UNIVERSITY OF OKLAHOMA

GRADUATE COLLEGE

THE INTEGRATED REALIZATION OF MATERIALS, PRODUCTS AND ASSOCIATED MANUFACTURING PROCESSES

A DISSERTATION

SUBMITTED TO THE GRADUATE FACULTY

in partial fulfillment of the requirements for the

Degree of

DOCTOR OF PHILOSOPHY

By

ANAND BALU NELLIPPALLIL
Norman, Oklahoma
2018

THE INTEGRATED REALIZATION OF MATERIALS, PRODUCTS AND
ASSOCIATED MANUFACTURING PROCESSES

A DISSERTATION APPROVED FOR THE
SCHOOL OF AEROSPACE AND MECHANICAL ENGINEERING

BY

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To my Parents

(Mrs. Usha Kumari S. and Dr. N.S. Balakrishnan Nair)

for their continuous love, support and sacrifice for me

Acknowledgements

This dissertation is a result of the continuous support, mentoring and encouragement from several people involved in my life. The associations with these people have helped me grow as a person and as a professional. They have played a huge role in helping me in my journey to realize myself. I express my gratitude to each of them and acknowledge them here.

I begin by thanking the two most influential people of my life during my doctoral journey – my academic parents. I thank my Ph.D. advisors Professors Janet K. Allen and Farrokh Mistree for their continuous encouragement, support and faith in me. Janet and Farrokh's passion to help students realize their full potential by providing them an opportunity to learn is truly amazing. Their dreams for me are beyond what I dream for myself. Both of them have helped me in defining long-term and short-term goals and helped me to realize these goals through their support and mentoring. They have always challenged me to go beyond my comfort zones. Through this experience I realized that it is fun to step out of one's comfort zone. Almost everyone who has interacted with Farrokh has heard him say "the best job in the world is to be a professor". Farrokh and Janet's passion for their profession is what I inherit the most from them. The fundamental principles embodied within the Systems Realization Laboratory that is co-directed by Janet and Farrokh is to focus on scholarship and critical thinking, viewing students as colleagues, and creating a family environment where everyone rises to their full potential. These principles have impacted me a lot and I plan to abide to these when I start my own research laboratory in future. As I reflect upon myself, I realize that I have significantly grown as a person both professionally and personally in the last four years with Janet and

Farrokh. My thanks to Janet and Farrokh, for accepting me as their academic son and providing me an opportunity to learn and grow. Both of them have been wonderful role models and mentors.

I thank my Ph.D. dissertation committee members Professors Kuang-Hua Chang, Shivakumar Raman, Zahed Siddique, Janet Allen and Farrokh Mistree for critiquing my doctoral work and providing their insightful comments and feedback. I thank Professor Chang for his comments during my Ph.D. General Exam which helped me to frame the problem properly leading to my first conference and journal paper. I thank Professors Chang, Raman and Siddique for the encouraging and supporting words that they always have for me. I also thank Dr. Jinsong Pei who had to unfortunately leave my committee due to her sabbatical at ETH, Zurich. The advice she gave for my work and the materials she shared with me for a successful future career as a professor are very valuable and I thank her for that.

I thank all the colleagues with whom I worked during my doctoral studies. I thank Professor Amarendra Kumar Singh of Indian Institute of Technology, Kanpur for selecting me as an intern at Tata Research Development and Design Centre during my masters and recommending me to Janet and Farrokh; which further paved way for my doctoral studies. I thank Dr. B.P. Gautham of Tata Consultancy Services (TCS) Research, Pune for being my mentor during my doctoral studies. Dr. Gautham has guided me throughout the process of my PhD dissertation research and provided me with assistance and help whenever needed. He provided me with the opportunity to carry out internship at TCS Pune, where I was able to formulate the comprehensive example problem discussed in my dissertation. The association with Dr. Gautham has encouraged me to be strongly grounded in fundamentals and ask fundamental questions. I thank Dr. Chung-Hyun Goh of University of Texas at Tyler for helping me realize my duties and responsibilities as a doctoral student during my first year at OU. I thank him for being critical of me during my first year which helped me to improve myself and become an independent researcher in terms of formulating problems for my research. I thank Dr. Zhenjun Ming, Dr. Ru Wang, Vignesh Rangaraj, Kevin Song, Pranav Mohan, Pramod Zagade, Rishabh Shukla, Surya Ardham and Tate Fonville for working closely with me during my PhD research and co-authoring several papers that are part of my dissertation. I thank Pramod Zagade and Rishabh Shukla of TCS for helping me by sharing the knowledge and insight they had about the project while at TCS.

I thank Professor Mark F. Horstemeyer of Mississippi State University and Dr. Jitesh Panchal of Purdue University for advising me on the fields of Integrated Computational Materials Engineering and Decision-making in Engineering Systems Design, respectively. I thank them both for providing me the opportunity to take their courses which helped me gain knowledge and insight in their respective fields that are foundational for my doctoral research. I thank past Systems Realization Laboratory members especially Drs. Jitesh Panchal, Warren Smith, Wei Chen, Kemper Lewis, and Carolyn Conner Seepersad for the advice that they gave me for my doctoral studies and future career goal of a life in academia.

I thank all the members of the Systems Realization Laboratory @ OU (starting Fall 2014) who were next to me, inspired and helped me during the last four years especially Pranav Mohan, Abhishek Yadav, Maryam Sabeghi, Dr. Jelena Milisavljevic, Dr. Zhenjun Ming, Dr. Chung-Hyun Goh, Dr. Shabnam Rezapour, Dr. Amirhossein

Khosrojerdi, Dr. Ru Wang, Professor Guoxin Wang, Lin Guo, Reza Alizadeh, Gehendra Sharma, Jackson Autrey, Ali Shahbazi, Xiwen Shang, Liangyue Jia, Shuting Chen, Kevin Song and Kelan Berry. I also thank researchers at Tata Consultancy Services especially Akash Gupta, Sharad Goyal, Ravikiran Anapagaddi, Danish Khan and Gerald Tennyson for their help, support and mentoring while at TCS. I thank the staff members of School of AME especially Melissa Foster, Bethany Burklund and Ellen McKenzie for all their help in the School. I thank Dr. Partha Sarathi De of IIT Bhubaneswar for mentoring me during my masters and supporting me towards my doctoral studies with Janet and Farrokh. I wouldn't be here without his support. I also thank Dr. Narayan R.L. (currently Post-Doctoral Fellow in Nanyang Technological University, Singapore) for his continued help and inspiration during my studies.

I thank my friends at OU especially Dr. Terry Dunn, Mortaza Saeidijavash, Pranav Mohan, Dhruv Sharma, Dr. Arun Bala, Ravi Soni, Bhanu Prasad Kotamraju, Shreyasi, Cindy Belardo, Abhishek Yadav, Saptarshi Mandal, Yi Hsu and Paul Calle for providing me an environment, where I never felt away from home. My life at OU wouldn't be so happy and cheerful without you all. I thank Deepak T. Abraham and Chinmaya Kathe for being such nice roommates and supporting me in all possible ways for my doctoral studies. I also thank my friends back home especially Rijin Wilson, Viswanathan P.O., Rahul Sathyanath, Athul Sathyanath and Arun Jose for being the wonderful friends that they are in my life.

Above all, I thank my family for all the love and support that they have given me. I thank my mother, Usha Kumari S. for sacrificing so much for raising my brother and me. I thank her for educating us, taking care of us and being there for our family all the time as a constant source of love. Her passion for education and teaching is what influenced me into a life in academia. I thank my father Dr. N.S. Balakrishnan Nair for raising my brother and me with values essential for the society. His commitment to the field of education and quest for knowledge is the inspiration for my doctoral studies. The discipline that he maintained in his career and life is something that I wish to emulate in my life. I thank him for being the role model that he is in my life. I thank my brother Harikrishnan N.B. (*Appu*) for being the most loving brother that one could ever ask for. I thank him for being next to me all these years and making me proud with his accomplishments in life. I have been blessed with my wonderful fiancée, Anju Vijayan Nair (*Ammus*), who came into my life last year. Each day with her is a blessing. I thank Anju for her continued and unfailing love, support and understanding especially during my final stages of doctoral studies.

Finally, I acknowledge the financial support that I received during my doctoral studies. I thank Janet and Farrokh for offering me a fully funded doctoral position with them at the Systems Realization Laboratory @ OU. My doctoral studies and the work carried out in my dissertation have been supported from Grant Number 105-4160-00 from Tata Consultancy Services, India and the funding from the John and Mary Moore Chair (Professor Janet K. Allen) and the L.A. Comp Chair (Professor Farrokh Mistree) at the University of Oklahoma respectively. I also thank the School of AME for awarding me the Frank Chuck Scholarship for outstanding academic and research performance for two academic years. I am grateful for the financial support from these organizations without which this work would not be possible.

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Summary

Problem: A materials design revolution is underway in the recent past where the focus is to design (not select) the material microstructure and processing paths to achieve multiple property or performance requirements that are often in conflict. The advancements in computer simulations have resulted in the speeding up of the process of discovering new materials and has paved way for rapid assessment of process-structure-property-performance relationships of materials, products, and processes. This has led to the simulation-based design of material microstructure (microstructure-mediated design) to satisfy multiple property or performance goals of the product/process/system thereby replacing the classical material design and selection approaches. The foundational premise for this dissertation is that systems-based materials design techniques offer the potential for tailoring materials, their processing paths and the end products that employ these materials in an integrated fashion for challenging applications to satisfy conflicting product and process level property and performance requirements. The primary goal in this dissertation is to establish some of the scientific foundations and tools that are needed for the integrated realization of materials, products and manufacturing processes using simulation models that are typically incomplete, inaccurate and not of equal fidelity by managing the uncertainty associated. Accordingly, the interest in this dissertation lies in establishing a ***systems-based design architecture*** that includes system-level synthesis methods and tools that are required for the integrated design of complex materials, products and associated manufacturing processes starting from the end requirements. Hence the primary research question: ***What are the theoretical, mathematical and computational foundations needed for establishing a comprehensive systems-based***

design architecture to realize the integrated design of the product, its environment, manufacturing processes and material as a system? Major challenges to be addressed here are: a) integration of models (material, process and product) to establish processing-structure-property-performance relationships, b) goal-oriented inverse design of material microstructures and processing paths to meet multiple conflicting performance/property requirements, c) robust concept exploration by managing uncertainty across process chains and d) systematic, domain-independent, modular, reconfigurable, reusable, computer interpretable, archivable, and multi-objective decision support in the early stages of design to different users.

Approach: In order to address these challenges, the primary hypothesis in this dissertation is to establish the theoretical, mathematical and computational foundations for: 1) forward material, product and process workflows through systematic identification and integration of models to define the processing-structure-property-performance relationships; 2) a concept exploration framework supporting systematic formulation of design problems facilitating robust design exploration by bringing together robust design principles and multi-objective decision making protocols;

3) a generic, goal-oriented, inverse decision-based design method that uses 1) and 2) to facilitate the systems-based inverse design of material microstructures and processing paths to meet multiple product level performance/property requirements, thereby generating the problem-specific inverse decision workflow; and 4) integrating the workflows with a knowledge-based platform anchored in modeling decision-related knowledge facilitating capture, execution and reuse of the knowledge associated with 1), 2) and 3). This establishes a comprehensive systems-based design architecture to realize

the integrated design of the product, its environment, manufacturing processes and material as a system.

Validation: The systems-based design architecture for the integrated realization of materials, products and associated manufacturing processes is validated using the validation-square approach that consists of theoretical and empirical validation. Empirical validation of the design architecture is carried out using an industry driven problem namely the '**Integrated Design of Steel (Material), Manufacturing Processes (Rolling and Cooling) and Hot Rolled Rods (Product) for Automotive Gears'**. Specific sub-problems are formulated within this problem domain to address various research questions identified in this dissertation.

Contributions: The contributions from the dissertation are categorized into new knowledge in four research domains: a) systematic model integration (vertical and horizontal) for integrated material and product workflows, b) goal-oriented, inverse decision support, c) robust concept exploration of process chains with multiple conflicting goals and d) knowledge-based decision support for rapid and robust design exploration in simulation-based integrated material, product and process design.

The creation of new knowledge in this dissertation is associated with the development of a systems-based design architecture involving systematic function-based approach of formulating forward material workflows, a concept exploration framework for systematic design exploration, an inverse decision-based design method, and robust design metrics, all integrated with a knowledge-based platform for decision support. The theoretical, mathematical and computational foundations for the design architecture are proposed in this dissertation to facilitate rapid and robust exploration of the design and solution spaces to identify material microstructures and processing paths that satisfy conflicting property and performance for complex materials, products and processes by managing uncertainty.

Chapter 1: Frame of Reference – Integrated Design of Materials, Products and Associated Manufacturing Processes

1.1 Motivation for Integrated Design of Materials, Products and Associated Manufacturing Processes

In practice, design involved the selection of a suitable material for a given application (Norton , Shigley 1972, Ashby and Cebon 1993, Pahl and Beitz 2013). The performance of many engineered systems involving materials and products is limited by the available properties of the constituent materials. The difficulty here with material selection is the inherent inability to tailor a material microstructure and constituents for satisfying application specific requirements. These requirements tend to conflict with the actual achievable performance from the material microstructure and properties. The discovery of new materials has always been arduous, fortuitous and instinctive for the people in this domain. The lead times for developing new materials have remained almost constant and unacceptably long when compared to the development cycle of a desired product. This has thus resulted in increased cost and time in the development of new materials and products which is partly due to the predominantly empirical, trial-and -error approach adopted by materials engineers and designers till now (McDowell and Story 1998, Olson 2000).

The U.S. National Science Foundation (NSF) defines *design* as a process by which products, processes and systems are created to perform desired functions through specification. In a design process, requirements also termed as ‘functions’ are transformed into design descriptions (Gero 1990). The ‘functions’ embody the expectations of the purposes of the resulting artifact. Gero (Gero 1990) describes design as a goal-oriented, constrained, decision making exploration, and learning activity that operates within a context that depends on the designer's perception of the context.

A materials design revolution is underway in the recent past where the focus is to ***design*** (not select) the material microstructure and processing paths to achieve multiple property or performance requirements that are often in conflict. Recent advancements in computational modeling tools and frameworks that support simulation-based, integrated design exploration of materials, products, and the manufacturing processes through which they are made have resulted in the speeding up of the process of discovering new materials and has paved way for rapid assessment of process-structure-property-performance relationships of materials, products, and processes. This has led to the simulation-based design of material microstructure (microstructure-mediated design) to satisfy multiple property or performance goals of the product/process/system thereby replacing the classical material design and selection approaches, see (Olson 2000, Panchal, Choi and coauthors 2005, Board 2008, McDowell and Olson 2008, Horstemeyer 2012). **The foundational premise therefore for this dissertation and the emerging field of materials design in general is that systems-based materials design techniques offer the potential for tailoring materials, their processing paths and the end products that employ these materials in an integrated fashion for challenging applications to satisfy conflicting product and process level property and performance requirements.**

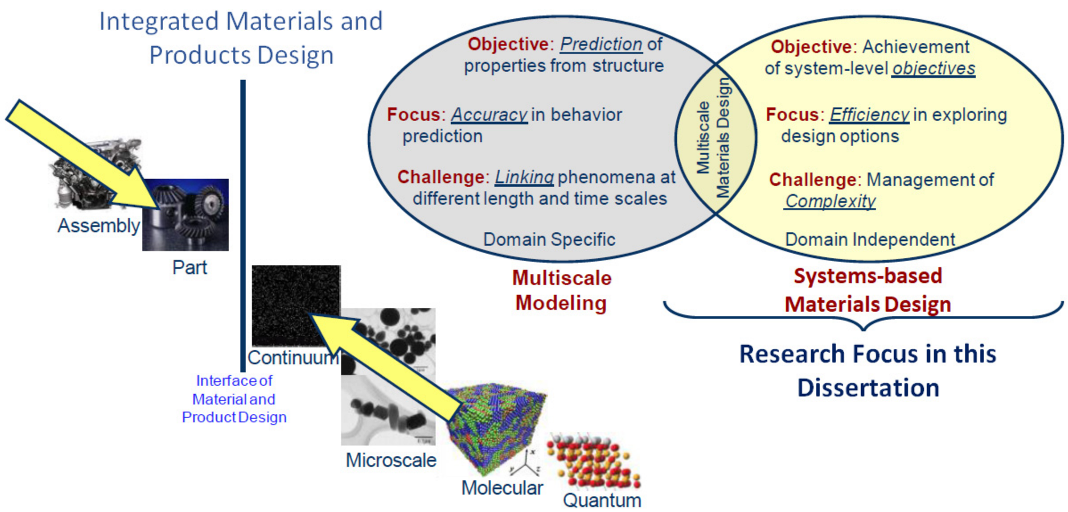


Figure 1.1: Distinction between multiscale modeling and systems-based materials design

At this point, it is important to recognize the distinction between multiscale modeling efforts which is the focus of materials scientists and engineers and systems-based materials design which is the focus of systems designers to be addressed in this dissertation. The focus of materials scientists and engineers is in creating increasingly sophisticated, realistic, physics-based and history dependent models that accurately predict the material microstructure and properties which can then be used to support a design process to satisfy ranged set of performance requirements. Systems designers recognize the potential of integrated design of materials, products and processes and focus on designing material microstructures that satisfy system-level design objectives. The distinction is captured in Figure 1.1. The major challenge arising in systems-based materials design is the management of uncertainty and complexity of design problems. Multiscale modeling approaches are usually domain-specific demanding considerable knowledge and insight in mechanisms, material hierarchy and information flow and thus corresponds to detailed design. Systems-based design approaches are mostly domain-independent and facilitates design "exploration" rather than detailed design.

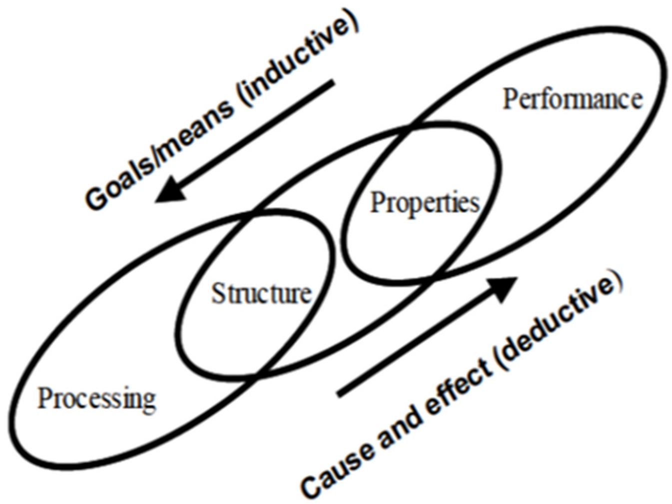


Figure 1.2: Olson's concept of Materials-By-Design (Olson 1997)

The conventional way of modeling hierarchical processes and systems is a "bottom-up", cause and effect (deductive) approach of modeling the material's processing paths, microstructures, resulting properties, and then mapping the property relations to performance functions, as shown in Figure 1.2. Such deductive links are necessary but not sufficient for materials design. Systems designers as discussed by Olson (Olson 1997) and illustrated in Figure 1.3, seek a "top-down", goals/means, inductive or inverse methods to explore the design space of processing paths and resulting microstructures of a material *satisfying* a set of specified performance requirements that could be conflicting in nature.

In this dissertation, design is defined as a *top-down, simulation-supported, integrated, decision-based process to satisfy a ranged set of product-level performance requirements* (McDowell, Panchal and coauthors 2009, Allen, Panchal and coauthors 2015). Keeping with this, the integrated design of materials, products and processes is defined in this dissertation as ***fundamentally an inverse, goal-oriented synthesis activity in which the designer (decision-maker) aims at identifying material structures and processing paths that achieve/satisfy certain required product and manufacturing process-level properties and performances***.

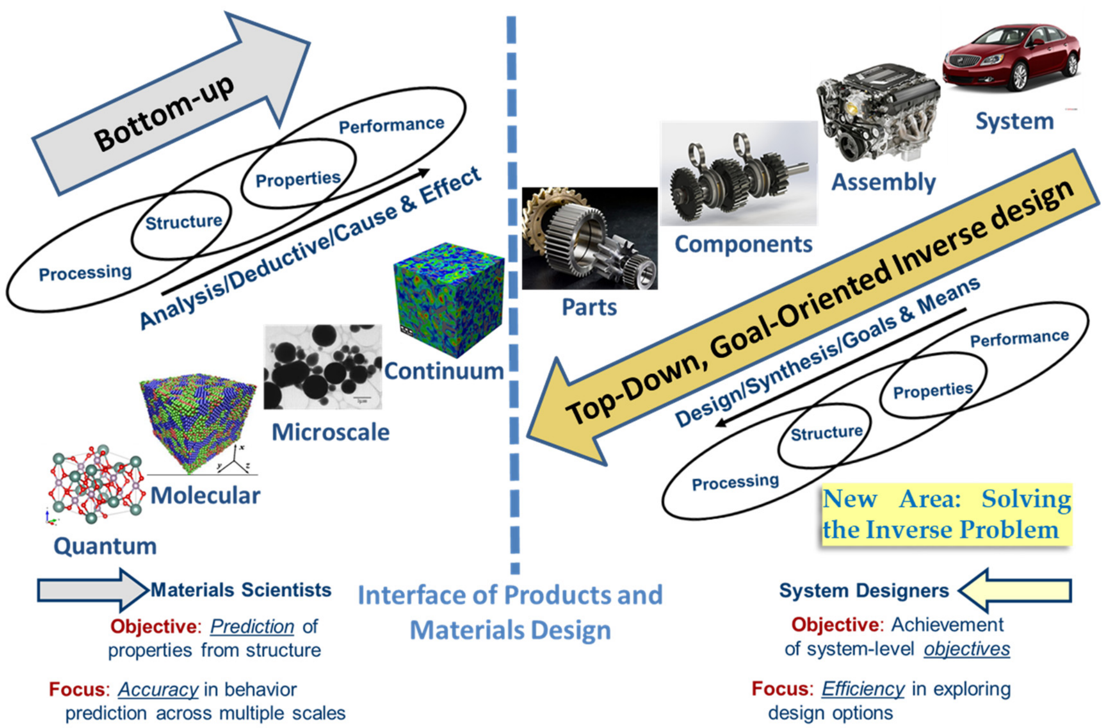


Figure 1.3: Top-down goal-oriented inverse design

1.1.1 The Integrated Material, Products and Manufacturing Process Design Focus in this Dissertation: Integrated Design of Steel (Material), Manufacturing Processes (Rolling and Cooling) and Hot Rolled Rods (Product) for Automotive Gears

Steel mills are involved in the production of semi-products like sheets or rods with certain grade of steel. Steel manufacturers are focused on developing newer grades of steels with improved properties and performances due to the increasing competition arising from new engineering materials. However, there has not been a decline in the popularity of steel as an engineering material in manufacturing industries as careful managing of material processing during steel manufacturing will lead to the development of diverse ranged sets of mechanical properties and microstructures resulting in improved performances of products.

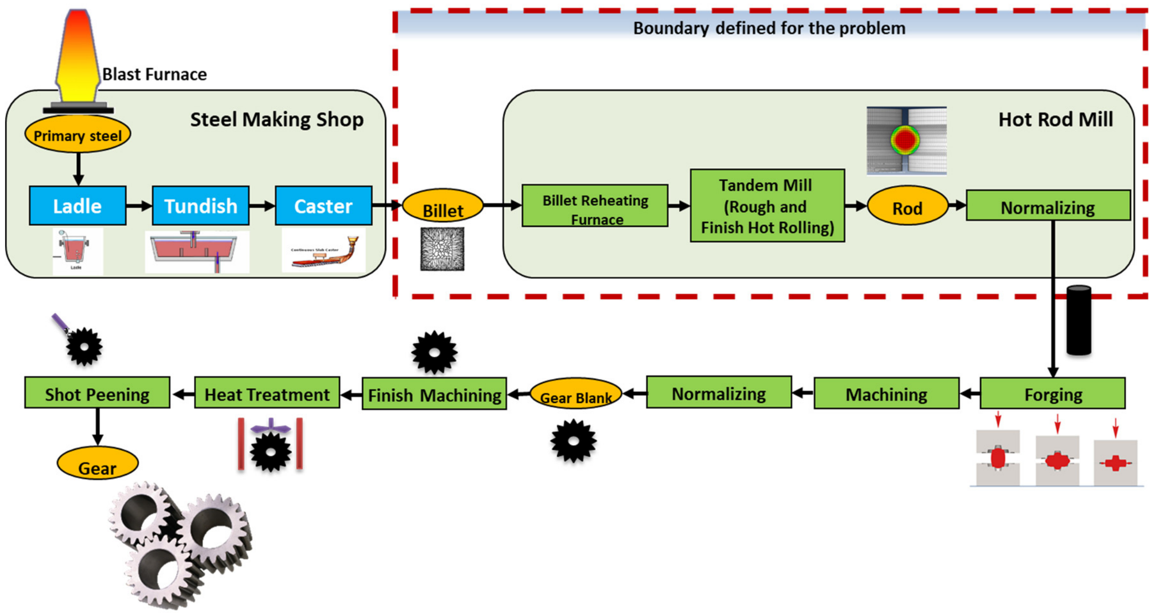


Figure 1.4: Steel Manufacturing Process Chain for Automotive Gear Production

Modern steelmaking for the production of automotive gears involves the following processes listed in sequential order as depicted in Figure 1.4.

Ironmaking: In the first stage known as ironmaking, the raw material inputs iron ore, coke (fuel) and lime (flux) are melted in a blast furnace. Blast furnace is a one type of metallurgical furnace used for smelting to produce industrial metals. The resulting molten iron contains 4-4.5% carbon and other impurities that make it brittle.

Primary Steelmaking: Primary steel making is carried out in two ways. The first involves Basic Oxygen Furnace (BOF) and the second involves the more modern Electric Arc

Furnace (EAF) methods. In BOF, recycled scrap steel is added to the molten iron in a converter. Oxygen is blown through the metal at very high temperatures, which reduces the carbon content to around 0-1.5%. In EAF, recycled steel scrap is fed through high power electric arcs that melts the metal converting it to high-quality steel.

Secondary Steelmaking: In secondary steelmaking (steel making shop in Figure 1.4) the molten steel produced from both BOF and EAF are further treated to refine the composition to the desired steel quality. This is carried out by adding or removing certain elements and/or manipulating the temperature and production environment. The count and nature of inclusions present and the levels of tramp elements such as sulfur, phosphorus and total oxygen present in the liquid steel are factors assessed for checking the quality of steel. The desired composition is maintained with respect to alloying elements (Ni, Cr, Mn, etc.) that are added to impart certain properties to the steel. The ladle furnace (in steel making shop, Figure 1.4) is one of the key unit operations for carrying out deoxidation and desulfurization to maintain the levels of oxygen and sulfur within a tolerable limit. The steel from basic oxygen furnace (BOF) or electric arc furnace (EAF) is tapped into the ladle where several operations such as addition of alloying and slag forming additives to meet the required steel composition, desulfurization to reduce Sulphur content through Argon purging, arcing to maintain the heat content in steel required for subsequent casting, ladle refining to reduce inclusions formed, etc. are carried out to meet the compositional and cleanliness requirements of steel (Shukla, Anapagaddi and coauthors 2015). The molten steel from the ladle is sent to the next unit, which is the tundish (see, Figure 1.4). A modern steelmaking tundish is used to facilitate inclusion removal, to maintain chemical and thermal homogeneity, and to provide the next unit, the continuous caster with the required amount of superheat in the steel (Anapagaddi, Shukla and coauthors 2013, Anapagaddi, Shukla and coauthors 2014).

Continuous Casting **(Hot melt to Billet)**: The hot melt from the tundish is passed to the continuous casting unit (see, Figure 1.4). The continuous casting unit includes a mold usually made of copper. The hot melt as it comes in contact with the mold gets cooled as heat is extracted by the mold (primary cooling) and solidifying of the metal starts at the mold-melt interface. Steel is withdrawn from the mold by a dummy bar. The mold is oscillated in the vertical direction in order to avoid sticking and to ensure separation of the solidified steel from the copper mold. The thickness of the solidified layer (shell thickness) continuously increases as the melt moves down the mold. The movement of the solidified block is guided and supported by rolls beyond the mold exit. The solidified metal block is cooled by water with the help of spray nozzles. The block is cut into desired lengths depending on application; slabs for flat products (plate and strip), blooms for sections (beams), billets for long products (wires) or thin strips. For automotive gear production, usually solidified billets of square/rectangular cross section, often in the range of 80-250 mm side are used. During the solidification process, the compositional elements segregate leading to a variation across the cross section. This segregation at macroscopic scale, i.e. width of the billet is called macro-segregation. Besides the macrosegregation, the chemistry will also segregate at the level of dendritic arm spacing leading to microsegregation. Besides the variation in the chemistry, due to the different cooling rates seen by different portions of the cross section, the microstructure across the cross section will also be inhomogeneous. Predominantly the cross section will have three zones consisting of central equiaxed morphology, surrounded by columnar region and finally a fine-grained chill zone on the surface. The variation of chemistry as well as cooling rate will impact the overall structure of the cast billet including formation of precipitates etc. Another aspect of importance is the distribution of inclusions present in the incoming steel melt across the cross section of the billet. All these aspects lead to a significant impact on the final product as some of these signatures stay till the end, even though modified to some extent.

Rolling Mill **(Billet to Rod)**: The steel billet that is cast is then sent to the rolling mill. The rolling mill includes a reheating furnace to heat the billet before rolling to ensure thermo-mechanical deformation and refinement of microstructure during rolling. The billet is formed into various shapes depending on the end application. The process is a high temperature, high strain rate process. The process eliminates cast defects and achieves the required shape, surface quality and microstructure for the semi-product after rolling. Microstructural phenomenon like dynamic, metadynamic and static recrystallizations and grain growth occur during rolling resulting in a change in the microstructure of steel. The rolled rods are further sent to a cooling unit, where the phase transformation of the steel takes place. The Hot rolled products are divided into flat products, long products, seamless tubes, and specialty products. Rods are one of the products from a rolling mill.

Forging **(Rod to Blank)**: Rolled rods of desired grade and diameter are the raw materials for the forging industry. The rods are cut to required length, forged in one or multiple steps for obtaining a desired shape and finally heat treated to relieve of the stresses and are known as blanks. For automotive gears the rods are forged to gear blanks. These blanks forged are machined to obtain desired final blank shape. One of the key factors influencing the process is the distortion of the forged piece subsequent after to forging and subsequent heat-treatment. Higher distortion leads to providing for higher machining allowances. The magnitude of distortion depends on the incoming material state, forging process sequence (die design and operations) and heat treatment and can be controlled by appropriate die design. However, the segregation and microstructural non-uniformity of the material will also be an important aspect in the final distortion as this signature will stay till the end and may cause distortion. One needs to look at all these aspects in tandem and recommend best status for incoming material (rod) state without adding to the cost.

Machining, Heat Treatment, and Finish Machining: Finally, secondary forming techniques give the steel its final shape and properties. These techniques include machining (e.g. drilling), joining (e.g. welding), coating (e.g. galvanizing), heat treatment (e.g. tempering), surface treatment (e.g. carburizing), shot peening, etc., to finally produce the product – a gear in this case.

A boundary is defined for the problem addressed in this dissertation within the hot rod rolling process with the billet coming from the casting unit as the input and the hot rolled rod as the output. The boundary defined is shown in Figure 1.4.

1.1.2 Defining Boundary – Hot Rolling Process Chain

Typical steel mills produce intermediate products such as slabs, billets, blooms and finished products such as sheets and rods/bars. The round rod produced in steel mills after passing the raw steel material through several manufacturing processes like casting, reheating, rolling and cooling forms the input material for the production of gears. The chemical composition of material including the segregation of alloying elements, the deformation history during rolling, the cooling after rolling and the microstructure generated define the end properties of the steel product that is rolled. The presence of large number of design variables, constraints and bounds, conflicting goals and sequential information/material flow during material processing makes the steel rod making process chain to be highly complex in nature. Large number of plant trials are therefore required to produce a product from a new steel grade having desired properties and performances. These trials are usually expensive and time-consuming. Process designers are very much aware of the operating constraints and process requirements for each of the operations as they are involved in the whole process day-in and day-out. Due to the advancements in material technology, new improved materials with enhanced properties are introduced to market and this has posed a serious challenge to steel manufacturers. Suppose, a situation happens that owing to the changed properties and performance requirements, manufacturers are asked to produce a semi-product like the rod with a newer grade of steel with enhanced properties. This new steel grade is used at laboratory scale to produce a rod, but the current challenge posed to a steel manufacturer is to scale-up the production of this rod from laboratory scale to industrial scale. This has created a requirement to explore the design set points of each unit operation involved in the production of the rod with some target properties at plant scale. Experimentations and plant trials are one way of achieving this requirement, which usually takes a lot of time and is mostly expensive. Usually for automotive applications, the materials research may take up to 8-10 years when this option is adopted. As per the information from Tata Steels, India; it takes around 20-25 plant trials to come up with these design set-points and each such trial will cost a $100,000 dollar. This is thus a huge challenge to industry.

To address this issue, there is a huge drive by industry especially in the past decade to use computational models for exploring the design set points for these operations and thereby reduce the time and cost involved in the development. The focus is to carry out simulation-based, integrated design exploration of the different manufacturing processes involved by exploiting the advancements in computational modeling tools and frameworks. The fundamental question addressed in this dissertation from the problem perspective for the integrated realization of steel (material), rolled rod (product) and hot rolling process chain (manufacturing process chain) is:

How to realize this complex system involving the material, product and manufacturing processes using simulation models that are typically incomplete, inaccurate and not of equal fidelity?

George Box (Box 1979) is reputed for his aphorism that "all models are wrong but some are useful". In keeping with George Box's observation, the challenge here is to determine the design and operating set points for the hot rolling process chain involving the material steel and end product rod using computational models and simulations that at best capture the essence of reality but not reality itself. Therefore, there is a need to explore solutions that are relatively insensitive to the inherent uncertainties embodied in the computational models and simulations while satisficing the conflicting goals associated with material, product and process. An integrated design exploration approach is needed, where ranged set of solutions are sought that satisfy the requirements identified for the steel manufacturing process as well as the end rod product. However, these models and simulations are specific for specific phenomena that happens during a process and an isolated design using individual models will not be a true representation of the whole system and the solution desired. Thus, there requires an integration of these models to allow information flow so as to explore the design and operating set points for the production of rod. For exploring the design and operating set points, knowledge of the operation constraints and requirements are necessary and for a newer grade of steel, this information is not readily available for a manufacturer. Therefore, the first task is to identify operating constraints and requirements for each operation, which is imposed by the subsequent unit operations as each process step is connected and information flows from one operation to another. To identify these operating constraints there needs to be information about each operation in sufficient details. This needs integration of different models which are at multiscale of an operation so as to obtain information in much greater details which can then be passed to other unit operations. This is termed as ***vertical integration*** of models for one particular unit operation. The integrated study possible by the flow of information from one-unit operation to other is termed as ***horizontal integration***.

Thus, in order to effectively couple the material processing-structure-property-performance spaces, there needs to be an interplay of the systems-based design of materials with enhancement of models of various manufacturing processes through multi-scale modeling methodologies and integration of these models at different length scales (vertical integration). This ensures the flow of information from process to another thereby establishing the integration of manufacturing processes (horizontal integration). Together these types of integration will support the decision-based design of the manufacturing process chain so as to realize the end product.

To achieve the vertical and horizontal integration of models, there must be analysis models and simulations that can link the different manufacturing processes by predicting the different material phenomenon associated thereby ensuring the proper forward flow of information. To predict the properties and performances of hot rolled steel product there needs to be modeling of the material flow behavior during hot rolling followed by the microstructural changes that happens during hot deformation and at the interstand region followed by the phase transformation phenomena that happens during the cooling process after rolling. Mathematical models and simulation programs for the different metallurgical events that happen during rolling and cooling when integrated into the right sequence will be able to help a designer predict the microstructure evolution as a function of process parameters. The integration of these models enables the designer to identify new processing routes, composition maps and mill sequences that will provide a microstructure and to track their impacts on the end mechanical properties of the product. Thus, using these analysis models, the designer will be able to solve the standard forward problem: given the input parameters related to the processing and microstructure models, what are the properties and performances of the end product? These standard forward problems are characterized by the availability of a single point solution and the designer iterates the analysis several number of times to identify a solution that meets the end property/performance requirements. Again, such an approach takes a huge amount of time and cost for the designer to make design decisions and is not top-down or goal-oriented.

Thus, the questions to be asked here is:

Given these analysis models and simulations that establish the forward material workflow for the system, how do a designer design the system from a systems perspective taking into account the end goals and requirements and make design decisions that are critical for the integrated simulation-based realization of materials, products and processes?

From a systems perspective, the interest therefore lies in formulating and solving the inverse design problem: given the required end properties/performances, what should be the input parameters and variables in terms of material microstructures and processing paths so as to achieve the model-based realization of the material, product, and the manufacturing processes?

There are several challenges in addressing these questions. The challenges are discussed in next section.

1.1.3 Challenges in Systems-based Integrated Design of Materials, Products and Processes

The philosophical underpinning of the goal-oriented approach to materials design has been provided by Olson (Olson 1997) and reiterated by many others (McDowell, Panchal and coauthors 2009, Horstemeyer 2012, Horstemeyer 2018, McDowell 2018). Several challenges associated with top-down, goal-oriented approach of materials design have been highlighted, see (Panchal 2005, McDowell, Choi and coauthors 2007, McDowell, Panchal and coauthors 2009, McDowell 2018). The challenges that need to be addressed for the integrated realization of materials, products and manufacturing processes from a systems-based, simulation-assisted, top-down design perspective are:

i. **Managing uncertainty** associated with material microstructure and behavior;

ii. **Managing uncertainty** associated with complex manufacturing processes resulting from its environment and the factors affecting the processes;

iii. Material, product and process models and simulations of complex systems are typically **incomplete, inaccurate and not of equal fidelity** and thus the models and simulations are **uncertain** – need to be managed;

iv. **Propagation of uncertainty** across multiple scales and across processing, microstructure, property and performance spaces – need to be managed;

v. Modeling different phenomenon related to a manufacturing process and integration of models for these different phenomenon (across scales mostly) to generate information specific to the manufacturing process – achieve **vertical integration**;

vi. Integration of different manufacturing processes and ensuring information (generated through vertical integration) flow across processing, microstructure, property and performance spaces to come up with the end product – achieve **horizontal integration**;

vii. **Non-linear, history dependent behavior** of metals and alloys limits extent of parametric study and imparts dependence on initial conditions;

viii. **Non-unique and large number of solutions** possible for a given property or performance requirement – need exploration of design and solution space;

ix. **Computational tractability of microstructure** (new) that satisfy conflicting property and performance requirements;

x. Availability of bottom-up models and deductive links that establishes forward information flow while **lack of generic and reliable inverse design techniques and tools for top-down materials design "exploration**";

xi. Dynamic design scenarios where the design goals change with time, thereby establishing the **need for reusable, flexible and adaptable design processes**;

xii. Balancing **model accuracy and computational cost**;

xiii. Modeling the physics associated with the materials system – ensuring the **capture of relevant information via modeling the appropriate number** of subsystems, components, parts and material phenomenon;

xiv. Identification and selection of **appropriate models, model parameters and the associated variabilities** at each scale/space of a complex material system;

xv. Managing **large quantities of information** especially related to material structure and properties at different levels of abstraction;

xvi. Capture, storage, reuse and updating of the **material, process and product knowledge and data base**;

xvii. **Verification and validation** of algorithms, models and design results;

xviii. Systems designers and materials engineers have different **backgrounds and expertise** and may not share the same "language" in terms of materials design;

Systems-based robust design methods are needed to address the major challenges arising due to i) uncertain material models (that includes input factors, parameters, responses, etc.) due to simplification/idealization or a lack of complete knowledge and ii) the propagation of uncertainty due to hierarchical information dependence in a multiscale model chain or in Olson's processing-structure-property-performance relations. An effective top-down, goal-oriented systems approach for materials design must be able to manage the uncertainty with regard to all relevant information ensuring feasible designs that meets specified ranges with high confidence. McDowell (McDowell 2018) asserts that such an approach must address ***uncertainty of models and experiments at each scale, as well as uncertainty propagation through a chain of models and/or experiments at different levels of hierarchy with the ability to provide decision support through rapid design space exploration***. The report by the U.S. National Academy of Engineering National Materials Advisory Board on Integrated Computational Materials Engineering (ICME) (Pollock, Allison and coauthors 2008) outlines a broad set of challenges and opportunities for the integrated realization of materials, products and processes from the emerging ICME perspective. In this dissertation, the systems-level strategies and their implications are explored for the integrated realization of materials, products and associated manufacturing processes, building on the foundational ideas laid by Olson on Materials by Design and the ICME community.

1.1.4 Addressing the Systems-based Material, Product and Process Design Challenges

To address many of the challenges associated with the integrated realization of materials, products and manufacturing processes, **a systems-based approach** is necessitated. Designing the materials cannot be done in an isolated fashion. Materials are subsystems of a larger system that includes parts, assemblies, product and physical systems. Engineering applications demand materials that satisfy multiple performance functions which requires a systems-level analysis to be defined properly. A hierarchical structure can be assigned to materials themselves where information passes from one scale to another and the desired end material properties and product performances often depend on the material phenomena that occurs at these different length and time scales. The challenge here is in developing/formulating a single model that predicts the material properties at macroscale by unifying information from all the length scales (McDowell and Story 1998). Atomistic and molecular level simulations based on first-principles predict structure and properties of materials. However, these simulations are computationally too expensive and often too idealized to model materials having heterogeneous structures (McDowell, Panchal and coauthors 2009). Similarly, continuum mechanics models and simulations predict properties of materials and products at macroscopic level, but are inappropriate for incorporating lower scale information that involves atoms, dislocations, defects, etc. Horstemeyer (Horstemeyer 2012) addresses the bridging between scales from the perspective of different disciplines/approaches like solid mechanics, numerical/concurrent methods, materials science, physics, mathematics and design. Horstemeyer coins the term “upscaling” for bottom-up approach of modeling and running simulations at each scale and averaging the results in some sense to be passed to next scale and the term “downscaling” for top-down approach of requirements driven simulation at macrostructural level taking into account lower length scale features.

Developing physics-based models that capture process-structure-property-performance relations at different length and time scales is challenging. The integration of these models across length and time scales is difficult owing to the complexity and limitations involved due to the different domains of application. The requirement here is to link these models in an integrated fashion that facilitates "***exploration***" of the systems-level design and solution space. The design and solution space exploration need to be carried out by distributing analysis and synthesis activities in a collaborative manner by a team of experts involving material scientists, product designers and engineers. This allows to leverage the different domain-specific knowledge and expertise associated with these experts related to may be length and time scales, multi scale modeling, material classes, and material functionalities, etc. The fundamental role of each of these domain-specific design experts is to make decisions given the information available. These decisions include synthesizing, analyzing and identifying design alternatives that satisfy conflicting material property and performance goals by carrying out trade-offs. Decisions taken for material systems depends on information available from different levels of hierarchy as the system is highly interconnected and interdependent. This demands the need for ***multi-objective decision protocols and workflows*** that allows the interfacing of individual decisions and decision-making experts so that information flows across the material hierarchy. A systems-based approach is sought for making these decisions by identifying solutions that satisfy ***systems-level*** objectives.

A deterministic approach to materials design is not sufficient as there is a certain degree of randomness in material systems. There is also uncertainty associated with the model-based realization of complex material systems. Model parameters are subject to variations associated with the variability of microstructure and variability due to processing. There is also uncertainty associated with model predictions due to various sources. The assumptions and approximations incorporated in a model also contributes to the uncertainty associated. Uncertainty associated can be magnified if a model is used in its boundary of applicability and when information is passed from one model to another resulting in propagation of uncertainty. Surrogate models developed to facilitate design space exploration of broad space also contributes to the uncertainty as fidelity is compromised for computational efficiency in such models. The experimental data available to verify and validate the model predictions may be sparse and may be affected by errors associated with measurements. Removing or mitigating these sources of uncertainty is expensive or impossible in most of the cases. The impact of these uncertainty sources however could be profound on the model predictions and final system performance. The need therefore is for system-level design methods that take into account these sources of uncertainty without removing or eliminating them. The method should support a designer to manage uncertainty and facilitate the identification of robust design solutions that are relatively insensitive to these sources.

One of the foundational elements for material, product and process design that is often neglected is databases for material structures, processing paths and properties based on both experiments and simulations. Databases serve the same purpose as models and simulations and are considered as instruments of informing design decisions. Databases should also convey uncertainty associated with the material-product-process system to facilitate systems-based robust design.

Design space exploration will be much more efficient if knowledge-guided assistance can be provided to designers at various decision points in the material system design process. Knowledge engineering plays a key role in enabling this with learning being an integral part of it. Previous design problems, methods, results, etc. can be systematically evaluated to gain knowledge that can thus make future design exploration process more efficient.

The ability to capture knowledge from various sources is also essential. A knowledge-based platform for decision support is therefore essential for the integrated design of materials, products and processes. The platform should serve as a computing infrastructure for simulation-based design process supporting decision making. The computing infrastructure should be easily extensible and platform independent serving systems-based design. The process of executing, linking models, exploring solution spaces, etc. should be automated by the computing infrastructure. It should also have the capability to archive and organize large amounts of data and should be able to capture the relevant information and knowledge associated. Sharing of data, information and knowledge with different types of users depending on their levels in the design process is necessary and the platform should facilitate real-time sharing, collaboration, communication, visualization, and search-based retrieval of design information and knowledge.

Based on the challenges identified in Section 1.1.3 and the needs identified to address the challenges in Section 1.1.4, key challenges to be addressed in this dissertation and the associated research gaps are identified to achieve the model-based integrated realization of materials, products and associated manufacturing processes. The key challenges identified are listed below.

1) Integration of Models Across Process Chain

- *Integrated design of materials and systems*: Design of the system/components and the design of the materials need to be connected enabling the integrated design of materials, product system and manufacturing processes. To achieve this models across scales for a specific process need to be integrated (vertical integration) for generating information that can be passed to subsequent manufacturing processes or material design space. Through this, designers will be able to incorporate model-based material microstructure and process design along with system and component design in a single, concurrent design process at the early stages of design thereby reducing the lead time and cost involved with product development.

- *Integration of manufacturing process chains to ensure a joined product development lifecycle*: The model-based integration (horizontal integration) of several manufacturing processes enabling communication of relevant design information across the different product processing stages allows for a faster, more efficient iterative product development process. The integration of the manufacturing process stages allows for a unified representation of the relevant data and knowledge with uncertainty managed to be shared across the manufacturing process chain to facilitate flexible, end-user specific product development process.

2) *Processing-Structure-Property-Performance Relationships*

- *Simulation-based definitions of material properties and performances at systems level using process-structure-property-performance relations – and exploiting them as system variables for designing materials and products with tailored performance characteristics*: Current practices use experimental and plant trials to define material properties and performances. These are often costly and time consuming. Such material property definitions are static and are unable to change with the design of the product at systems level. The material data generated/available is often in the past and are not updated with the current trends and practices resulting in a gap between research and design. Simulation/model-based definitions of material property do not rely on such plant trials and are dynamic in nature that respond to changes in design process at systems level in early stages of design. Verification and validation of individual models and models at different levels is critical which further allows to define the "design space" for material definitions and consider the management of uncertainty across the process-structure-property-performance spaces. The variables associated with the models are used as system variables to carry out the design of the material to tailored properties and performances.

Table 1.1: Research gaps in systematic model integration and information flow

Research Gaps	
G1	Systematic approaches to identify and integrate material, process and product models based on their function structures to frame system-level structure
G2	Systematic approaches to define the forward processing-structure-property-performance relationships and develop material and product workflows

3) Domain-independent Design Methods and Tools

- *Design methods, tools, mathematical constructs and frameworks, and ontologies that are domain-independent*: Currently materials design methods, tools, constructs, frameworks and ontologies that describe material and product related data, information and knowledge are domain-specific and are not favorable for design exploration at early stages of design. There is a need for domain-independent design methods, tools, constructs, frameworks and ontologies that are standard and interoperable ensuring easy storage, accessibility and reusability of information and knowledge among designers, tools, domains, and different communities with different design school of thoughts.

4) ***High-Throughput Decision Support and Inverse Methods Supporting Exploration***

- *High-throughput decision support and goal-oriented, inverse methods for materials design exploration*: High-throughput decision support is critical in all stages of material, product and process design. There is a need for decision-based design exploration protocols and workflows and inverse design methods that provides robust decision support for top-down design for process-structure-property-performance relations using bottom-up simulations, models and experiments. Uncertainty management, verification and validation are foundational to address this requirement.

5) ***Managing Uncertainty***

- *Robust Design of Materials, Products and Processes under Uncertainty*: Robustness of materials, products and processes with respect to variations in boundary or operating conditions, material properties, or material microstructures or processing paths are important to consider during design process because they can have significant impacts on the final performance of the end product. Typically, robustness is not considered during a material and product design process, and the design problems are usually formulated as deterministic optimal design problems. The need therefore is for system-level design methods that take into account these sources of uncertainty without removing or eliminating them. The method should take into account uncertainty of models and experiments at each scale, as well as uncertainty propagation through a chain of models and/or experiments at different levels of hierarchy with the ability to provide decision support through rapid design space exploration.

Table 1.2: Research gaps in systematic "robust" concept exploration

Research Gaps	
G3	Support systematic and rapid concept exploration of materials, products and processes to generate satisficing design specifications
G4	Systematic design methods to carry out inverse design exploration of materials, products and processes meeting end goals
G5	Systematic strategies to carry robust concept exploration of material, product and process system in inverse manner by managing uncertainty

6) Reusable, Flexible, Adaptive Design Processes

- Product and process requirements are subject to dynamic changes due to changing market requirements. This necessitates the need to design products by reusing existing knowledge for other products; flexible enough to dynamic market changes and accommodate them; adaptive enough to work satisfactorily in the changing environment that is prone to uncertainty.

7) Capture, Storage and Reuse the Knowledge

- *Knowledge-Based Platforms for Decision Support in the Design of Complex Material and Product Systems*: Decision making is a knowledge-intensive process, with knowledge playing a significant role in speeding up and effecting decisions. Capturing, managing, and reusing of decision related knowledge such as alternatives, parameters, constraints, goals, dependencies, and the design process in the design of complex material and product systems is an effective way for providing decision support. Hence there is a need for a decision-based computational framework to manage (off-line and in real-time) complexity and risk associated with the realization of complex (cyber-physical-social) material and product systems that necessitate the integration of information technology and operational technology.

Table 1.3: Research gaps knowledge-based decision support

Research Gaps	
G6	Constructs and tools to capture and reuse the knowledge associated with material and product systems design
G7	Facilitation of original, adaptive and variant design decision support
G8	Facilitation of systematic design exploration through decisions that are robust, flexible and modifiable particularly in the early stages of design.

1.1.5 Research Gaps and Overview

The focus in this dissertation is on the integrated model-based realization of materials, products and associated manufacturing processes from a systems perspective. Knowledge-based decision support during early stages of design by managing uncertainty has not attracted adequate research attention. How to define the product, material, manufacturing process or design-process amidst customer, engineering, and production uncertainty remains largely an open question. In the preceding sections, the challenges to achieve integrated model-based realization of materials, products and associated manufacturing processes have been reviewed and research gaps are identified. The mapping between the challenges and the research gaps identified is shown in Figure 1.5. Research gaps thus identified are summarized below.

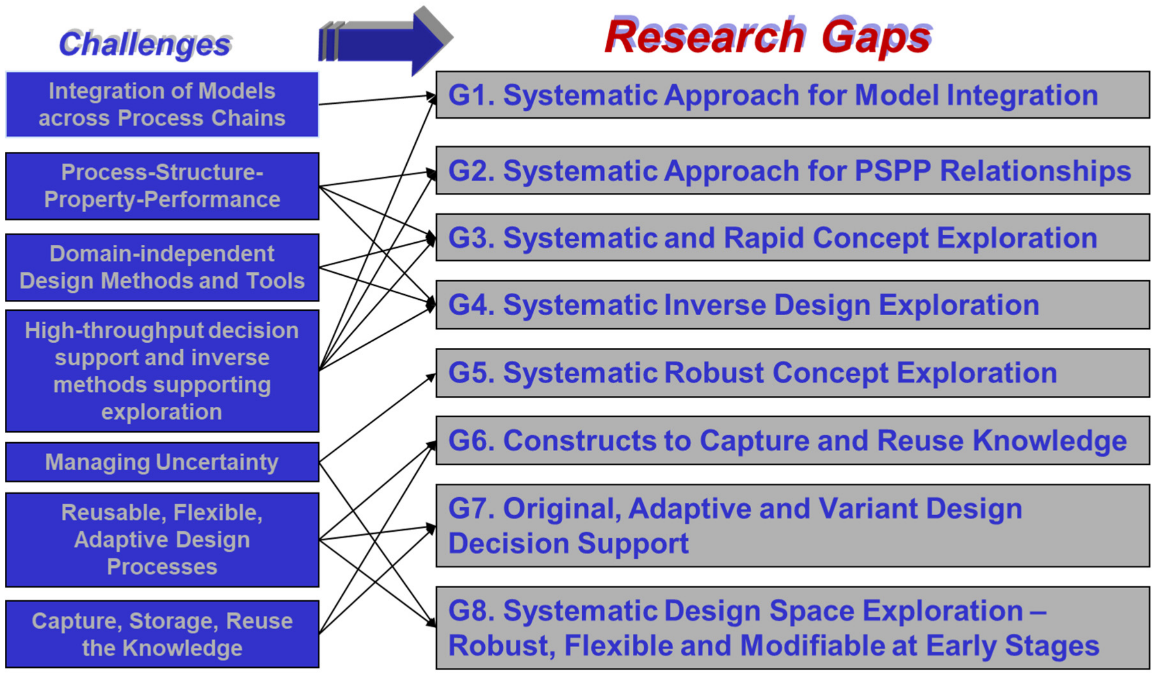


Figure 1.5: Mapping between research challenges and research gaps

G1. Systematic approaches to identify and integrate material, process and product models based on their function structures to frame system-level structure

G2. Systematic approaches to define the forward processing-structure-property-performance relationships and develop material and product workflows

G3. Support systematic and rapid concept exploration of materials, products and processes to generate satisficing design specifications

G4. Systematic design methods to carry out inverse design exploration of materials, products and processes meeting end goals

G5. Systematic strategies to carry robust concept exploration of material, product and process system in inverse manner by managing uncertainty

G6. Constructs and tools to capture and reuse the knowledge associated with material and product systems design

G7. Facilitation of original, adaptive and variant design decision support

G8. Facilitation of systematic design exploration through decisions that are robust, flexible and modifiable particularly in the early stages of design.

Based on the research gaps identified, nine key elements for the integrated realization of materials, products and manufacturing processes is identified and listed in Table 1.4. In this dissertation, these nine key elements will be discussed in the context of the materials design problem of focus in this dissertation, namely the integrated design of steel (material), manufacturing process (rolling and cooling) and hot rolled rods (product).

Table 1.4: Key elements for the integrated model-based realization of materials, products and manufacturing processes

	KEY ELEMENTS	Ties to Research Gaps
1	Individual Models and Multiscale Models and Modeling Methods	***G1***
2	Integration of Models across Process Chains to establish forward Process-Structure-Property-Performance relationships	***G2***
3	Systems-based Mathematical and Computational Frameworks for Decision-making	***G3, G4, G5***
4	Generic Goal-Oriented, Inverse Design Exploration Methods	***G3, G4***
5	Uncertainty Management and Robust Design	***G5***
6	Data, Information and Knowledge Capture, Storage, Access, Reuse, Management and Visualization	***G6, G7, G8***
7	Material Workflows and Decision Workflows	***G6, G7***
8	Knowledge-based Platforms for Decision Support	***G6, G7, G8***
9	Verification and Validation	***G1 to G8***

1.2 Research Questions

As discussed in previous section, the primary goal in this dissertation is to establish some of the scientific foundations and tools that are needed for the integrated realization of materials, products and manufacturing processes using simulation models that are typically incomplete, inaccurate and not of equal fidelity by managing the uncertainty associated. To realize the design of such complex engineering systems and make design decisions requires domain-specific knowledge, expertise and multi-scale (length and time scales) models with the consideration of not only the products themselves, but also the manufacturing processes, the constituent materials, and the operating environments as a system. Accordingly, the interest in this dissertation lies in establishing a ***systems-based design architecture*** that that includes system-level synthesis methods and tools that are required for the integrated design of complex materials, products and associated manufacturing processes starting from the end requirements. Keeping with this interest, focus is put in this dissertation to establish synthesis techniques that facilitate exploration of the design and solution spaces starting from the end performance to identify satisficing material microstructures and processing paths by managing the different types of uncertainty associated and thereby carry out robust decision-making in the design of complex material, product, and process systems.

The primary requirement for systems-based design architecture for integrated model-based realization of materials, products and associated manufacturing processes gives rise to the following primary research question for this dissertation:

Primary Research Question: *What are the theoretical, mathematical and computational foundations needed for establishing a comprehensive systems-based design architecture to realize the integrated design of the product, its environment, manufacturing processes and material as a system?*

The primary hypothesis defined in this dissertation to answer the primary research question is:

By establishing the theoretical, mathematical and computational foundations for,

1) *forward material, product and process workflows through systematic identification and integration of models to define the processing-structure-property-performance relationships;*
2) *a concept exploration framework supporting systematic formulation of design problems facilitating robust design exploration by bringing together robust design principles and multi-objective decision making protocols;*
3) *a generic, goal-oriented, inverse decision-based design method that uses 1) and 2) to facilitate the systems-based inverse design of material microstructures and processing paths to meet multiple product level performance/property requirements, thereby generating the problem-specific inverse decision workflow; and*

integrating them with a knowledge-based platform anchored in modeling decision-related knowledge facilitating capture, execution and reuse of the knowledge associated with 1), 2) and 3), a comprehensive systems-based design architecture to realize the integrated design of the product, its environment, manufacturing processes and material as a system can be achieved

Based on the analysis of the primary research question and hypothesis, the following requirements are specifically laid out:

i. *Integrated design by considering the material, product and the processes by which the material/product are made*
ii. *Integration of models (material, process and product) to establish processing-structure-property-performance relationships – establishing the material information workflow*
iii. *Consideration of end performance requirements for the material, product and process*
iv. *Support the goal-oriented, inverse decision-based design of material microstructures and processing paths to meet multiple conflicting performance/property requirements*
v. *Facilitation of robust concept exploration and decision making*
vi. *Accepting the notion that the models are typically incomplete, inaccurate and not of equal fidelity and managing the uncertainty associated*
vii. *Facilitation of rapid concept exploration when design requirements changes*
viii. *providing systematic, domain-independent, modular, reconfigurable, reusable, computer interpretable, archivable, and multiobjective decision support in the early stages of design to different users.*

Based on these key requirement, the primary research question is divided into four secondary research questions, **Research Question 1, Research Question 2, Research Question 3** and **Research Question 4**:

RQ1. *What are the foundations needed for* ***systematically identifying*** *and* ***integrating*** *material models with models of the rest of the system (product, manufacturing processes, and environment), so as to define the* ***processing-structure-property-performance*** *relationships and associated* ***information workflow*** *at early stages of design?*

RQ2. *What are the computational foundations needed for performing the* ***systematic*** *and* ***rapid concept exploration*** *of complex engineered systems involving the material, product and manufacturing processes* ***satisfying certain end performance requirements****, when simulation models are typically* ***incomplete, inaccurate and not of equal fidelity****?*

RQ3. *What are the requirements for an* ***inverse, goal-oriented design approach*** *for realizing the* ***robust design exploration*** *of the material, product and process as a system by managing the associated uncertainties?*

RQ4. *What are the foundations needed for maintaining* ***structural consistency*** *of the decision-based design workflow for the manufacturing process chain involving the material and product, ensuring* ***robust, flexible and modifiable*** *decisions while incorporating newer* ***data, information and knowledge*** *associated with the system?*

1.2.1 Research Area 1: Systematic Model Integration and Information Flow

Secondary Research Question 1 is focused on addressing research gaps 1 and 2 (G1 and G2). In response to Secondary Research Question 1, ***Research Hypothesis 1*** is:

> ***R.H1.1.*** *Through a systematic approach from a systems perspective, consisting of concept generation which includes*
>
> *a) functional decomposition to generate multilevel function structures across the process chain for the end performance requirements, followed by*
>
> *b) identifying material and process phenomenon associated with function structures and systematically mapping them to solution principles (models identified from literature or developed through experiments),*
>
> *and framing the system structure for problem via,*
>
> *c) vertical integration of identified/developed material models and horizontal integration of identified/developed process models to systematically map material processing to material microstructure phenomena and next to macrolevel properties and performances,*
>
> *the design of product, process and material concepts are integrated, and conceptual materials design is rendered more systematic* (To address **G1** and **G2**).

Materials design approaches in its current form do not address the conceptual design phase in a systematic fashion. Conceptual design phase is considered as the most crucial design stage as the decisions taken here affect the entire product's life cycle and resources. Advanced methodologies for material selection was the focus in the materials design communities before (Ashby and Cebon 1993, Ashby, Evans and coauthors 2000, Ashby and Johnson 2013). A paradigm shift has started towards materials design with the objective of tailoring the chemical composition, constituent phases, microstructure and processing paths to obtain materials with desired properties for particular applications (Rühle, Dosch and coauthors 2001, Panchal 2005, Panchal, Choi and coauthors 2005, McDowell, Panchal and coauthors 2009, Kalidindi, Niezgoda and coauthors 2011, McDowell and Kalidindi 2016, McDowell 2018). However, even now materials design is mostly exercised in the embodiment phase with focus on multiscale modeling techniques and simulations (Panchal, Choi and coauthors 2005).

Materials design as an automated search space is a very limited viewpoint as observed by (Eberhart and Clougherty 2004, Messer 2008). This is because of the fact that a supercomputer searching for an optimum property using accurate analysis models of an infinite number of materials, will still require infinite time to perform the search. Now the question arises whether there is a need for complex multiscale models to carry out materials design? The answer will be 'No'. Complex multiscale models might not be necessary in many materials design cases because the goal in materials design is to not accurately predict material properties but to satisfy a range of performance requirements. To this argument, we include the second fact that bottom-up modeling is not design but analysis. Thus, we believe that the key to materials design is an interplay of multiscale modeling and bottom-up analysis along with top-down, goal-oriented inverse design and human decision making.

A detailed review of materials design is presented in Chapter 2. In order to achieve materials design starting from the conceptual design phase, a function-based systematic approach is needed. This requirement is addressed in Research Question 1. The interest therefore by answering this research question is to propose a systematic approach to identify and classify material processing-structure-property-performance relations on multiple length scales to facilitate the design of material concepts to be further explored through systems-based top-down or inverse design exploration methods.

The function-based approach proposed in this dissertation for systematic model integration and information flow is based on the foundational work carried out by Matthias Messer in his dissertation (Messer 2008). The intention in this dissertation is to enable designers identify underlying phenomena and associated solution principles (models) to achieve systematic model integration for materials design exploration. Materials models and simulations evolve over time. Also, interdisciplinary research involving different fields such as mechanical engineering, materials engineering, systems engineering, design, etc. form a part of the emerging materials design research. By focusing on phenomena and associated solution principles embodying identified functional relationships, we are able to overcome such disciplinary boundaries and technological evolution.

Systematic design methods support designers to formulate and solve problems efficiently and effectively (Beitz, Pahl and coauthors 1996, Pahl and Beitz 2013). Pahl and Beitz (Beitz, Pahl and coauthors 1996), describe function-based design i.e, function-based analysis, abstraction, synthesis and systematic variation as most effective and efficient in the mechanical and electrical engineering domains. Achieving integrated material, product and process design involving phenomena and associated solution principles on the material level to systematically integrate models and establish information flow have not been addressed. Rendering materials, products and process design more systematic and domain independent by enhancing existing function-based systematic design approaches is addressed in Chapters 4 as proposed in Research Hypothesis 1.

1.2.2 Research Area 2: Concept Exploration and Inverse Design Exploration

Secondary Research Question 2 is focused on addressing research gaps 3 and 4 (G3 and G4). In response to Secondary Research Question 2, Research Hypothesis 2 is:

R.H2.1. *Developing a concept exploration framework anchored in decision-based design construct – the cDSP can support the designer in formulating the design problem systematically and exploring the solution space to generate satisficing design specifications* (To address **G3**). ***R.H2.2.*** *Developing a goal-oriented inverse design method that uses the concept exploration framework to facilitate the systems-based inverse design exploration of material microstructures and processing paths to meet multiple product level performance/property requirements* (To address **G4**).

In general, concept exploration is the process of evaluating different design concepts and providing top-level design specifications to meet overall system design requirements (Chen 1995). Determining top-level specifications is strongly influenced by the way in which overall design requirements (goals and constraints) can be used to control solutions. Overall design requirements can be used in two ways (Amarel 1990):

- By constraining *a priori,* the generation of possible design structures to be consistent with them, and
- By testing *a posterior* whether a candidate design satisfies them.

This relationship is shown in Figure 1.6.

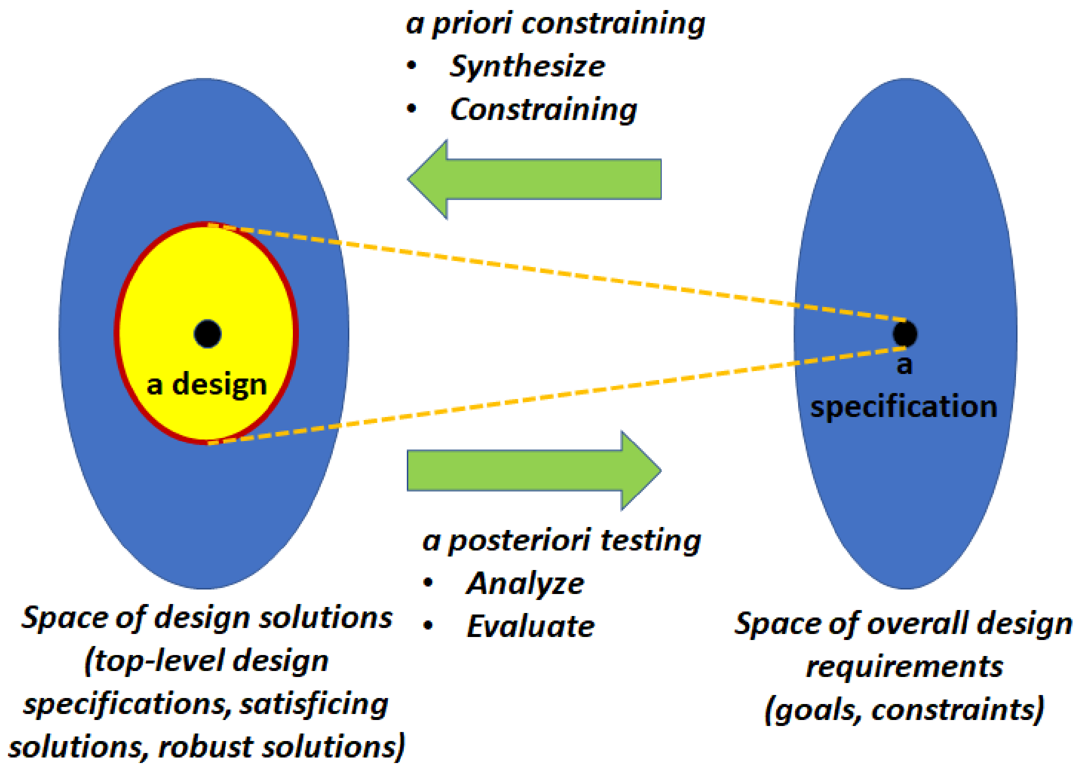


Figure 1.6: Relationship between space of overall design requirements and space of design solutions

The *a priori* use of design requirements involve *analysis* and *transformation* of the design requirements so as to enable them to control directly the generation of solutions. Relating this to the materials design mapping across processing, structure, property and performance spaces, this is equivalent to forward mapping using bottom-up modeling (deductive/cause and effect). This is systematically achieved using Research Hypothesis 1. The *a posteriori* use of design requirements involve *synthesis* and *evaluation* of a candidate solution or set of candidate solutions, and an assessment to the degree to which the candidate satisfies the design requirements. Relating this to the materials design, this is equivalent to inverse or inductive mapping using top-down design methods where the focus is to design the material to satisfy certain performance requirements. To achieve the integrated materials and product design both of these are required.

In this dissertation, the focus is to develop a concept exploration framework that is based on simulation-based design approach for designing complex systems. An ideal concept exploration framework should support both the activities of *a priori* analysis and *a posterior* evaluation/synthesis in concept exploration. The focus however in this dissertation is to use the concept exploration framework to support systems-based top-down design to generate "***satisficing design specifications***". The first proposed concept exploration model was in the ship design field to evaluate design alternative and generate top-level design specifications (Georgescu and Boonstra 1990). Smith (Smith and Mistree 1994) based on their detailed study on modeling and exploration of ship concepts, came to an important finding that a single-point design solution/approach as followed in optimization yields limited knowledge of the possibilities of the true solution space. The conclusion that was made therefore was that a greater emphasis is hence needed on concept exploration. However, due to expensive computational burden associated with complex engineering design problems, there should also be a way to manage the complexity associated during concept exploration. Therefore, concept exploration framework for complex, high dimensional engineering design problems requires efficient ways to manage the complexity – alternative to the extensive factorial grid search and effective data analysis tools, screening experiments. The framework should offer the capability to the designer to visualize the entire design space and further generate information about the *satisficing* regions of the design space.

In this dissertation, the compromise Decision Support Problem (DSP) provides a means for mathematically modeling, formulating, and supporting design decisions that involve seeking *satisficing design solutions* among multiple conflicting goals. The cDSP is the foundational mathematical construct for decision support and concept exploration in this dissertation. The compromise DSP is a domain-independent, multi-objective decision model that is a hybrid formulation based on Mathematical Programming and Goal Programming (Mistree, Hughes and coauthors 1993). It is used to determine the values of design variables that satisfy a set of constraints while achieving a set of conflicting goals as closely as possible. The compromise DSP is discussed in detail in Chapter 3. In this dissertation, it is shown that the compromise DSP can be used as a foundational, mathematical construct for structuring the systematic exploration for families of satisficing solutions for materials design problems. The focus in this dissertation is on making consistent compromise decisions in the integrated design exploration of materials, products and associated manufacturing processes.

Research Efforts in Inverse Design Exploration Approaches for Materials, Products and Processes

The need for inverse design exploration in process chains involving complex materials, products and processes is to identify adjustable ranges of control factor (design variables) that satisfies end performance requirements. As discussed in Section 1.1, inverse methods to identify microstructures and processing paths of a material satisfying a set of specified performance requirements is the focus in materials design communities and there are several works to this credit. Adams and coauthors (Adams, Kalidindi and coauthors 2013) present a framework that utilizes highly efficient spectral representations to arrive at invertible linkages between material structure, its properties, and the processing paths used to alter the material structure. Materials Knowledge Systems approach by Kalidindi and coauthors (Kalidindi, Niezgoda and coauthors 2010, Kalidindi, Niezgoda and coauthors 2011) showcase advances in rapid inverse design to estimate local responses. However, all these approaches including the strategy proposed by Olson (McDowell and Olson 2008) fall to specific classes of materials design problems and demands considerable knowledge and insight in mechanisms, material hierarchy and information flow. Thus, these classes of inverse design approaches are mostly suited for detailed design and not for “design exploration” (McDowell 2018).

In this dissertation, we seek “top-down”, goals/means, inductive or inverse methods especially at early stages of design to explore the design space of processing paths and resulting microstructures of a material satisfying a set of specified performance requirements. Approaches to pursue inverse design exploration by employing multiscale modeling and systems-based design especially at early stages of design are limited and need further evaluations to address hierarchical material design problems with consideration of robustness. Choi and coauthors (Choi, Mcdowell and coauthors 2008, Choi, McDowell and coauthors 2008) propose the Inductive Design Exploration Method (IDEM); a multi-level, robust design method that considers propagation of all three types of uncertainty, such as that arising in hierarchical materials design problems that incorporates process-structure-property relations. The two major design objectives using the IDEM for material and product design is (McDowell and Olson 2008): i) to guide bottom-up modeling so as to conduct top-down, goal-oriented design exploration, ii) manage the uncertainty in chains of process-structure-property relations. Kern and coauthors (Kern, Priddy and coauthors 2017) propose pyDEM a generalized implementation of the IDEM as an open-source tool in the Python environment. In pyDEM, the authors adopt the general procedure of IDEM as multi-level robust design tool and expands the algorithm for improved functionalities like arbitrary feasible boundary representation, improved computational efficiency, multi-platform availability, etc. to suit for practical engineering problems. In this dissertation, an inverse decision-based design method to achieve the integrated design exploration of materials, products and manufacturing processes through the vertical and horizontal integration of models is proposed (Nellippallil, Song and coauthors 2017, Nellippallil, Rangaraj and coauthors 2018). The inverse method is supported by the Concept Exploration Framework to systematically explore design alternatives and generate '***satisficing***' design solutions across process chains that involve process-structure-property-performance relations (Nellippallil, Rangaraj and coauthors 2018). The inverse decision-based design method for design exploration is addressed in Chapters 6 and 7 of this dissertation.

1.2.3 Research Area 3: Robust Concept Exploration

Secondary Research Question 3 is focused on addressing research gap 5 (G5). In response to Secondary Research Question 3, Research Hypothesis 3 is:

R.H3.1. *Introduction of specific robust design goals and constraints anchored in the mathematical constructs of error margin indices and design capability indices to determine ''satisficing robust design'' specifications for given performance requirement ranges using the goal-oriented, inverse design method can bring in robustness for multiple conflicting goals across process chains* (To address **G5**).

Uncertainty could be either *Aleatory* (irreducible) or *Epistemic* (reducible), depending on their causes. Improving the measurements and/or model formulation and/or increasing the accuracy are ways to diminish Epistemic uncertainty. Aleatory uncertainty, however is inherent in the physical system and can only be quantified in a statistical sense. Extending the classification by Isukapalli and coauthors (Isukapalli, Roy and coauthors 1998), we classify the types of uncertainty in simulation-based integrated design of material, product and processes as (Choi, Austin and coauthors 2005, McDowell, Panchal and coauthors 2009):

- *Natural Uncertainty* (NU): uncertainty due to the inherent randomness or unpredictability of a physical system; Aleatory in nature.
- *Model Parameter Uncertainty* (MPU): incomplete knowledge of model parameters/inputs due to insufficient or inaccurate data; reducible by sufficient data or accurate measurements; uncertainty in design variables or control factors.
- *Model Structure Uncertainty* (MSU): uncertain model formulation due to approximations in a model; reducible by improving model formulation; uncertainty in function relationship between control/noise and response.
- *Propagated Uncertainty* (PU): uncertainty compounded by the combination of all the above three types of uncertainty in a chain of models that are connected through input output relations; interdependent responses and shared control/noise factors as one model interacts with another, see (Allen, Seepersad and coauthors 2006) for their modes of interaction.

Two approaches are followed in dealing with these sources of uncertainty – mitigating uncertainty and managing uncertainty. In first approach, the focus is to reduce/mitigate the uncertainty. This is achieved by seeking “perfect” models, collecting more data, developing improved methods to model, calculate and quantify uncertainty through expensive computations. Modern data science methods for materials and microstructure informatics along with multiscale modeling techniques are being developed to provide decision support and address the issue of uncertainty in hierarchical materials design (Panchal, Kalidindi and coauthors 2013, Kalidindi 2015, McDowell and Kalidindi 2016, McDowell and LeSar 2016). Seepersad and coauthors (Shahan and Seepersad 2012, Matthews, Klatt and coauthors 2016) considers Bayesian network classifiers to design materials with hierarchy and to treat uncertainty propagation in multilevel material design. Mahadevan and coauthors (Li and Mahadevan 2016, Mullins and Mahadevan 2016) address the issue of uncertainty integration across multilevel and the role of calibration, validation and relevance in multilevel uncertainty integration for hierarchical material design problems. Even though there are several such recent efforts to address the issue of uncertainty, McDowell (McDowell 2018) observes that quantifying uncertainty in schemes for linking models at different length and time scale is still an immature field and formal mathematical approaches for doing this are largely undeveloped. The recommendation therefore made for simulation-assisted materials design is to focus on understanding the sensitivity of material properties to material microstructure and to capture dominant mechanisms and transitions that affect material responses or properties instead of focusing on accurately predict mean properties at higher scales. Sensitivity analysis of responses is important because of several reasons (McDowell 2018):

- It is challenging to isolate response sensitivity experimentally at specific scales in the material hierarchy,

- The identification of key design variables across material structure hierarchy is possible via sensitivity analysis, and
- Core to the concept of robust design is the sensitivity of process-structure and structure-property relations, where the focus is to explore a range of solutions that meet conflicting response requirements and identify satisficing design solution that are relatively insensitive to uncertainty (McDowell, Panchal and coauthors 2009).

This demands the need for the second approach of managing uncertainty in integrated design of materials, products and processes with focus on sensitivity of key properties or responses to variation in microstructure which in turn connects to variation in processing paths.

In second approach, the focus is to manage uncertainty by designing the system to be insensitive to the sources without reducing or eliminating them. This is done by exploring the solution space and studying the sensitivity of responses to variations in noise, control factors and models themselves and understanding the tradeoffs required with various compromises; this is called robust design (Chen, Allen and coauthors 1996, Choi, Austin and coauthors 2005, Murphy, Tsui and coauthors 2005, Allen, Seepersad and coauthors 2006, Choi, McDowell and coauthors 2008, Nellippallil, Allen and coauthors 2017). There are several practical implications with this approach. Robust solutions are not focused on extensive optimization searches at individual levels and do not necessarily involve large number of iterations (McDowell and Olson 2008). The practical interest here is for ranged set of solutions that showcase good performance under variability rather than single-point solutions that are valid for narrow range of conditions, while performing poorly when the conditions are changed slightly. The human designer plays the role of an interpreter of value of information in this approach. Concepts and mathematical constructs from information economics (Howard 1966, Panchal, Paredis and coauthors 2006, Sinha, Bera and coauthors 2013) are used to manage uncertainty by studying the value of information for cost/benefit tradeoff to make design decisions in the presence of uncertainty.

Research Efforts in Robust Design of Materials, Products and Processes – Design Under Uncertainty

In robust design (RD), the quality of products and processes are improved by reducing their sensitivity to variations without eliminating the sources (Taguchi 1986, Taguchi and Clausing 1990, Nair, Abraham and coauthors 1992, Tsui 1992). The robust design principles and methods are founded on the philosophy of Genichi Taguchi (Taguchi 1986).

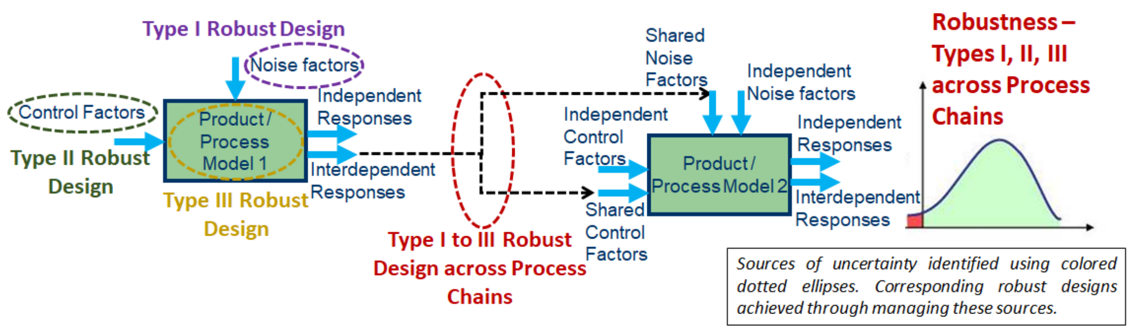


Figure 1.7: **The sources of uncertainty and corresponding robust designs in complex material, product and process systems**

Three categories of information interact with the system model in robust design (McDowell, Panchal and coauthors 2009): i) control factors, also known as design variables are parameters that the designer adjusts to move towards a desired product, ii) noise factors, are exogenous parameters that affect the performance of product/process but cannot be controlled by the designer, iii) responses are performance measures for the product or process. We have captured these information in Figure 1.7 with their interactions in complex material, product and process systems. Over the years robust design have been categorized into (McDowell, Panchal and coauthors 2009):

Type I Robust Design (Taguchi 1993)**:** To identify control factor (design variable) values that satisfy a set of performance requirement despite variations in noise factors. Though Type I robust design principles as proposed by Taguchi are advocated widely, his statistical techniques that includes orthogonal arrays and signal-to-noise ratio are widely criticized. Many researchers (Box 1988, Vining and Myers 1990, Welch, Yu and coauthors 1990, Shoemaker, Tsui and coauthors 1991, Tsui 1992, Parkinson, Sorensen and coauthors 1993, Sundaresan, Ishii and coauthors 1995, Chen, Allen and coauthors 1996) have actively worked on improving the statistical techniques in robust design and thus have over the years developed mathematical constructs that bring in robust design into a systematic framework.

Type II Robust Design (Chen, Allen and coauthors 1996, Chen, Simpson and coauthors 1999)**:** To identify control factor values that satisfy a set of performance requirements target despite variation in control factors themselves. Chen and coauthors (Chen, Allen and coauthors 1996) propose a procedure for robust design Types I and II by minimizing variations of noise and control factors and formulate the problem as multi-objective decision problem using mean on targets and variances as separate goals. The foundational mathematical construct for decision support in their work is the compromise Decision Support Problem (cDSP) proposed by Mistree and coauthors (Bras and Mistree 1993, Mistree, Hughes and coauthors 1993) for robust design with multiple goals. The Robust

Concept Exploration Method (RCEM) is further proposed for Type I and II robust designs and includes systematic steps to identify design alternatives and generate robust design solutions (Chen, Allen and coauthors 1997). Mathematical constructs known as Design Capability Indices (DCIs) are further incorporated in RCEM to determine whether a ranged set of design specifications satisfies a ranged set of design requirements (Chen, Simpson and coauthors 1999). Nellippallil and coauthors (Nellippallil, Rangaraj and coauthors 2018) propose the Concept Exploration Framework (CEF); inspired from the RCEM with addition of features (processors) to consider different material and product models and options to explore the solution space for different design scenarios by weighing multiple goals. The CEF is addressed in Chapter 5 of this dissertation.

Type III Robust Design (Choi, Austin and coauthors 2005)**:** To obtain design solutions that are insensitive to variability or uncertainty embedded within the model used. Choi and coauthors (Choi, Austin and coauthors 2005) propose the robust concept exploration method with error margin indices (RCEM-EMI) for Type I, II and III robust designs. Error margin indices are mathematical constructs that indicates the location of the mean response and the spread of the response considering the variability associated with design variables and system models. These are then incorporated as goals in the cDSP formulation to design the system under model structure and model parameter uncertainty. The inverse decision-based design method for robust design exploration is addressed in detail in Chapter 7 of this dissertation.

1.2.4 Research Area 4: Knowledge-based Platform for Decision Support

Secondary Research Question 4 is focused on addressing research gaps 6, 7 and 8 (G6, G7 and G8). In response to Secondary Research Question 4, Research Hypothesis 4 is:

R.H4.1. *Using ontology to represent decision-related knowledge that is modeled as Decision Support Problem (DSP) templates can capture, analyze, archive and update the decision-based design workflow as per the needs of the individual decision-maker. Separation of declarative (problem specific) knowledge and procedural (process specific) knowledge in the information flow scheme can help in generalizing the decision models in the design workflow* (To address **G6**).

R.H4.2. *Defining three types of users, namely Template Creators, Template Editors, and Template Implementers, and providing customized decision support to these users during the design of engineering systems can help perform original design, adaptive design, and variant design respectively* (To address **G7**).

R.H4.3. *Developing an ontology for design space exploration and a template-based ontological method that supports systematic design space exploration ensuring the determination of the right combination of design information that meets the different goals and requirements set for a process chain* (To address **G8**).

Design of engineering systems is increasingly recognized as a decision-making process (Daskilewicz and German 2012, Afshari, Peng and coauthors 2016, Berg and Vance 2016, Soria, Colby and coauthors 2017). The fundamental research philosophy in this dissertation is that the principal role of a human designer is to make decisions. Providing decision support is of critical importance for augmenting this role, by speeding up the design process and generating quality designs. One of the challenges in providing decision support in the design of engineering systems, especially complex systems that are, by definition, made up of inter-related subsystems (Kuppuraju, Ganesan and coauthors 1985), arises because of the complexity embodied in the decision workflows that embody multiple coupled decisions networked in various degrees of complexity. The networked decision workflows may include different types of decisions, e.g., selection of design alternatives and improvement of an alternative considering multiple goals. The decisions are coupled together due to the dependency existing among systems and subsystems. The different types of decisions and their associated dependencies in the decision workflows make it difficult to provide appropriate decision support.

Decision making is a knowledge-intensive process, knowledge plays a significant role in speeding up and effecting decisions. Capturing, managing, and reusing of decision related knowledge such as alternatives, parameters, constraints, goals, dependencies, and the design process in the design of complex systems is an effective way for providing decision support. Many research efforts have been made to develop knowledge-based decision support in designing engineering systems, these efforts are typically categorized as follows: 1) application of reasoning techniques for dealing with a large number of rules in design (Gero 1990, Tong and Sriram 1997), 2) integrating design knowledge with decision based design processes (Zha, Lim and coauthors 2003, Zha, Sriram and coauthors 2003), and 3) representing semantic knowledge to facilitate communication and interoperability of integrated decision support systems (Schoop, Becks and coauthors 2002, Chiu, Cheung and coauthors 2005, Rockwell, Grosse and coauthors 2010). In addition to the efforts on decision support in design, many others are contributed to support organizational decisions by managing enterprise resources, such as (Liu, Duffy and coauthors 2008, Liu, Duffy and coauthors 2009). Despite the fact that many knowledge-based systems have been developed for decision support from different perspectives, the challenge of supporting the decision workflow in the design of complex engineering systems is not yet well addressed, mainly, by the following reasons:

1) Lack of a both reusable and executable decision knowledge representation schemes. Knowledge reusability is critical for adaptive and variant design wherein only a small portion of the original decision workflows need to change while the rest remains the same and can be reused. Some authors have proposed to represent decision knowledge as ontologies (e.g., (Rockwell, Grosse and coauthors 2010)), but they mainly focus on capturing the semantic information of design decisions while failing to represent the execution process information which is necessary for effecting new decisions, especially in a computational environment whereby some degree of automation is realized.

2) Lack of a classification of users for decision support. The needs of designers for decision support vary according to how much novelty is involved in the design and how much knowledge they have about the design process. For example, an expert has much knowledge about design and can perform the decision-making process independently, thus the support this designer needs from the computer system is very different from a novice designer who only has the basic knowledge about design and needs to get most of the knowledge from the system. Very few of knowledge-based systems recognized this difference and provide appropriate decision support.

To address the aforementioned needs, a Knowledge-Based Platform for Decision Support in the Design of Engineering Systems (PDSIDES) is proposed by Zhenjun Ming in his dissertation and reported in (Ming, Nellippallil and coauthors 2018). The industry inspired problem for integrated design of materials, product and manufacturing processes formulated and studied in this dissertation is used as a test example to illustrate the efficacy of the PDSIDES platform; addressed in Chapter 8 of this dissertation.

In order to achieve an intelligent environment for designing complex engineering systems, a good understanding of predicting process behavior is paramount. Achieving this using decision-based design necessitates a systematic, flexible, dynamic, and adaptive designing of the decision workflows involved. The decision-based design results associated with these workflows should be robust i.e. relatively insensitive to the uncertainties involved. The design results should also be flexible enough to accommodate any risk of errors that may accumulate along the decision workflows. To address above demands, an ontology for design space exploration and a template-based ontological method that supports systematic design space exploration in the model-based realization of complex engineered systems is proposed by Ru Wang in his dissertation and reported in (Wang, Nellippallil and coauthors 2018). Using this proposed method, a designer is able to determine the right combinations of design information that meets the different goals set thereby satisfying the end requirements for each stage of the process, and also adjust the design space to achieve solutions that are robust and flexible enough to manage any risk of error propagation in continuous multi-stage design. The efficacy of this method is illustrated by using the example associated with the design of a multi-stage hot rod rolling system addressed in this dissertation. The ontology for design space exploration and the template-based ontological method that supports systematic design space exploration in the model-based realization of complex engineered systems is addressed in Chapter 9 of this dissertation.

1.2.5 Fundamental Research Philosophies and Assumptions

The fundamental philosophies on which research questions and hypotheses are based are summarized in this section. The general philosophies are:

- *Analysis models are incomplete, inaccurate and of differing fidelity*: The foundational philosophy for this research is accepting the fact that models are but abstractions of reality and are typically incomplete, inaccurate and not of equal fidelity. Given this the role of a human designer in this dissertation is to provide computational support to make decisions for exploring the solution space.
- *Emergent properties*: A complex system has emergent properties. Complex systems embody systemic features (emergent properties) that cannot be predicted or deduced. Hence, designers need to know how to account for emergent properties associated with the realization of a complex system. The key emergent properties in a complex system are "complexity" and "uncertainty". Therefore, for the model-based realization of complex systems, it is essential to know how to identify and manage complexity and to identify and manage uncertainty.
- *Design is a goal-oriented activity and design requirements are subject to change*: As observed by Gero (Gero 1996), design can be conceived of as a purposeful, constrained, decision making, exploration and learning activity. Decision making here refers to the process of deciding the values of a set of design variables. Exploration here refers to changing the problem or design spaces within which

decision making takes place. Learning here implies the restructuring of the knowledge generated through the design process. The context in which the designer operates partially depends on the designer's perceptions of purposes, constraints, goals and related requirements. Thus, the designer starts with some goals that he/she wishes to satisfy and thus design is a goal-oriented activity. These perceptions are bound to change as the designer explores the emerging relationships between possible designs and the context and as learning happens while exploring the design space.

Given the fundamental research philosophies, the question addressed in this dissertation from the simulation-based design perspective is:

What is the role of a human designer in simulation-based design?

The question is investigated in this dissertation and the answer to which depends on certain fundamental research assumptions, listed below:

- A human designer should make decisions using information provided by computational decision support models that are typically incomplete and inaccurate.
- There are two types of decisions that a human designer can make - selection or compromise.
- Do not eliminate uncertainty – manage it.
- Explore multiple possible solutions and their consequences rather than identifying a single unique solution.

1.2.6 Overview Research Hypothesis

Research requirements, questions and hypotheses are summarized in Table 1.5. In Table 1.6, it is illustrated which constructs of the systematic approach and which validation examples address the research requirements identified in Section 1.2. The secondary research hypotheses and example problems are mapped to the overall systematic approach to integrated product, materials and manufacturing process design, given here as an overview in Figure 1.8 and described in greater detail in Chapter 4. The relationship between hypotheses and dissertation chapters is illustrated in Table 1.7.

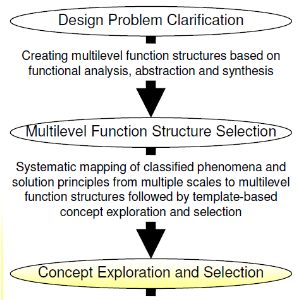
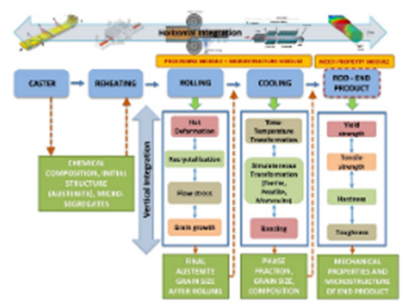
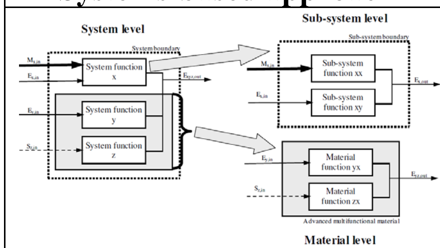
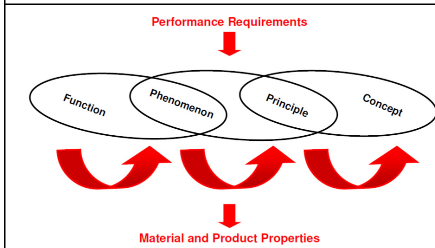
Table 1.5: Research Gaps, Research Hypothesis, Research Questions and Expected Contributions

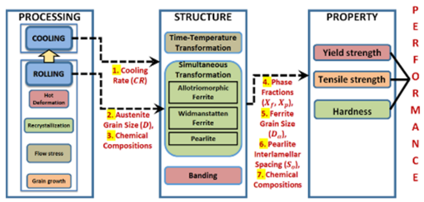
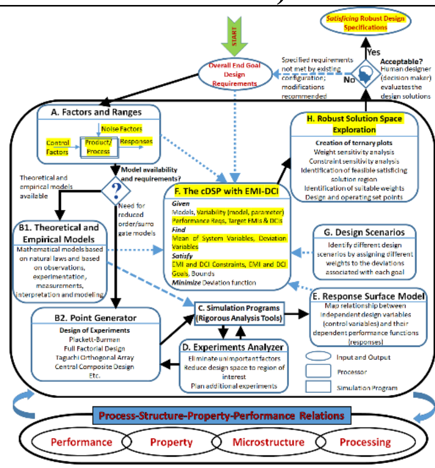
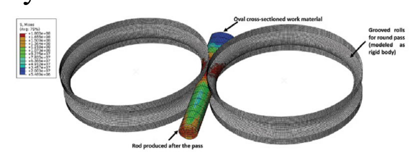
<table>
<tr><td rowspan="3">Primary</td><td>Requirement</td><td colspan="3">Systems-based design architecture for integrated model-based realization of materials, products and associated manufacturing processes</td></tr>
<tr><td>Research Question</td><td colspan="3">What are the theoretical, mathematical and computational foundations needed for establishing a comprehensive systems-based design architecture to realize the integrated design of the product, its environment, manufacturing processes and material as a system?</td></tr>
<tr><td>Research Hypothesis</td><td colspan="3">By establishing the theoretical, mathematical and computational foundations for,
1) forward material, product and process workflows through systematic identification and integration of models to define the processing-structure-property-performance relationships;
2) a concept exploration framework supporting systematic formulation of design problems facilitating robust design exploration by bringing together robust design principles and multi-objective decision making protocols;
3) a generic, goal-oriented, inverse decision-based design method that uses 1) and 2) to facilitate the systems-based inverse design of material microstructures and processing paths to meet multiple product level performance/property requirements, thereby generating the problem-specific inverse decision workflow; and
and integrating them with a knowledge-based platform anchored in modeling decision-related knowledge facilitating capture, execution and reuse of the knowledge associated with 1), 2) and 3), a comprehensive systems-based design architecture to realize the integrated design of the product, its environment, manufacturing processes and material as a system can be achieved.</td></tr>
<tr><td></td><td>Research Gaps</td><td>Research Hypothesis addressing the Research Gaps</td><td>Secondary Research Questions Framed from Research Hypothesis</td><td>Contributions (New Knowledge)</td></tr>
<tr><td>I</td><td>G1. Systematic approaches to define the forward processing-structure-property-performance relationships and develop material and product workflows

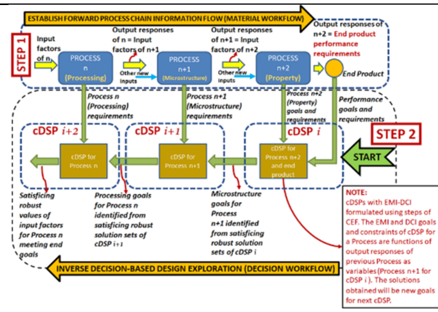
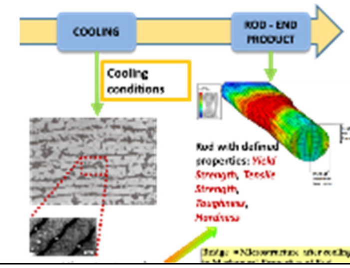
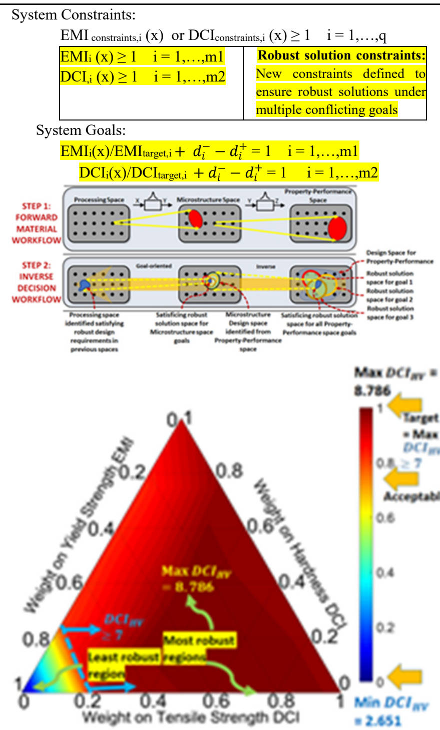
G2. Systematic approaches to identify and integrate material, process and product models based on their function structures to frame system-level structure</td><td>H1.1. Through a systematic approach from a systems perspective, consisting of concept generation which includes
a) functional decomposition to generate multilevel function structures across the process chain for the end performance requirements, followed by
b) identifying material and process phenomenon associated with function structures and systematically mapping them to solution principles (models identified from literature or developed through experiments),
and framing the system structure for problem via,
c) vertical integration of identified/developed material models and horizontal integration of identified/developed process models to systematically map material processing to material microstructure phenomena and next to macrolevel properties and performances,
the design of product, process and material concepts are integrated, and conceptual materials design is rendered more systematic.</td><td>RQ1. What are the foundations needed for systematically identifying and integrating material models with models of the rest of the system (product, manufacturing processes, and environment), so as to define the processing-structure-property-performance relationships and associated information workflow at early stages of design?</td><td>Systematic identification and integration of material, process and product models and workflows to define processing-structure-property-performance mapping.</td></tr>
</table>

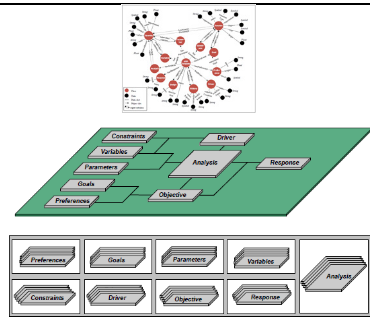
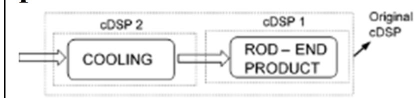
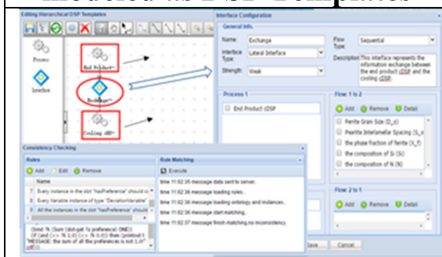
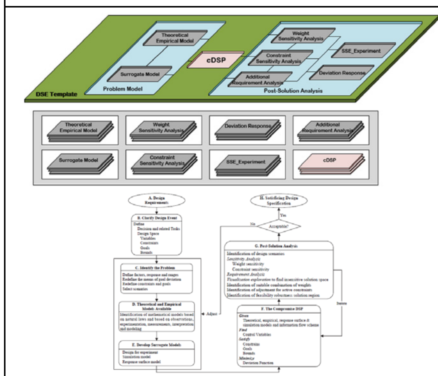
II	**G3.** Support systematic and rapid concept exploration of materials, products and processes to generate satisficing design specifications **G4.** Systematic design methods to carry out inverse design exploration of materials, products and processes meeting end goals	***H2.1.*** Developing a concept exploration framework anchored in decision-based design construct – the cDSP can support the designer in formulating the design problem systematically and exploring the solution space to generate satisficing design specifications (To address **G3**). ***H2.2.*** Developing a goal-oriented inverse design method that uses the concept exploration framework to facilitate the systems-based inverse design exploration of material microstructures and processing paths to meet multiple product level performance/property requirements (To address **G4**).	***RQ2.*** What are the computational foundations needed for performing the ***systematic*** and ***rapid concept exploration*** of complex engineered systems involving the material, product and manufacturing processes ***satisfying certain end performance requirements***, when simulation models are typically ***incomplete, inaccurate and not of equal fidelity***?	1. A framework for systematic design and solution space exploration 2. A generic method for inverse design of materials and products across process chains
III	**G5.** Systematic strategies to carry robust concept exploration of material, product and process system in inverse manner by managing uncertainty	***H3.1.*** Introduction of specific robust design goals and constraints anchored in the mathematical constructs of error margin indices and design capability indices to determine "satisficing robust design" specifications for given performance requirement ranges using the goal-oriented, inverse design method can bring in robustness for multiple conflicting goals across process chains	***RQ3.*** What are the requirements for an ***inverse, goal-oriented design approach*** for realizing the ***robust design exploration*** of the material, product and process as a system by managing the associated uncertainties?	1. Metrics, robust design constraints and goals for facilitating robust design across process chains for multiple conflicting goals
IV	**G6.** Constructs and tools to capture and reuse the knowledge associated with material and product systems design **G7.** Facilitation of original, adaptive and variant design decision support **G8.** Facilitation of systematic design exploration through decisions that are robust, flexible and modifiable particularly in the early stages of design.	***H4.1.*** Using ontology to represent decision-related knowledge that is modeled as Decision Support Problem (DSP) templates can capture, analyze, archive and update the decision-based design workflow as per the needs of the individual decision-maker. Separation of declarative (problem specific) knowledge and procedural (process specific) knowledge in the information flow scheme can help in generalizing the decision models in the design workflow (To address **G6**). ***H4.2.*** Defining three types of users, namely Template Creators, Template Editors, and Template Implementers, and providing customized decision support to these users during the design of engineering systems can help perform original design, adaptive design, and variant design respectively (To address **G7**). ***H4.3.*** Developing an ontology for design space exploration and a template-based ontological method that supports systematic design space exploration ensuring the determination of the right combination of design information that meets the different goals and requirements set for a process chain (To address **G8**).	***RQ4.*** What are the foundations needed for maintaining ***structural consistency*** of the decision-based design workflow for the manufacturing process chain involving the material and product, ensuring ***robust, flexible and modifiable*** decisions while incorporating newer ***data, information and knowledge*** associated with the system?	1. Capture knowledge in original design, maintain consistency in adaptive design and provide a package of documented knowledge in variant design. 2. Template-based ontological method for systematic design space exploration

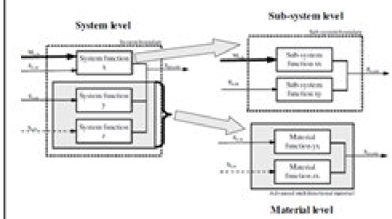
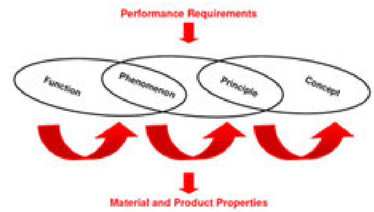
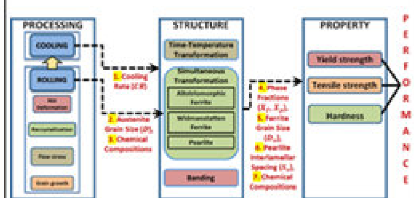
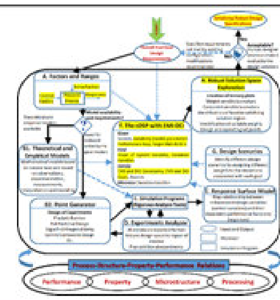
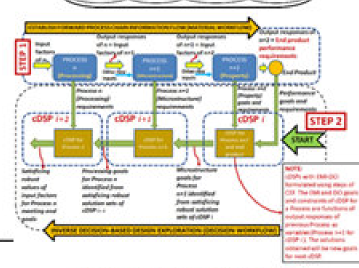
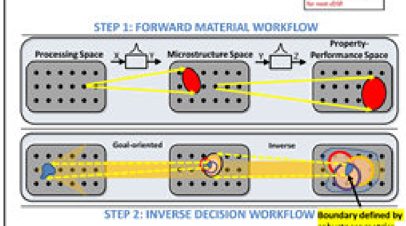
Table 1.6: Constructs of the Systems-Based Architecture to Address the Requirements and Validation Examples

Requirements	Constructs of the Systems-based Design Architecture developed in this Dissertation	Research Hypotheses	Validation Examples
1.Systematically define the forward processing-structure-property-performance relationships 2.Systematic integration of material, process and product models	 **Systems-based approach**	**RH.1.** a systematic approach from a systems perspective, consisting of concept generation	1. Steel Manufacturing Process Chain Problem - Integrated design of steel (material), manufacturing processes (rolling and cooling) and hot rolled rods (product) for automotive gears 
	 **Systematic generation of multilevel function structures**	**RH1.1. a)** functional decomposition to generate multilevel function structures across the process chain for the end performance requirements,	
	 **Systematic design mappings to identify models**	**RH1.1. b)** identifying material and process phenomenon associated with function structures and systematically mapping them to solution principles (models identified from literature or developed through experiments)	

	 **Systematic integration of identified models to develop processing-structure-property-performance mapping (forward material workflow)**	framing the system structure for problem via, **R.H.1. c)** vertical integration of identified/developed material models and horizontal integration of identified/developed process models to systematically map material processing to material microstructure phenomena and next to macrolevel properties and performances	
Systematic concept exploration	 **Concept Exploration Framework**	**RH2.1.** a concept exploration framework anchored in decision-based design construct – the cDSP can support the designer in formulating the design problem systematically and exploring the solution space to generate satisficing design specifications.	**1.** Integrated design of steel (material), manufacturing processes (rolling and cooling) and hot rolled rods (product) for automotive gears **AND** **2.** Horizontal Integration of a Multistage Hot Rod Rolling System  **AND**

Inverse design exploration	 **Goal-oriented Inverse Design (GoID) Method**	**RH2.2.** a goal-oriented inverse design method that uses the concept exploration framework to facilitate the systems-based inverse design exploration	**3.** Explore the Solution Space for Microstructure After Cooling Stage to Realize the End Mechanical Properties of Hot Rolled Product 
Robust concept exploration of process chains in an inverse manner under uncertainty for multiple conflicting goals	 **Robust Concept Exploration**	**R.H3.1.** Introduction of specific robust design goals and constraints anchored in the mathematical constructs of error margin indices and design capability indices to determine ‘‘satisficing robust design’’ specifications for given performance requirement ranges using the goal-oriented, inverse design method can bring in robustness for multiple conflicting goals across process chains	1. Steel Manufacturing Process Chain Problem - **Focus on robust exploration across process chains** 

1.Knowledge capture and reuse 2.Facilitation of original, adaptive and variant designs 3.Facilitation of systematic design exploration through decisions that are robust, flexible and modifiable particularly in the early stages of design.	 **Ontology to represent decision-related knowledge modeled as DSP Templates**	**RH4.1.** Ontology to represent decision-related knowledge that is modeled as Decision Support Problem (DSP) templates can capture, analyze, archive and update the decision-based design workflow	1. Steel Manufacturing Process Chain Problem – **Focus on cooling process and end rod product** 
	 **Editing Design Templates in PDSIDES**	**RH4.2.** Defining three types of users, namely Template Creators, Template Editors, and Template Implementers, and providing customized decision support to these users during the design of engineering systems can help perform Original Design, Adaptive Design, and Variant Design respectively.	
	 **Ontology and template-based method for Design Space Exploration**	**RH4.3.** Ontology for design space exploration and a template-based ontological method that supports systematic design space exploration	1. Integrated design of steel (material), manufacturing processes (rolling and cooling) and hot rolled rods (product) for automotive gears

Systematic Model Integration and Information Flow *-Research Question 1-*	**Design Problem Clarification** Creating multi-level function structures based on functional analysis, abstraction and synthesis **Multi-level Function Structure Selection and Integration** Systematic mapping of classified phenomena and solution principles from multiple scales to multilevel function structures (models identified) **Frame System-level Function Structure** Vertical and horizontal integration of models to systematically map processing-structure-property-performance spaces (Information flow)	  
Systematic Concept Exploration and Inverse Design Exploration *-Research Question 2-*	**Systematic Concept Exploration** Systematic formulation and exploration of the design space to generate satisficing design specifications **Systematic Inverse Design Exploration** A goal-oriented inverse design method to facilitate the systems-based inverse design exploration	 
Robust Concept Exploration *-Research Question 3-*	**Systematic Robust Concept Exploration** Generating "satisficing robust design" specifications across process chains using robustness metrics	

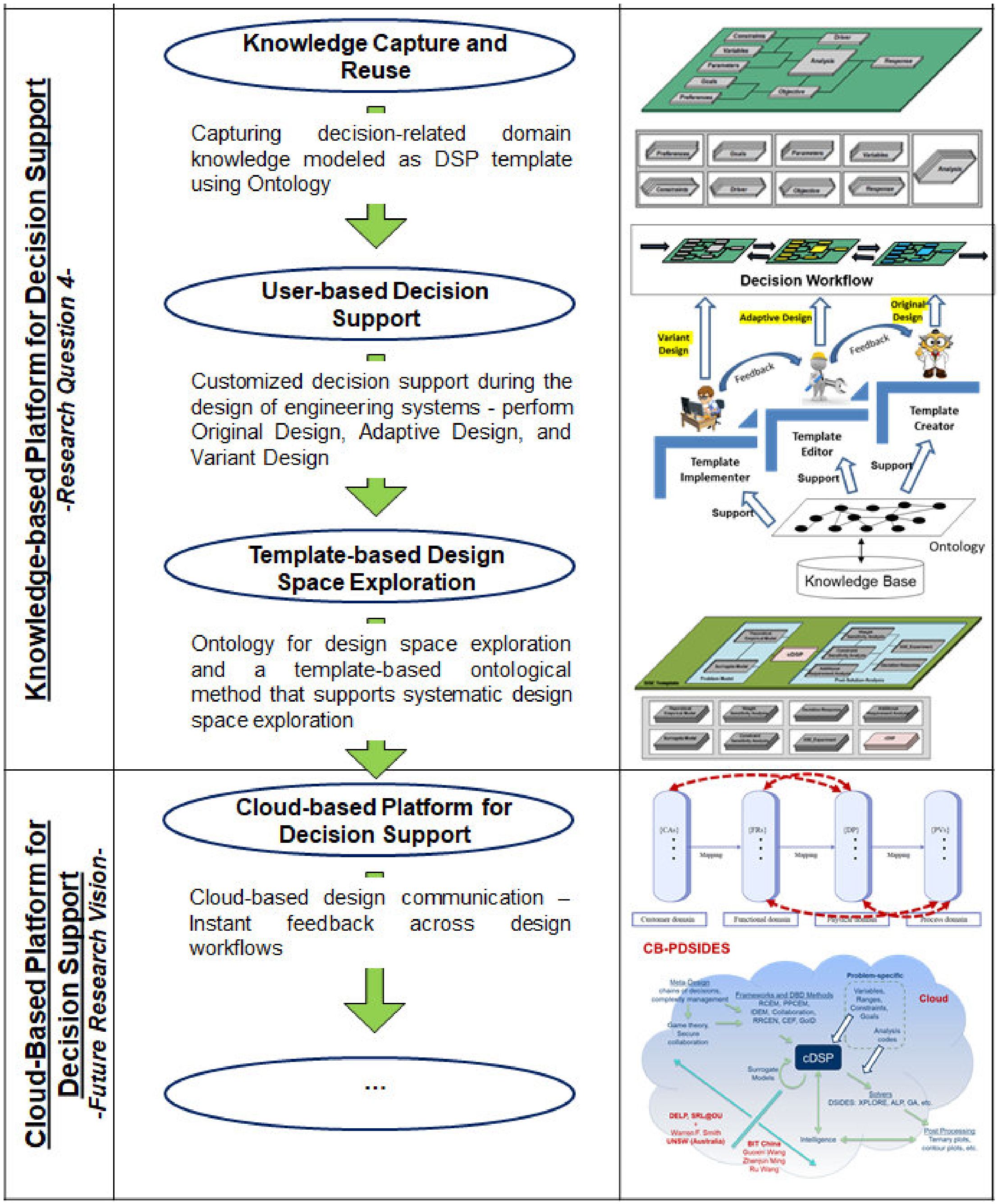


Figure 1.8: Systematic approach towards integrated design of materials, products and manufacturing processes

Table 1.7: Relation between Research Hypothesis and Dissertation Chapters

Hypothesis	Foundations Reviewed	Chapters Approach Developed	Approach Tested
1	3	4	6
2	2, 3	4	6
3	3, 7	7	7
4	3, 8	8, 9	8, 9

1.2.7 Research Contributions

As described in Section 1.1, the main contribution in this dissertation is the development of a systems-based design architecture for the integrated design of materials, products and associated manufacturing processes. The foundational premise for this dissertation is that systems-based materials design techniques offer the potential for tailoring materials, their processing paths and the end products that employ these materials in an integrated fashion for challenging applications to satisfy conflicting product and process level property and performance requirements. The primary goal in this dissertation is to establish some of the scientific foundations and tools that are needed for the integrated realization of materials, products and manufacturing processes using simulation models that are typically incomplete, inaccurate and not of equal fidelity by managing the uncertainty associated. Accordingly, the interest in this dissertation lies in establishing a systems-based design architecture that includes system-level synthesis methods and tools that are required for the integrated design of complex materials, products and associated manufacturing processes starting from the end requirements.

The contributions from the dissertation are categorized into new knowledge in four research domains: a) systematic model integration and information flow (vertical and horizontal) for integrated material and product workflows, b) goal-oriented, inverse decision support, c) robust concept exploration of process chains with multiple conflicting goals and d) knowledge-based decision support for rapid and robust design exploration in simulation-based integrated material, product and process design.

The creation of new knowledge in this dissertation is associated with the development of a systems-based design architecture involving systematic function-based approach of formulating forward material workflows, a concept exploration framework for systematic design exploration, an inverse decision-based design method, and robust design metrics, all integrated with a knowledge-based platform for decision support. The theoretical, mathematical and computational foundations for the design architecture are proposed in this dissertation to facilitate rapid and robust exploration of the design and solution spaces to identify material microstructures and processing paths that satisfy conflicting property and performance for complex materials, products and processes by managing uncertainty.

Specific contributions in this research include:

- Systematic identification and integration of material, process and product models and workflows to define processing-structure-property-performance mapping and information workflow,
- A reusable, expandable computational framework supporting vertical and horizontal integration of models to identify material structures and processing paths that satisfy ranged set of product and manufacturing process-level property and performance requirements,
- A framework supporting systematic design and solution space exploration,

- A generic method for inverse design of materials and products across process chains,
- Metrics, robust design constraints and goals for facilitating robust design across process chains for multiple conflicting goals,
- Capture knowledge in original design, maintain consistency in adaptive design and provide a package of documented knowledge in variant design,
- Template-based ontological method for systematic design space exploration.

Based on these contributions a designer now has the following abilities the baseline designer did not have before:

- Designing materials and products in a systematic fashion during the early stages of design by looking at information flow and mapping across models,
- Designing products, materials and their processing paths in a function-based, systematic, integrated fashion from a systems perspective by satisfying specific end performance requirements,
- The capability to carry out rapid, integrated design exploration of material and products using simulation models that we accept are typically incomplete and inaccurate,
- The capability to support a human designer under complex material system's random variability and/or model parameter uncertainty and/or model structure uncertainty in making decisions that satisfies multiple conflicting goals,
- The capability to model decision-related knowledge with templates using ontologies to facilitate execution and reuse,
- The capability to coordinate information and human decision making.

Therefore, crucial to this dissertation are:

i) The requirements driven, "top-down" design of system and associated subsystems by taking a goal-oriented, inverse approach which is different to the standard practice of bottom-up modeling and design of material and product systems,

ii) the management of uncertainty in the system without removing the sources and supporting in identifying robust design solutions across process chains,

iii) Platformization of decision templates to support different types of users to facilitate original, adaptive and variant designs in materials and product design.

The systems-based design architecture for integrated model-based realization of materials, products and associated manufacturing processes is validated using an industry-inspired example problem from the steel manufacturing domain, namely: *the integrated design of steel (material), manufacturing processes (rolling and cooling) and hot rolled rods (product) for automotive gears*.

However, potential applications are numerous and compelling, and not limited to the one addressed in this dissertation. The framework and method developed in this dissertation is generalizable for industries in which mechanical, structural, and thermal systems are essential. The applications include the manufacturing of lightweight, high performance, low cost and reliable parts and machine components, for example automobile gear box, shafts, etc. More details on the validation strategy used in this dissertation are described in the following Section.

1.3 Verification and Validation of Dissertation Chapters

The verification and validation strategy used in this dissertation is based on the validation square framework introduced by Pederson and co-authors (Pedersen, Emblemsvag and coauthors 2000, Pedersen, Emblemsvag and coauthors 2000, Seepersad, Pedersen and coauthors 2006). The validation square construct is illustrated in Figure 1.9.

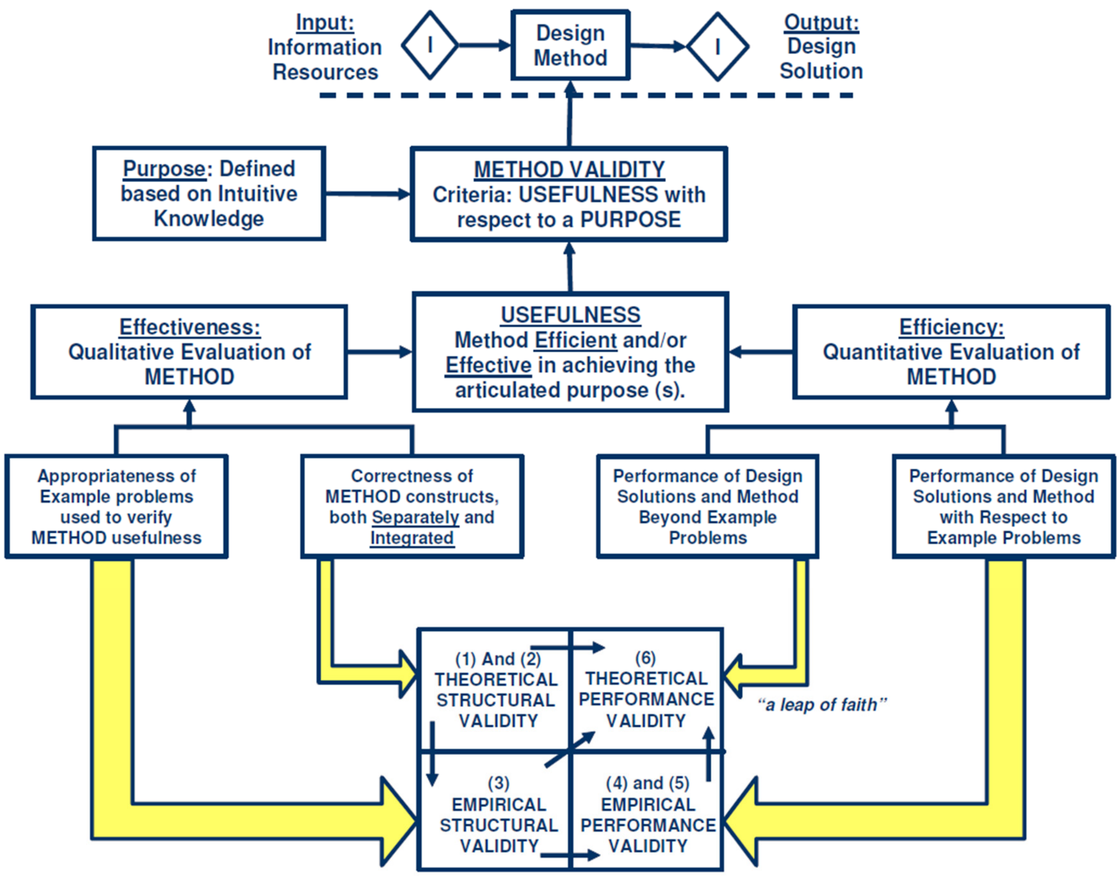


Figure 1.9: Validation square framework used to validate design method adapted from Seepersad and co-authors (Seepersad, Pedersen and coauthors 2006)

From modeling perspective, verification refers to "*internal consistency*" and validation refers to "*justification of knowledge claims*". Pedersen and co-authors propose a framework for validating design methods in which the usefulness of a design method is associated with whether the method provides design solutions correctly (structural validity) and whether it provides correct design solutions (performance validity) (Seepersad, Pedersen and coauthors 2006). The "validation square" consists of four quadrants: Theoretical structural validity, Empirical structural validity, Empirical performance validity and Theoretical performance validity. The corresponding verification involves checking for internal consistency.

Theoretical Structural Verification and Validation (TSV)**:** Accepting the individual constructs constituting a method as well as the internal consistency of the integration of all constructs to form an overall method. Thus, TSV consists of:

- Establishing requirements for the design method,
- Carrying out literature review,
- Establishing logical soundness of constructs used – individually and integrated

Empirical Structural Verification and Validation (ESV)**:** Building confidence in the appropriateness of the test example problems chosen for illustrating and verifying the performance of the design method. ESV consists of:

- Checking the appropriateness of the test example problems selected to test design method,
- Accepting the design methods and constructs.

Empirical Performance Verification and Validation (EPV)**:** Building confidence in the usefulness of the method using example problems. EPV consists of:

- Checking the ability of the method to provide useful results for selected example problems.

***Theoretical Performance Verification and Validation (EPV)*: ** Building confidence in the generality of the design method and accepting that the method is useful beyond the example problems considered. EPV consists of:

- Checking the ability to provide useful results beyond example problems,
- Showcasing the generic form of method.

How can the verification and validation framework used to verify and validate the chapters in this dissertation?

This question is answered and discussed in detail in Table 1.8 and summarized in Figure 1.10. In Figure 1.11, an overview of the verification and validation tasks to be carried out in this dissertation is shown.

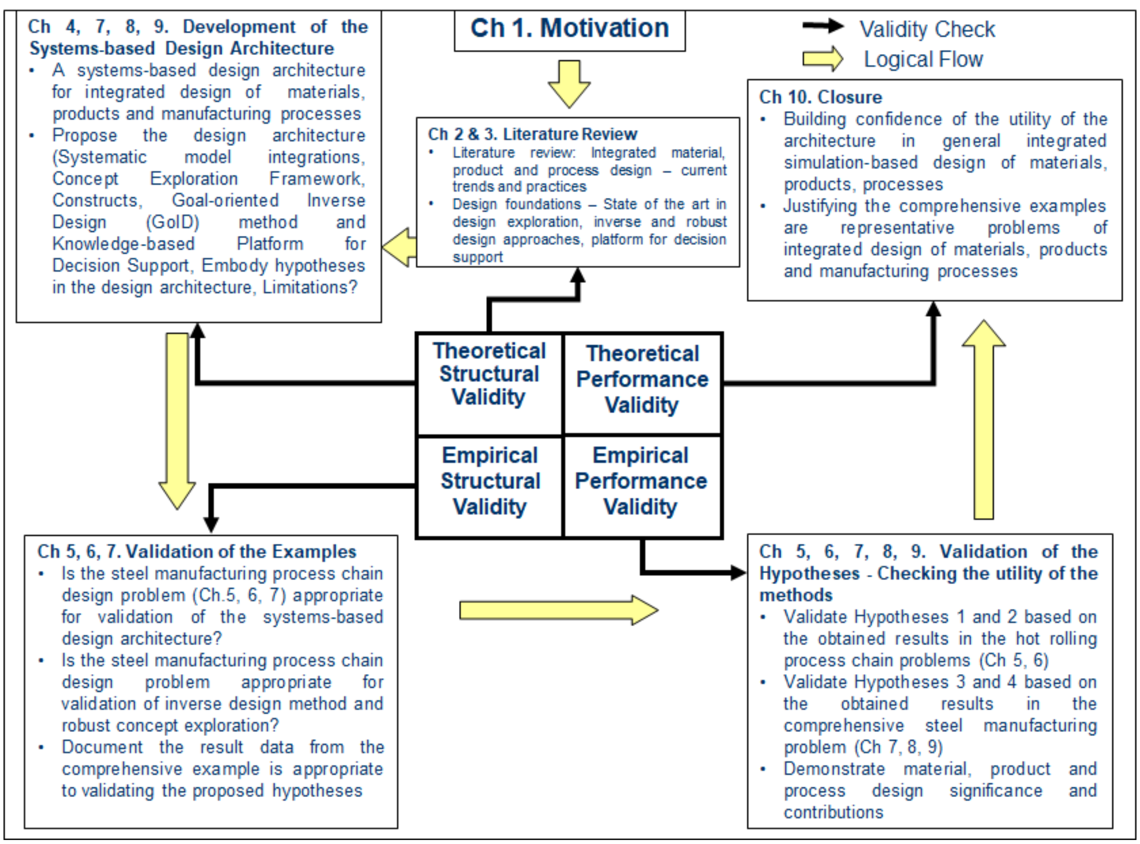


Figure 1.10: Organization of Dissertation Chapters according of Verification and Validation Square

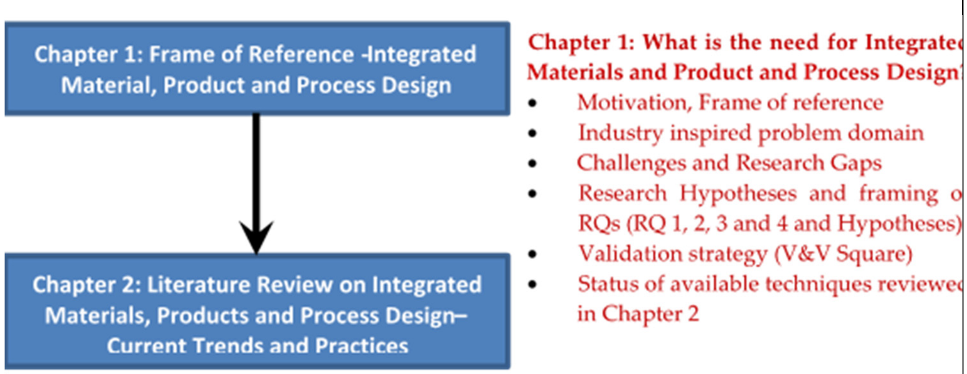
Table 1.8: Overview of Dissertation Chapters and Verification and Validation Strategy

Chapters	Overview of Dissertation Chapters and Verification and Validation Strategy
Chapter 1	***Overview***: In Chapter 1, a foundation is laid for achieving the goals addressed in this dissertation, where motivation, background and frame of reference in Sections 1.1, and 1.2, are presented which contains literature review and discussion on following topics: (1) Integrated design of materials, products and associated manufacturing processes, (2) Distinction between multiscale modeling and systems-based materials design, (3) Challenges and research gaps in systems-based integrated design of materials, products and processes. The industry inspired problem of focus in this dissertation, namely the integrated design of steel (material), manufacturing processes (rolling and cooling) and hot rolled rods (product) for automotive gears is introduced in Chapter 1. The principal goal in this dissertation is identified by carrying out a gap analysis and hypotheses are laid to address these gaps. Research questions worthy of investigation are framed and the expected new knowledge on answering the research questions are identified. An overview of the hypotheses, expected contributions and validation strategy are discussed in Sections 1.2 and 1.3 respectively. The organization of the dissertation and a road map for accomplishing the chapters planned are presented in Section 1.4.

This chapter is revisited for checking structural soundness of the dissertation where literature review, design approach, developed method, and validation of hypotheses are discussed in following chapters.

Theoretical Structural Validity of Research Questions 1, 2, 3 and 4 and Hypotheses in Chapter 1:

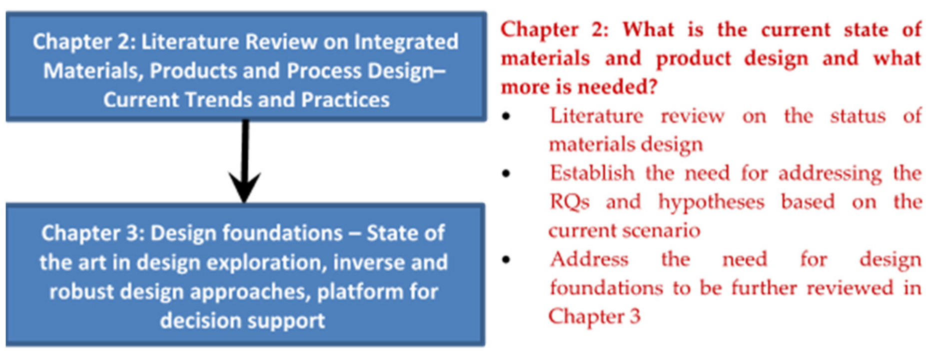
- Justifying the necessity for systematic integration of material, process and product models to establish processing-structure-property-performance relationship
- Justifying the necessity of systems-based design exploration and need for goal-oriented, inverse design methods
- Justifying the necessity of robust concept exploration across process chains for multiple conflicting goals
- Justifying the need for a knowledge-based platform for decision support for original, adaptive and variant designs and template-based ontological method for systematic design exploration.



<table>
<tr>
<td>Chapter 2</td>
<td>Overview: In Chapter 2, a review of the existing efforts associated with materials and product design is given. Several critical issues associated with the current capabilities of materials design is discussed in this chapter. Some of the major elements of modern materials design like material informatics, uncertainty management, verification and validation, multiscale modeling, systems design, etc. are discussed in this chapter.

Theoretical Structural Validity in Chapter 2

▪ Literature review on the status of materials design domain and identify research opportunities
▪ Justify that the four hypotheses are logically formulated to appropriately cover the research opportunities.
▪ Discussion about the advantages, limitations of current tools and establish the need for the research in this dissertation.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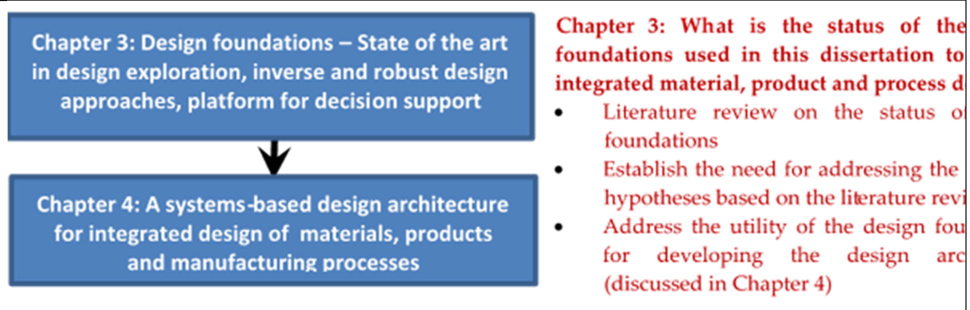
<tr>
<td>Chapter 3</td>
<td>Overview: In Chapter 3, the theoretical foundations for designing simulation-based design processes are discussed. These foundations include existing design constructs such as decision-based design, meta-design and Decision Support Problem Technique, robust design,</td>
</tr>
</table>

	compromise Decision Support Problem, robust concept exploration method, robust design metrics, indices for robust design – error margin indices, design capability indices, hyper-dimensional error margin index, inductive design exploration method. Also explored in this chapter is regarding design process modeling. Foundational constructs are reviewed from this area. This includes: template-based decision centric design, design concept flexibility, function-based systematic design, solution generation approaches. Relevant literature for each of these areas is referenced, discussed, and critically evaluated to show the appropriateness of use of these constructs for the design architecture developed in the dissertation. The literature review in Chapter 3 is used to identify availability, strengths, and limitations of these constructs in the context of integrated design of materials, products and design processes, and becomes an essential component of theoretical structural validation. **Theoretical Structural Validity in Chapter 3** ▪ Literature review on the status of design foundations used in this dissertation and identify research opportunities ▪ Justify that the four hypotheses are logically formulated to appropriately cover the research opportunities. ▪ Discussion about the advantages, limitations of current design tools, methods and approaches, establish the need for the research in this dissertation.

	
Chapter 4	***Overview:*** In Chapter 4, the components of the systems-based design architecture are presented: 1) a systematic function-based approach of integrating models (vertically and horizontally) to formulate forward material workflows establishing process-structure-property-performance relations, 2) a concept exploration framework for systematic design problem formulation and exploration along with a goal-oriented inverse design (GoID) method for designing materials for satisficing property and performance goals. The discussion in this chapter is focused on answering the first two research questions in this dissertation. **Theoretical Structural Validity in Chapter 4** Theoretical structural validation refers to accepting the validity of individual constructs used in the systematic approach and accepting the internal consistency of the way the constructs are put together. Theoretical structural validation is carried out in this chapter using a systematic procedure consisting of i) identifying the method's scope of application, ii) reviewing the relevant literature and identifying the strengths and limitations of the constructs in the literature, and iii) identifying the gaps in existing literature, and iv) determining which constructs are leveraged

	in the systematic approach while exploring the advantages, disadvantages, and accepted domain of application. The internal consistency of the individual constructs is checked by a critical review of the literature.
Chapter 5	***Overview***: In this chapter, Research Hypotheses 1 and 2 are tested using two test example problems: horizontal integration of multi-stage hot rolling process and product design. The horizontal integration is systematically achieved using well-established theoretical and empirical models and response surface models developed through simulation experiments (finite-element based). The illustration of the efficacy of the constructs proposed is carried out by the decision-based design of a multistage rolling system and the circular rod product. **Empirical Structural Validity of Chapter 5** Empirical structural validation involves accepting the appropriateness of the example problems used to verify the performance of the method. **Empirical Performance Validity of Chapter 5** Empirical performance validation consists of accepting the usefulness of the outcome with respect to the initial purpose and accepting that the achieved usefulness is related to applying the method.
Chapter 6	***Overview:*** In Chapter 6, the design architecture in terms of Research Questions 1 and 2 developed in the dissertation is applied to a multiscale, multistage materials design problem - vertical and horizontal integration and integrated design of hot rod rolling process chain, steel and rolled rod. In this chapter, the industry inspired problem of focus in this dissertation

	is addressed. The bigger picture of the problem of interest and how integrated materials; product and process design can be applied at industrial scale is discussed in beginning. A discussion on the specific problem (vertical and horizontal integration of hot rolling process chain) is carried out in detail. A literature review on hot rod rolling process is carried out. The problem– impact of segregation along the rolling to forging process chain is discussed in detail. This will be followed by creating a requirements list (both macro and micro level) for the integrated realization of the rod, steel and hot rolling process. The problem is to design the material microstructure and processing paths to satisfy conflicting product and process related end performances and properties in an inverse manner. The problem is modeled as an integrated design of materials, products, and manufacturing processes. In addition to the validation of design methods, the chapter is also crucial from the standpoint of the major theme addressed in this dissertation. In this chapter, we discuss the validation of the proposed systematic method of model integration, inverse design method and concept exploration framework. **Empirical Structural Validity of Chapter 6** Empirical structural validation involves accepting the appropriateness of the example problem used to verify the performance of the goal-oriented, inverse design method for integrated material, product and process design.

	In this context, it is to be validated that the examples fall within the scope of integrated product and materials design as well as decision-centric design-process design. **Empirical Performance Validity of Chapter 6** Empirical performance validation consists of accepting the usefulness of the outcome with respect to the initial purpose and accepting that the achieved usefulness is related to applying the method.
Chapter 7	***Overview:*** In this chapter, a variation to the existing goal-oriented inverse decision-based design method (Chapter 6) to bring in robustness for multiple conflicting goals from the stand-point of Type I to III robust design across process chains is introduced. The variation embodies the introduction of specific robust design goals and constraints anchored in the mathematical constructs of error margin indices and design capability indices to determine ''satisficing robust design'' specifications for given performance requirement ranges using the goal-oriented, inverse design method. The design of a hot rolling process chain for the production of a rod is used as an example to verify and validate the approach proposed. This chapter addressed Research Question 3 and validates the hypothesis proposed. **Theoretical Structural Validity in Chapter 7** Theoretical structural validation refers to accepting the validity of individual robust design constructs, goals and constraints used and accepting the internal consistency of the way the constructs are put

	together. Theoretical structural validation is carried out in this chapter using a systematic procedure consisting of i) identifying the method's scope of application, ii) reviewing the relevant literature and identifying the strengths and limitations of the constructs in the literature, and iii) identifying the gaps in existing literature, and iv) determining which constructs are leveraged in the systematic approach while exploring the advantages, disadvantages, and accepted domain of application. The internal consistency of the individual constructs is checked by a critical review of the literature. **Empirical Structural Validity of Chapter 7** Empirical structural validation involves accepting the appropriateness of the example problem used to verify the performance of the robust concept exploration across process chains for integrated material, product and process design. **Empirical Performance Validity of Chapter 7** Empirical performance validation consists of accepting the usefulness of the outcome with respect to the initial purpose and accepting that the achieved usefulness is related to applying the robust concept exploration constructs.
Chapters 8 and 9	**Theoretical Structural Validity in Chapter 8 and 9** Theoretical structural validation refers to accepting the validity of individual constructs in the platform PDSIDES and accepting the internal consistency of the way the constructs are put together. Theoretical

	structural validation is carried out in this chapter using a systematic procedure consisting of i) identifying the platform's scope of application, ii) reviewing the relevant literature and identifying the strengths and limitations of the constructs in the literature, and iii) identifying the gaps in existing literature, and iv) determining which constructs are leveraged in the systematic approach while exploring the advantages, disadvantages, and accepted domain of application. The internal consistency of the individual constructs is checked by a critical review of the literature. **Empirical Structural Validity of Chapter 8 and 9** Empirical structural validation involves accepting the appropriateness of the example problem used to verify the performance of the PDSIDES for original, adaptive and variant designs. **Empirical Performance Validity of Chapter 8 and 9** Empirical performance validation consists of accepting the usefulness of the outcome with respect to the initial purpose and accepting that the achieved usefulness is related to using PDSIDES for original, adaptive and variant designs. **Theoretical Performance Validity of Dissertation 8 and 9** Building confidence of the utility of the architecture in general integrated, simulation-based design of materials, products, processes.
Chapter 10	***Overview:*** In Chapter 10, the dissertation is summarized, and the intellectual contributions are critically reviewed. The advantages and limitations of the methods, metrics, and constructs are discussed. For

	theoretical performance validation, it is argued that these constructs are valid beyond the example problems selected for empirical validation. Finally, avenues for future research and broader applications of the fundamental ideas in this dissertation are discussed from the context of ***cloud-based design and manufacturing***. The focus in this chapter is in furthering the research vision by exploring the opportunities for ***automated realization of decision workflows for product design using the cloud***. ***I statement***: In this chapter, the author plans to determine if the objectives planned for the dissertation are addressed. The author plans to carry out a self-reflection of what have been achieved in past chapters and identify enabling technologies that requires advancement to further develop the vision of integrated design of materials, products and processes. In this chapter, the author plans to summarize some of the key concepts that form the basis of integrated design and materials research and the emerging interdisciplinary field of integrated computational materials engineering. Finally, the author's vision for research in systems-based design architecture is addressed from the context of a Cloud-Based Platform for Decision Support in the Design of Engineered Systems (CB-PDSIDES). **Theoretical Performance Validity in Chapter 10** By building confidence in the systems-based design architecture proposed in the dissertation for examples beyond that is discussed in this dissertation. This includes applications of the architecture proposed in

	robust product design (using a helmet design example) and by exploring the opportunities available via cloud-based design for automated realization of decision workflows for product design across the four axiomatic design domains. Through this, the author takes "*a leap of faith*" to build confidence in the general usefulness of the design architecture.

Theoretical Structural Validity (TSV) Validity of the constructs of the systems-based architecture • **Literature review** (Chapters 2, 3, 7, 8, 9) • **Gap analysis** (Chapters 1, 2, 3, 7, 8, 9) • **Checking internal consistency** • **Reasoning on applicability of constructs** (Chapters 2, 3, 4, 7, 8, 9)	**Theoretical Performance Validity (ESV)** Usefulness of the architecture beyond examples • **Generalizing Findings** (Chapters 9, 10) • **Arguing the validity of the systems-based design architecture developed beyond the example problems used in different domains** (Chapter 10)
Empirical Structural Validity (ESV) Appropriateness of the examples chosen to verify the architecture • **Horizontal Integration of Hot Rod Rolling Process Chain** (Chapter 5) • **Exploration of Microstructure Space for End Mechanical Properties of Rod** (Chapter 5) • **Vertical and Horizontal Integration of Hot Rod Rolling Process Chain** (Chapters 6, 7, 8, 9)	**Empirical Performance Validity (EPV)** Usefulness of the architecture in examples • **Systematic model integration** (Chapter 6) • **Inverse Design** (Chapters 5, 6) • **Robust Concept Exploration** (Chapter 7) • **Knowledge Capture, Reuse and Systematic Design Exploration** (Chapters 8, 9)

Figure 1.11: Overview of verification and validation tasks in this dissertation

The connections between research questions, dissertation chapters and the verification and validation square quadrants is shown in Table 1.9.

Table 1.9: Connections between research questions, chapters and validation square

Research Questions (RQ) / Chapters	1	2	3	4	5	6	7	8	9	10
RQ1: What are the foundations needed for systematically identifying and integrating material models with models of the rest of the system (product, manufacturing processes, and environment), so as to define the processing-structure-property-performance relationships and associated information workflow at early stages of design?	TSV	TSV	TSV	TSV	ESV, EPV	ESV, EPV				TPV
RQ2: What are the computational foundations needed for performing the systematic and rapid concept exploration of complex engineered systems involving the material, product and manufacturing processes satisfying certain end performance requirements, when simulation models are typically incomplete, inaccurate and not of equal fidelity?	TSV	TSV	TSV	TSV	ESV, EPV	ESV, EPV		EPV	EPV	TPV
RQ3: What are the requirements for an inverse, goal-oriented design approach for realizing the robust design exploration of the material, product and process as a system by managing the associated uncertainties?	TSV	TSV	TSV	TSV		ESV	ESV, EPV			TPV
RQ4: What are the foundations needed for maintaining structural consistency of the decision-based design workflow for the manufacturing process chain involving the material and product, ensuring robust, flexible and modifiable decisions while incorporating newer data, information and knowledge associated with the system?	TSV	TSV	TSV	TSV		ESV		EPV	EPV	TPV

1.4 Organization of Dissertation

An overview of this dissertation is presented as roadmap in Figure 1.12. The figure is intended to help navigate through the dissertation and develop an overall picture as to what is discussed in each chapter thereby establish context. The relationship of research efforts with the constructs of the design architecture developed is shown in Figure 1.13.

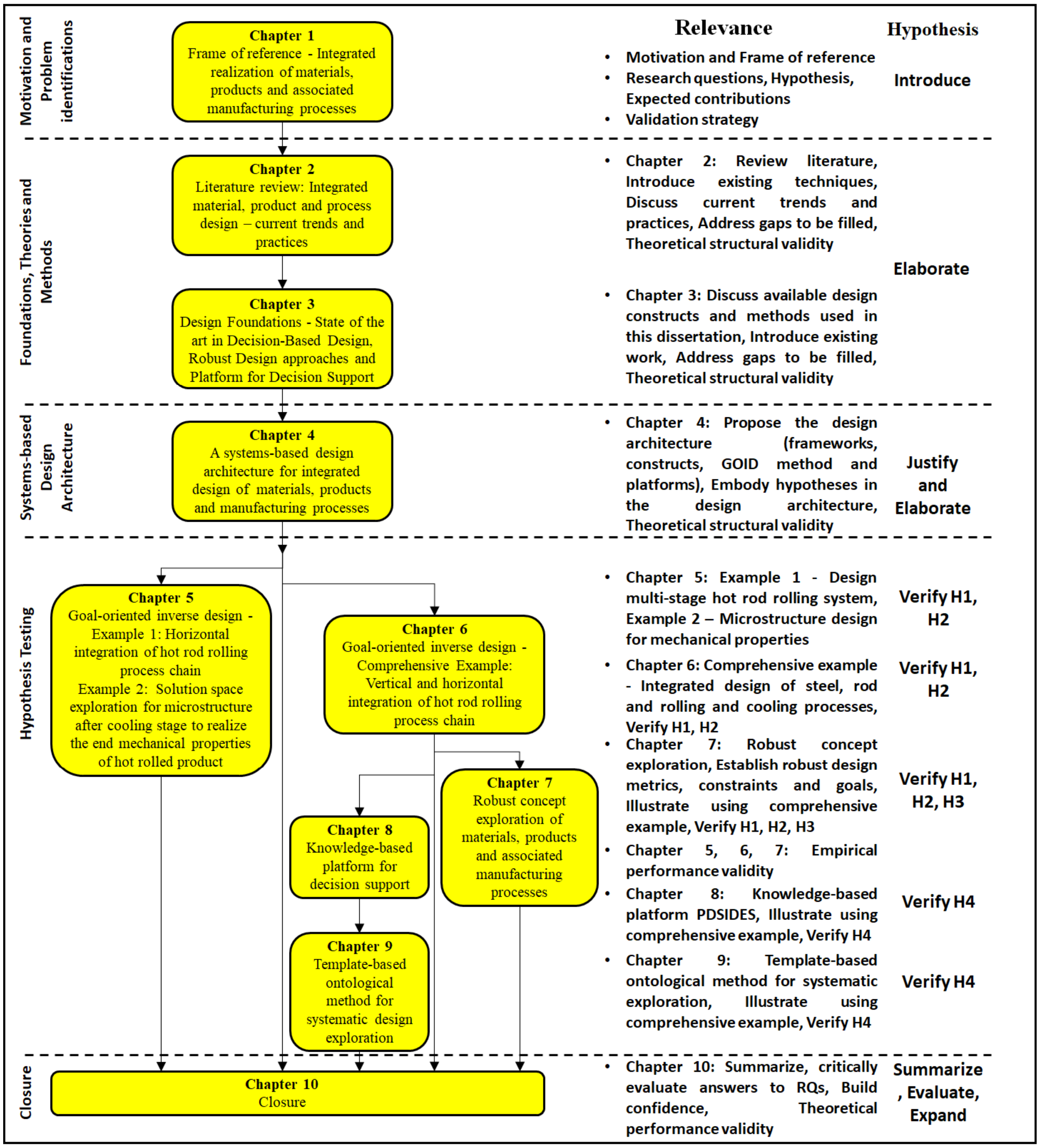


Figure 1.12: Dissertation Overview and Roadmap

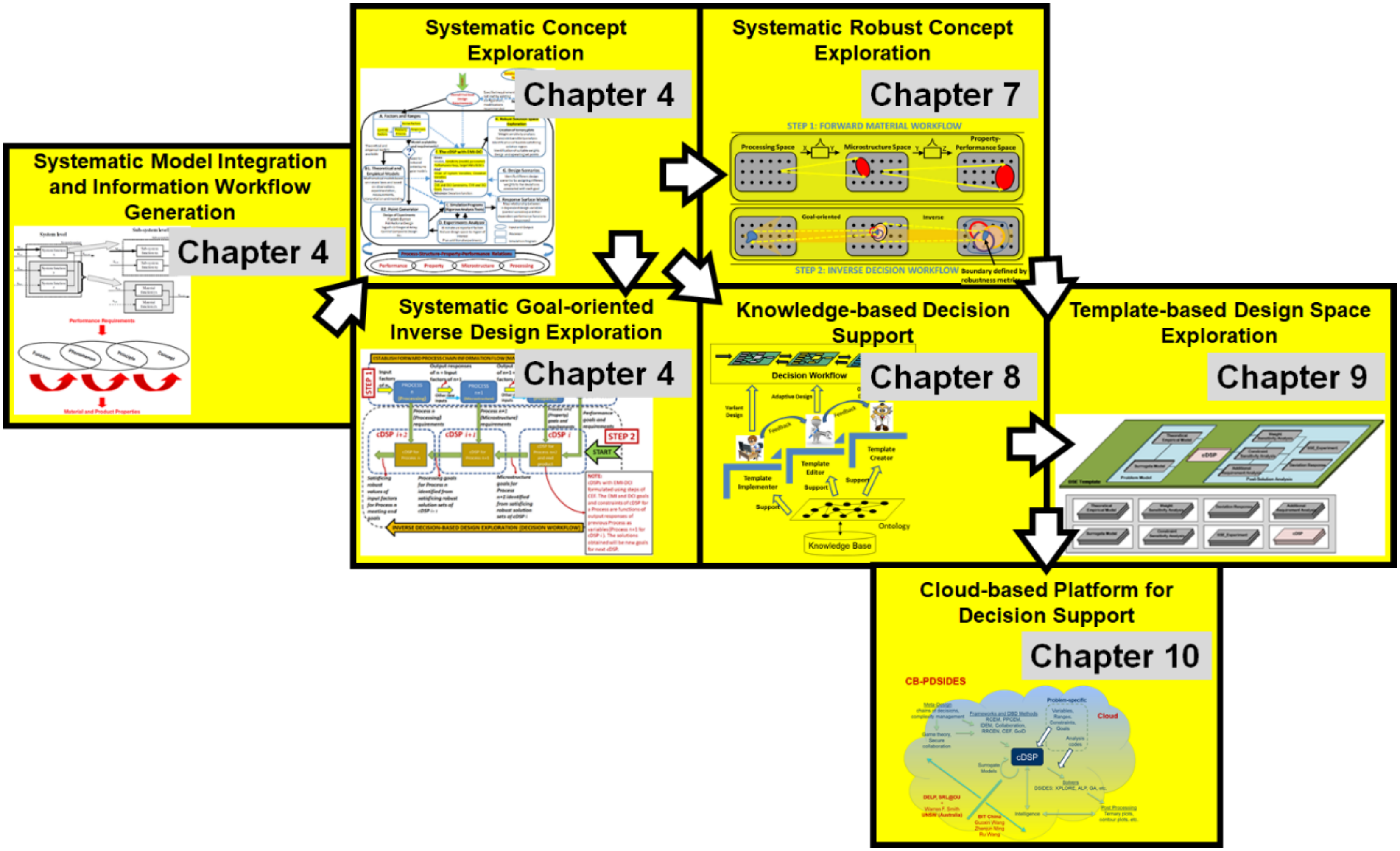


Figure 1.13: Relationship of research efforts with the constructs of the systems-based design architecture and connection between chapters of the dissertation

Chapter 2: Literature Review - Integrated Design of Materials, Products and Manufacturing Processes – Current Trends and Practices

The objective in this chapter is to review the current trends and practices in the integrated design of materials, products and manufacturing processes. In Section 2.1, the field of integrated materials and product design is discussed from the perspective of the emerging ICME domain. A detailed discussion on the current capabilities, the associated limitations and the research opportunities that are worthy of investigation from the standpoint of material models, simulations and databases; multiscale materials models and information linking; and materials design under uncertainty is carried out. In Section 2.2, the need for the research addressed in this dissertation is established. This is followed by a review of vertical and horizontal integration of models as defined by different authors and defining these terms for this dissertation in Section 1.3. In Section 1.4, verification and validation from the perspective materials design and model-based realization of multi-scale systems is discussed. In Section 1.5, remarks on the current status of materials design is presented based on the review carried out in this chapter.

2.1 The Emerging Field of Integrated Materials and Products Design

There has been a rapid fall in the time needed to develop a product due to the advancements in design and manufacturing procedures in the last two-three decades. The concept of *Integrated Computational Materials Engineering* (ICME) (Pollock, Allison and coauthors 2008, Horstemeyer 2012) is being widely discussed in the materials, manufacturing and design communities as a tool to reduce the lead time in development of a new product or component. The schematic structure of ICME is shown in Figure 2.1;

adopted from (National Research Council 2008). A major area of focus where ICME is intended to play a crucial role is the process scale-up of mill products. Even though there is a fall in the time required to develop a product, the time required to develop a new material however has remained relatively constant. This has necessitated the need to ask this question – *Have we fully realized the potential of ICME at an industrial scale?*

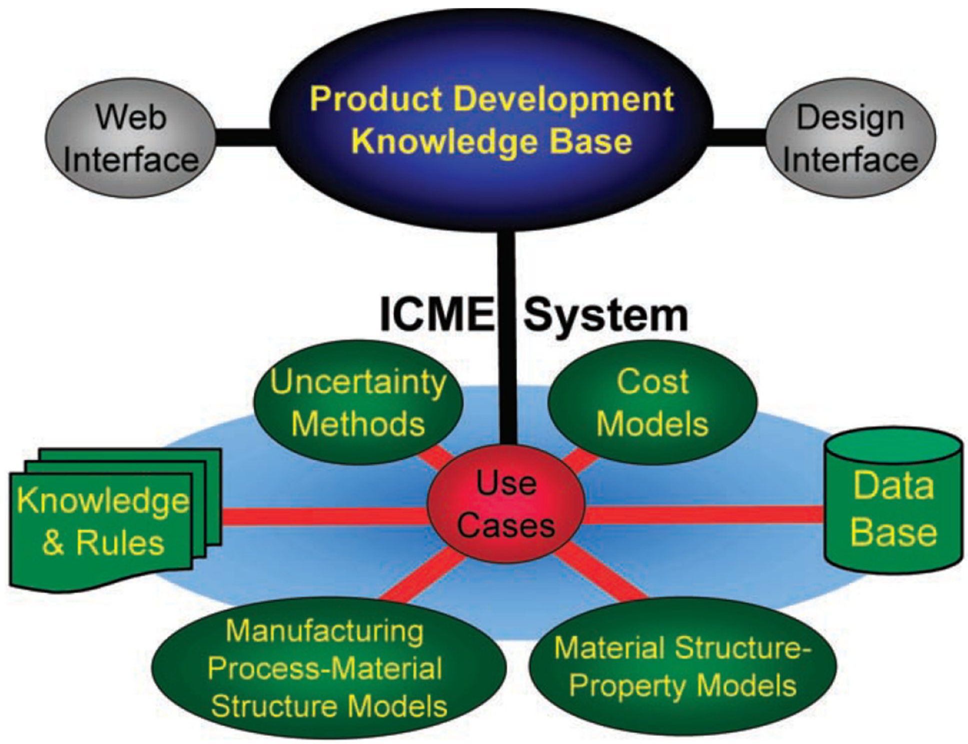


Figure 2.1: Schematic structure of an ICME system that unifies materials information into a holistic system that is linked by means of a software integration tool to a designer knowledge base containing tools and models from other engineering disciplines (National Research Council 2008)

The answer to this question can vary when asked to different communities as the definition and scope of ICME and the boundary that it holds itself has not been set properly as of now. However, there is a strong realization that to develop new materials for use in new products, there is a need to develop the ***capability of developing the product and material concurrently***. This requires us to address the challenges involved in realizing ICME fully at an industrial scale. If we look at any major manufacturing procedure for a product, we see that there is a host of unit operations involved and the end properties and performances of the product is influenced and linked by the processing steps at the final as well as intermediate stages. An example for this is the manufacture of a steel product mix (rod, bar, sheet) that involves a series of unit operations like continuous casting, reheating, rolling, annealing etc. In recent years there has been a tremendous increase in the computational power available along with physics-based models that are "good" enough to define the processing-structure-property and performance relationship of a material. Also, there has been advances in comprehensive robust, multidisciplinary, system exploration methods that facilitate the development of multi-scale materials that can achieve robust, multifunctional performances in varying product development environments. Enhancing these available models across multi-scales and integration at various length scales (vertical integration) ensures the flow of information from one unit operation to another thereby ensuring the integration of these individual processes (horizontal integration). Accordingly, the design of products and materials are not mutually exclusive and independent events but synergistic components of an integrated product, process and materials design endeavor, as noted by (McDowell, Panchal and coauthors 2009). This necessitates a philosophical and cultural shift towards **inductive (inverse), goal-oriented** synthesis of products, their constituent materials and their processing paths from a systems perspective. Several critical issues that need to be addressed to achieve this are identified in Chapter 1. In this Chapter, we discuss some of the current capabilities, the associated limitations and the research opportunities that are worthy of investigation in this dissertation:

- Models and simulations on different length and time scales for different set of functions that a material and product system must satisfy;
- Tools, techniques and systematic approaches for integrating and linking models and simulation tools across length and time scales, functional domains and material hierarchies;
- Systems design tools, constructs, methods and frameworks that support the integrated design of materials, products and manufacturing processes;
- Techniques, constructs and methods for characterizing and managing uncertainty in material and product variables, models, and their propagation across workflows.

2.1.1 Material Models, Simulations and Databases

Emphasis is placed in integrated materials and products design on developing and linking models, simulations and databases for processing-structure-property relations at multiple length scales to satisfy specific performance requirements of products. To meet application-specific performance requirements, the hierarchical scheme proposed by Olson is essential with top-down, goal-oriented approaches to carry out microstructure-mediated design of materials. An early vision for this was laid out at the 1998 National Science Foundation (NSF) workshop (McDowell and Story 1998). In 2008, the National Academy of Engineering (NAE) National Materials Advisory Study Group (National Research Council 2008) recognized ICME as a way to integrated, concurrent design of materials and products.

The essential building blocks of simulation-supported materials design are i) thermodynamics, ii) kinetics, and iii) kinematics (McDowell and Olson 2008). Thermodynamics provides information on stable and metastable phases, characterization of structures and energies of interfaces, and driving forces (transition states) for rearrangement of structure due to thermally activated processes; and therefore is considered as the fundamental building block of simulation-supported materials design (Olson 1997, McDowell, Choi and coauthors 2007, McDowell and Olson 2008). Preliminary design exploration of solutions to concurrent materials and products design problems is facilitated by it. First principles calculations support exploration of multicomponent systems for which empirical models are not yet established (Asta, Ozolins and coauthors 2001, Liu and Chen 2007). Data mining tools are also established and integrated with material modeling software to explore candidate solutions (Rajan 2005, Liu, Chen and coauthors 2006). Multiscale modeling methods are developed to model multiple levels of materials hierarchy (Cuitino and Ortiz 1993, Liu, Karpov and coauthors 2004, McDowell 2008, Horstemeyer 2012, Horstemeyer 2018). Current research efforts in each of these modeling areas are rather extensive and highly domain dependent.

Improving the fidelity and accuracy of models is the focus of material scientists in this domain. However, it is not practical to allocate time in improving all models and simulations. It is also difficult to prioritize which all models need to be selected for investing on improving fidelity and accuracy. In this regard, a very important player in the integrated model-based realization of materials and products is uncertainty – which is usually neglected and not given much attention.

2.1.2 Multiscale Models and Information Linking in Materials Design

For integrated materials and products design, it is essential to integrate and link models, databases and simulation tools across length and time scales, functional domains and material hierarchies. Materials design at multiple levels of hierarchy is a much broader activity than multiscale modeling (McDowell, Panchal and coauthors 2009).

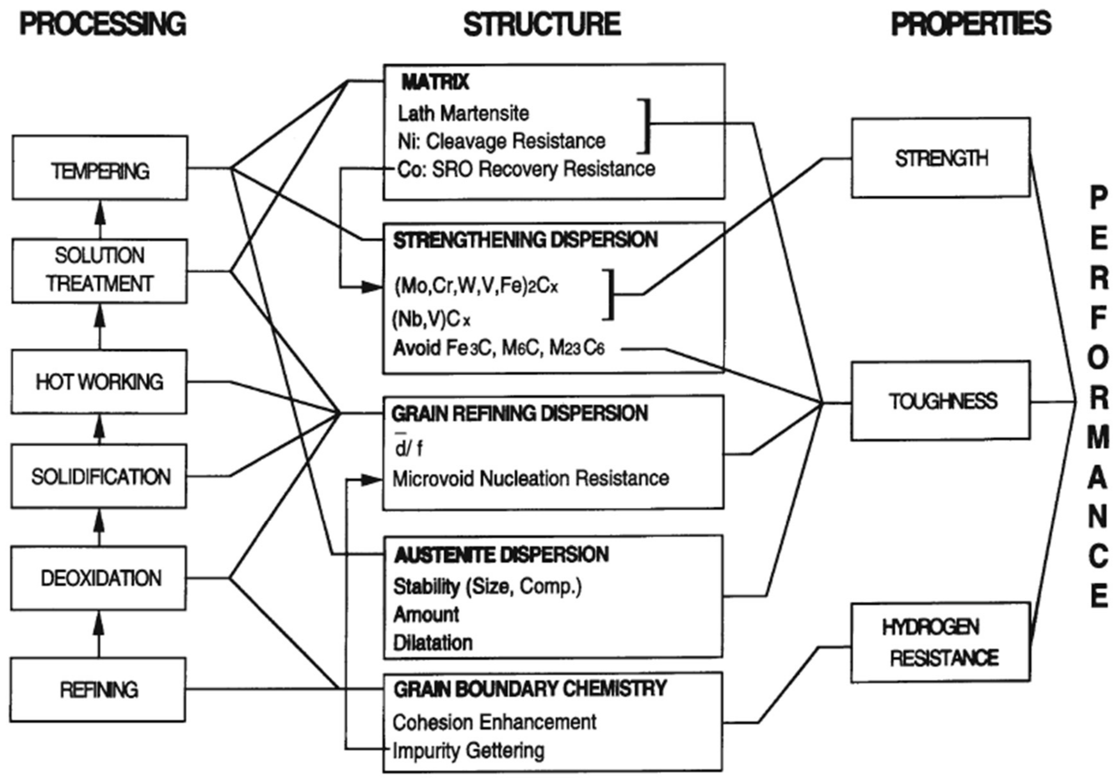


Figure 2.2: Process-structure-property-performance hierarchy for design of high strength steels for multiple objectives of strength, toughness and hydrogen resistance. From the SRG at Northwestern University (Olson 1997, Olson 2000)

Using Figure 2.2, Olson (Olson 2000) depicts the process-structure-property-performance hierarchy for design of high strength steels for multiple objectives. ***Now is this a representation of the hierarchy of length scales in materials design?*** McDowell (McDowell 2018) clarifies that the processing-structure-property-performance mapping shown in Figure 2.2 should not be confused with the hierarchy of length scales in materials design. The hierarchy of length scales is shown in Figure 2.3; adopted from (Horstemeyer 2012).

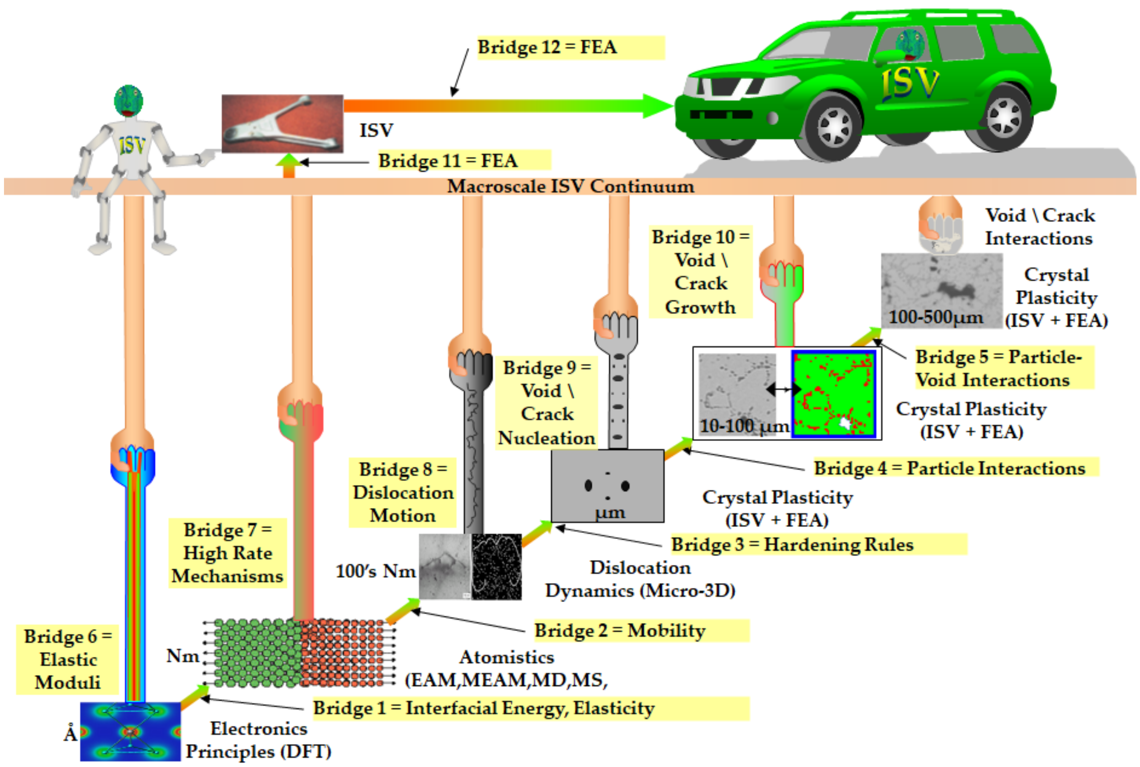


Figure 2.3: Multiscale modeling example of a metal alloy used for design in an automotive component. The hierarchical methodology illustrates the different length scale analyses used and various bridges needed. (ISV=internal state variable, FEA=finite element analysis, EAM=Embedded Atom Method, MEAM=Modified Embedded Atom Method, MD=Molecular Dynamics, MS=Molecular Statics, and DFT=Density Functional Theory) (Horstemeyer 2012)

To establish processing-structure-property-performance mapping at a scale or across two scales will probably require models or set of simulation experiments that span the entire hierarchy of length scales. The collection of all such models that serve the purpose of bridging information to higher-scale response is called as hierarchical multiscale models. Several research labs and government organizations have created their own computational frameworks focused on multiscale materials design. Some example of these include: The *Materials by Design*™ initiative by Olson (Olson 1997) for advanced steels using THERMOCALC software system to integrate models from quantum level to continuum level. The MatCASE (Material Computation and Simulation Environment) developed by Liu and co-authors (Liu, Chen and coauthors 2004, Liu, Chen and coauthors 2006) integrates software from atomic scale to continuum scale and evaluates finite element mechanical responses of designed microstructures. The MSU DMG ISV model developed by Horstemeyer and co-authors (Bammann, Chiesa and coauthors 1993, Horstemeyer, Lathrop and coauthors 2000) is another framework to capture the history effects of stresses, strains and microstructures to model the sequential processing of material during manufacturing processes. The model is based on the ISV plasticity formulation of Bammann (Bammann, Chiesa and coauthors 2010). The viscoplasticity model by Bammann and co-authors (Bammann 1990) coupled with the damage model by Horstemeyer (Horstemeyer 2012) has the capability to capture the non-linear response of material during processing. Horstemeyer (Horstemeyer 2012) presents the hierarchical multiscale modeling carried out to relate the history effects of a material through its processing to performance life cycle. The framework addresses the issue of handling bridging between scales by using thermodynamically constrained ISVs (Internal State Variables) that are physically based on microstructure-property relations. The ISV modeling framework takes a top-down approach as the ISVs exist at macroscale but reach down to various subscales to receive pertinent information. Using Figure 2.3, Horstemeyer depicts the hierarchical multiscale modeling methodology illustrating the different bridges and analyses required to capture the pertinent plasticity, damage, and failure aspects of metal alloys for use in design of automotive component.

The frameworks reviewed till now are aimed at "hard" computing by use of physics-based models that are linked at multiple scales. There is also increasing focus in "soft" computing aspects of materials design. Statistical or heuristic based relationships between materials design parameters for different applications is the major focus in soft computing research domain. The *Material Informatics* approach by Rajan and co-authors (Rajan 2005, Liu, Chen and coauthors 2006, Rajan 2013) have paved the way for objective (data-driven) formulation of surrogate PSP linkages. These linkages exhibit a remarkable combination of high accuracy and low computational cost through advances in material data sciences. The application of the same for the design of new alloys and catalysts are demonstrated. Definitely, increasing a materials designer's insight and perspective can happen through these soft computing techniques, but they still have to be paired with hard computing techniques for the true realization of new materials and products.

What are the difficulties associated with these hard and soft computing techniques for new material and product realization from a design perspective?

- They are customized for specific applications and are not transferrable;
- They are highly domain and platform dependent;
- They facilitate detail design of materials and products and is not suitable for early stages of design;
- There are issues of uncertainty that needs to be addressed;
- Developing such models/frameworks and integration of models consumes a lot of time and resources; and

- These techniques demand problem/platform-specific knowledge and skills which is not the focus/expertise of design engineers.

2.1.3 Materials Design under Uncertainty

Uncertainty can be classified as stochastic (aleatory) and epistemic in materials design. Improving the measurements and/or model formulation and/or increasing the accuracy are ways to diminish epistemic uncertainty. Aleatory uncertainty, however is inherent in the physical system and can only be quantified in a statistical sense. In order to realize the integrated model-based realization of materials, products and processes, it is very essential to characterize and manage both these types of uncertainty.

Engineering design communities have focused over the years on simulation-based design in the presence of uncertainty and a lot of research work is there to this credit. However, this body of knowledge have not found much applications in materials design under uncertainty due to certain significant challenges. The major reason here is because of the lack of expertise that exist for researchers in engineering design domains on materials design. In order to characterize and manage the uncertainty in materials design problems, there should be close collaboration and transfer of knowledge between material engineers/scientists and design engineers so that the nuances and sources of uncertainty related to designing materials can be clearly understood. Several challenges associated with materials design under uncertainty is highlighted by Allen and co-authors (Allen, Seepersad and coauthors 2006). Extending the classification by Isukapalli and coauthors (Isukapalli, Roy and coauthors 1998), the types of uncertainty in simulation-based integrated design of material, product and processes can be classified as (Choi, Austin and coauthors 2005, McDowell, Panchal and coauthors 2009): i) *Natural Uncertainty*, ii)

Model Parameter Uncertainty (MPU), iii) *Model Structure Uncertainty* (MSU) and iv) *Propagated Uncertainty* (PU). Techniques for addressing model uncertainty is addressed by Du and Chen in (Du and Chen 2000, Du and Chen 2002). Metrics known as Design Capability Indices (DCIs) for managing parameter uncertainty was developed by Chen and co-authors (Chen, Simpson and coauthors 1999). The metrics were later expanded to manage model uncertainty and its propagation by Choi and co-authors (Choi, Austin and coauthors 2005, Choi, Mcdowell and coauthors 2008); named as Error Margin Indices (EMIs). Gu and co-authors (Gu, Renaud and coauthors 2000, Gu, Renaud and coauthors 2006) studied the propagation of uncertainty through a series of models spanning across scales and/or disciplines. Studies on collaborative decision making under uncertainty by coupling robust design methods and game theory protocols were carried out Chen and Lewis (Chen and Lewis 1999). This was later extended by Xiao (Xiao 2003) by using Design Capability Indices and game theory protocols to facilitate flexible, robust and interactive decision making among multiple, distributed engineers. Kalsi and co-authors (Kalsi, Hacker and coauthors 2001) carry out collaborative, multidisciplinary systems design by treating shared variables as noise factors in their study. Chang and Ward (Chang, Ward and coauthors 1994, Chang and Ward 1995) in their work support designers to carry out robust collaborative decisions by considering the coupled parameters as noise and using robust design types I and II to manage the effects of coupling.

Even though there are research focused on addressing the issue of uncertainty, there are several challenges associated with the successful application of this knowledge in simulation-based design of materials under uncertainty. One major challenge is the propagation of uncertainty as information is shared from one model to another. This is amplified by the fact that the models in materials design are already sensitive due to the underlying physics-based assumptions, the lack of proper input data and the approximations made during model development because of computational cost and time. Materials design due to all these reasons should be viewed as a human decision making and collaborative activity with the assistance of computers. There are some recent efforts in this direction as briefly discussed in Chapter 1. Modern data science methods for materials and microstructure informatics along with multiscale modeling techniques are being developed to provide decision support and address the issue of uncertainty in hierarchical materials design (Panchal, Kalidindi and coauthors 2013, Kalidindi 2015, McDowell and Kalidindi 2016, McDowell and LeSar 2016). Panchal and co-authors (Panchal, Kalidindi and coauthors 2013) address some of the key computational modeling issues in Integrated Computational Materials Engineering and address the research efforts in mitigating and managing uncertainty. One important message delivered in their work is that ***materials design in its current form with the advent of ICME is not just an assemblage of tools as such tools do not have natural interfaces to material structure nor are they framed in a way that quantifies sources of uncertainty and manages uncertainty in representing physical phenomena to support decision-based design*** (Panchal, Kalidindi and coauthors 2013). Seepersad and coauthors (Shahan and Seepersad 2012, Matthews, Klatt and coauthors 2016) considers Bayesian network classifiers to design materials with hierarchy and to treat uncertainty propagation in multilevel material design. The approach incorporates Bayesian network classifiers (BNC) for mapping design spaces at each level and flexibility metrics for intelligently narrowing the design space as the design process progresses. The approach supports top-down design exploration of material hierarchy under uncertainty to make design decisions. Mahadevan and coauthors (Li and Mahadevan 2016, Mullins and Mahadevan 2016) address the issue of uncertainty integration across multilevel and the role of calibration, validation and relevance in multilevel uncertainty integration for hierarchical material design problems. Even though there are several such recent efforts to address the issue of uncertainty, McDowell (McDowell 2018) observes that quantifying uncertainty in schemes for linking models at different length and time scale is still an immature field and formal mathematical approaches for doing this are largely undeveloped. The recommendation therefore made for simulation-assisted materials design is to focus on understanding the sensitivity of material properties to material microstructure and to capture dominant mechanisms and transitions that affect material responses or properties instead of focusing on accurately predict mean properties at higher scales. Even though techniques are available for sensitivity analysis and uncertainty quantification, there still need to be research efforts to address materials design problems and infuse these knowledge into computational mechanics and materials science domains. In this dissertation, fundamentals of robust design and uncertainty management are discussed in Chapters 3 and 7 with robust concept exploration techniques for materials application in Chapter 7.

2.2 The Need for the Research addressed in this Dissertation

Materials design is viewed as fundamentally ***a goal-oriented*** synthesis activity, where requirements or goals for a product (or material or component or part or assembly or system) in terms of performance or properties are translated into suitable material microstructures and corresponding processing paths. A systems perspective is therefore needed for linking the information associated with multiscale and multilevel models, tools, and databases that are developed. It is equally important to develop design methods that allow systematic and strategic coordination of information and human decision making for the design of material structure, processing paths, and parent products. Design methods thus developed should support:

- Co-ordination of information and human decision-making across material and product hierarchies/levels;
- Bridging the gap between materials design and product (system) design;
- Goal-oriented design exploration, where the designer starts with the end goals that needs to be achieved for product performance;
- Systematic solution space exploration and design trade-offs from a large set of possible solutions and visualization of solution regions of interest;
- Management of uncertainty associated with materials and products;
- Management of complexity via reduced order material, process and product models and simulations;
- Propagation of robust solution regions of interest across material process chain;
- Support decision making and distributed solution space exploration for distributed decision makers;
- Support the inverse design exploration thereby achieving the integrated microstructure-mediated design of materials and products; and
- Domain-independent design of any complex material-product system.

As discussed in previous sections, a lot of researchers over the years have looked at materials design from different perspectives. Most of these are focused on detailed design of material behavior and not on early stage design exploration. There are only very few who have addressed the need for developing domain-independent design methods, tools and frameworks that support systematic and comprehensive early stage design of broad classes of materials and products, as noted by (McDowell, Panchal and coauthors 2009). A systems approach for materials design by taking into account the processing-structure-property-performance relationship was advocated by Olson in his seminal work on Materials-by-Design (Olson 1997, Olson 2000). This was later reiterated by many others in their work and forms one of the underlying philosophies for the emerging ICME domain. However, strategies to explore the design space and coordinate distributed human decision-making remains an open question in Olson's work. Olson's lead was followed by Subbarayan and Raj (Subbarayan and Raj 1999) to design system and subsystems sharing variables as links between the levels of hierarchy. The design of a tungsten filament is used an example to illustrate the approach. To formalize the relationships between the subsystems in the tungsten filament example, Lu and Deng (Lu and Deng 2004) use variable dependency graphs and thereby adding to the systems-based approach. Gall and Horstemeyer (Gall and Horstemeyer 2000) picks up Olson's systems philosophy and illustrate the design of cast component using multiscale modeling approach by establishing relationships at the component level and the microstructural level.

Adams and coauthors (Adams, Kalidindi and coauthors 2013) present a framework that utilizes highly efficient spectral representations to arrive at invertible linkages between material structure, its properties, and the processing paths used to alter the material structure. The authors address how the material microstructure can be tailored to meet stringent properties and performance requirements of complex components and systems. Materials Knowledge Systems approach by Kalidindi and coauthors (Kalidindi, Niezgoda and coauthors 2010, Kalidindi, Niezgoda and coauthors 2011) showcase advances in rapid inverse design to estimate local responses. However, these approaches are focused on problems where the structure-property relations can be inverted in some manner. For problems involving non-linear relationships and path dependencies across length and time scales and nonequilibrium microstructural evolution, the application of these ideas remains an open question. Other efforts in systems-based microstructure-mediated design includes the design of aluminum alloy microstructures for targeted properties using genetic algorithms, by Kulkarni and co-authors (Kulkarni, Krishnamurthy and coauthors 2004), topology and microstructure design of materials and products for specified properties, by (Sigmund 1994, Sigmund 1995, Sigmund and Torquato 1997, Hyun and Torquato 2002). Although, these systems-based approaches are the focus in materials design communities, they are still in the infancy stage. Thus,

Systematic methods for materials design are needed that support a human designer in exploiting the power of computational materials and product models to carry out simulation-supported, integrated, decision-based, inverse design exploration of material microstructures and processing paths to satisfy specific product and process level properties and performance requirements.

Systems-based design architecture (complete with frameworks, mathematical constructs, design methods and computational tools) is presented in Chapter 4 of this dissertation addressing this requirement.

2.3 Vertical and Horizontal Integrations and Information Flow in Materials Design

The development in computational tools have led to systems-based design methods that are simulation based so as to realize complex products with less lesser development cycle times and improved quality. The simulation models available with the revolution in computational techniques are "good" enough to predict the behavior of systems at multiple scales and the requirement at this stage is to systematically use these simulation models to design the behavior of the overall system by integrating the information that are obtained from each of these individual simulation models. Complex systems are mostly characterized by the hierarchical coupling between systems, subsystems and components. The hierarchical systems design is meant to simulate the performance of the system over multiple levels of hierarchically partitioned system so as to reduce the time needed to achieve that system level performance. The hierarchical system is differentiated from multiscale system in this study. By multiscale system we mean the systems simulated at multiple length and time scales, see Figure 2.4. In Figure 2.4, we see that the end performance of the automobile depends on the functionality of its individual components like the gear box assembly and the gear parts in it. The functionality of these parts in turn depends on the corresponding material properties. These material properties depend on the behavior of material at different scales ranging from quantum scale to the microstructure of the material. The interactions at the quantum scale affects the microstructure of the material which in turn affects the continuum behavior thereby affecting the mechanical properties of the material and the product. The variation of time scale may be in the order of few femtoseconds in the quantum scale and can go up to months or years at the system level. The need for simulation models at each of these levels is very essential due to this mapping and since these scales are linked, there needs to be a coupling between the models. The coupling of these models to allow information flow has been categorized as “Vertical Integration” and “Horizontal Integration”.

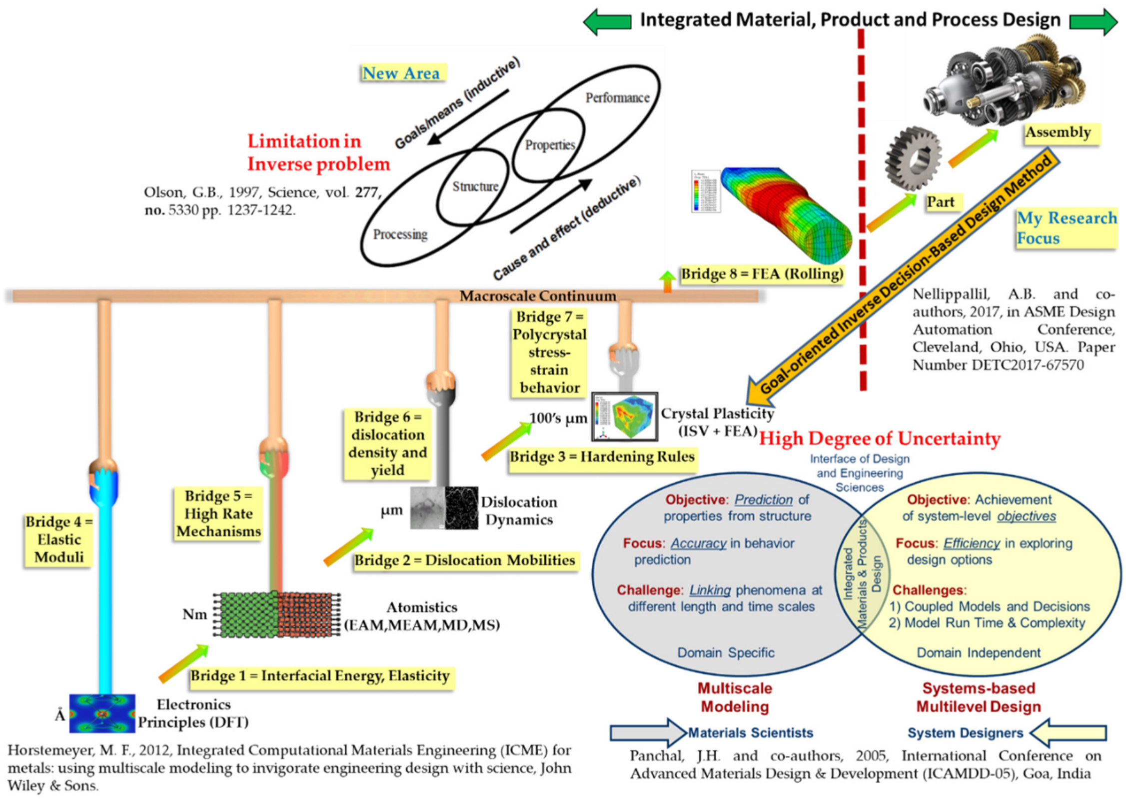


Figure 2.4: A multi-scale automobile system depiction with information flow across scales

Different researchers have defined these two types of integrations in different ways by looking at different perspective. In this Section, we review the definitions by Panchal (Panchal 2005), Shukla and co-authors (Shukla, Kulkarni and coauthors 2015), and Horstemeyer and Wang (Horstemeyer and Wang 2003).

Panchal in his Ph.D. dissertation (Panchal 2005) describe the coupling in hierarchical system as primarily between physical components and the multiscale coupling as that which exists within physical phenomena at different scales for the same component. In hierarchical systems coupling exits between systems, subsystems and components in the same scale known as horizontal coupling, while in multiscale systems an additional element of coupling exists over the length and time scale to designing the individual components known as vertical coupling, Figure 2.5 (Panchal 2005). Hence the requirement here is to establish vertical coupling along with horizontal coupling in multiscale systems to effectively establish the integrated information flow from the physical phenomena at different scales in order to make decisions.

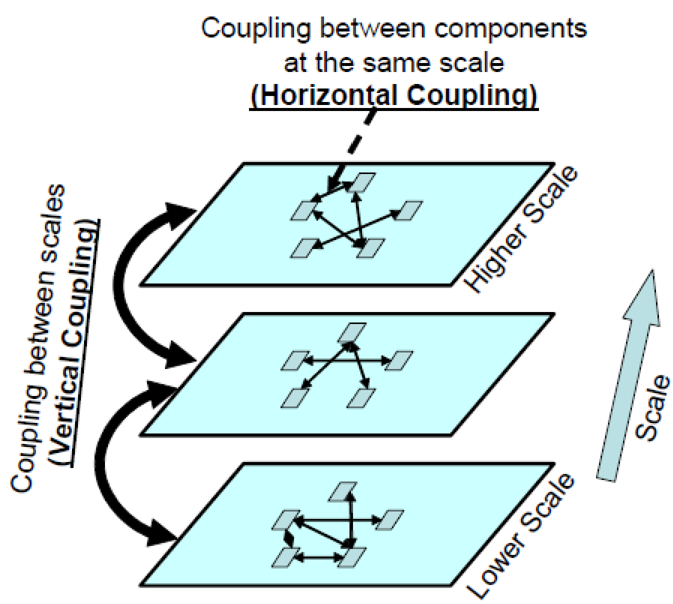


Figure 2.5: Horizontal and vertical couplings in multiscale systems (Panchal 2005)

An example for this can be visualized from the hot rolling problem perspective. The main aim in hot rolling is to breakdown the columnar grain structure to equiaxed grains by rolling the hot semi-product (slab, billet or bloom) through a set of rollers. The formation of new grains depends on the rolling load applied, the percentage reduction that is targeted, the rolling speed, etc. at the macro level. At the micro level, recrystallization phenomena (dynamic, metadynamic, and static) will take place resulting in new grain formation. A finite element model at the macro level can give significant information regarding all this. The finite element model thus needs to integrate all the rolling information at the macro level to simulate the process accurately. The analysis results from the finite element model, say the rolling load, the temperature profile along the workpiece or the strain developed, etc. is used by a microstructural evolution model at micro level to predict the recrystallization and the evolution of grain size. This requires integration at the micro level between recrystallization models for dynamic, static recrystallizations and the grain growth model. There needs to be a constant back and forth information flow between models at these two scales while carrying out the simulation. Thus, vertical integration at the two different scales and horizontal integration within models at the same scale helps in simulating the process effectively. Some of the challenges associated with multiscale modeling are (leveraged from Panchal's dissertation (Panchal 2005) and Sinha's thesis (Sinha 2011)):

- balancing the prediction accuracy with computational cost;
- modelling physical phenomena and interaction between scales;
- achieving collaborated decision making, achieving collaborative computational infrastructure;
- managing uncertainty and its propagation; and
- framing and solving the inverse problem (Sinha 2011).

Shukla and co-authors (Shukla, Kulkarni and coauthors 2015) have defined vertical and horizontal integration based on their study of the steel making process chain. The manufacture of a steel product mix (rod, bar, sheet) involves a series of unit operations like continuous casting, reheating, rolling, annealing etc. The flow of information from one unit operation to another is very essential to carry out an integrated study of each of these unit operations (Shukla, Kulkarni and coauthors 2015, Tennyson, Shukla and coauthors 2015). This has been termed as horizontal integration – the integration of different unit operations. To carry out horizontal integration there needs to information in a far greater detail from each of these unit operation. Thus there should be modeling of the important phenomenon that occur during a particular unit operation which are at different length scales with a very deep insight (Tennyson, Shukla and coauthors 2015). This has been termed as vertical integration, see Figure 2.6. Thus, vertical integration of a unit operation helps in adding information to the unit operation by integrating the different phenomenon and also results in information that can be passed to other unit operations thus helping in achieving horizontal integration. An example for this type of integration is illustrated in Figure 2.6 (Tennyson, Shukla and coauthors 2015). Inclusions are generally non-metallic compounds that are formed during the refining and pouring stages in the upstream process (ladle-tundish) stage of steel making. They are usually formed due to chemical reactions or due to presence of impurities in the melt. The total oxygen content present is a measure of the inclusions present. Simple chemistry model is used to control the ladle refining and predict the operating set points for the ladle that meets the required oxygen content. However, during an integrated study, the size, shape and morphology of the inclusions needs to be known and are to be modeled and this information has to pass to the subsequent stages like rolling where it is important to know the size and morphology of the inclusions, if present.

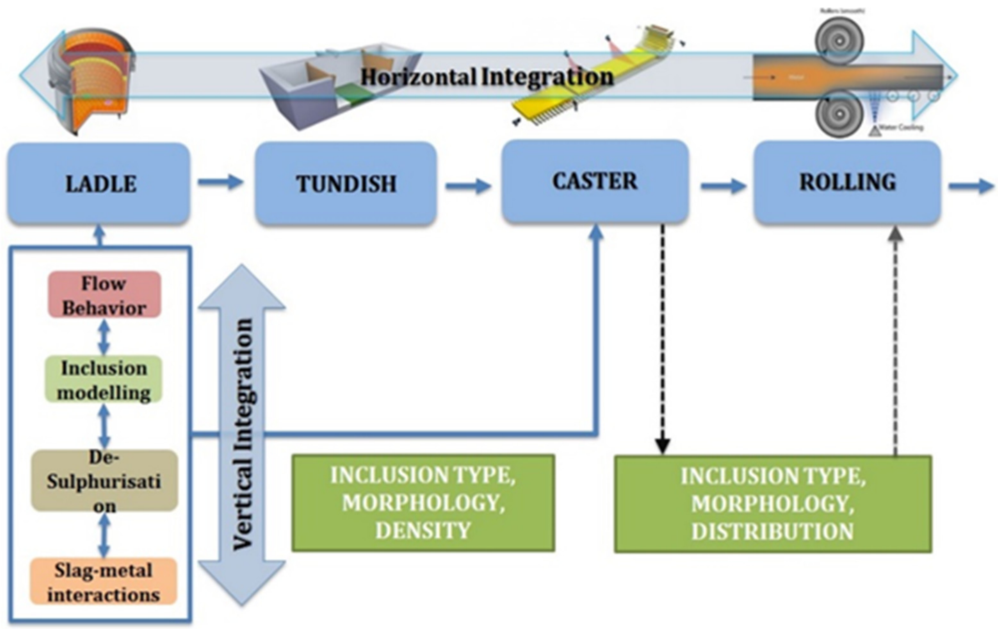


Figure 2.6: Vertical and horizontal integration as defined by Shukla and co-authors (Shukla, Kulkarni and coauthors 2015, Tennyson, Shukla and coauthors 2015)

Similarly, desulphurization is another important phenomenon during ladle refining. Argon purging at a high rate is essential for sulphur removal. However, argon purging at high rate results in inclusions through oxygen pick up. Hence it is essential to model the desulphurization phenomena and integrating it with inclusion model before information flow to rolling operation. Thus, a detailed vertical integration of unit operation is essential for information flow to subsequent operations and also to understand and model the corresponding unit operation in the best way.

Horstemeyer and Wang (Horstemeyer and Wang 2003) defines ICME as the bridging of information from two or more experimentally validated models or simulation codes in which structure-property information passes from one code to another. They describe "Horizontal ICME" as the integration in which simulation codes connect the sequential material processes with their structure which is at multiscale to their mechanical properties that is used in the performance life cycle evaluation (Horstemeyer and Wang 2003). The “Vertical ICME” is described as the integration in which simulation codes connect the multiple length scales, see Figure 2.7. The integration of both “Horizontal ICME” and “Vertical ICME” is described as the “Hybrid ICME”.

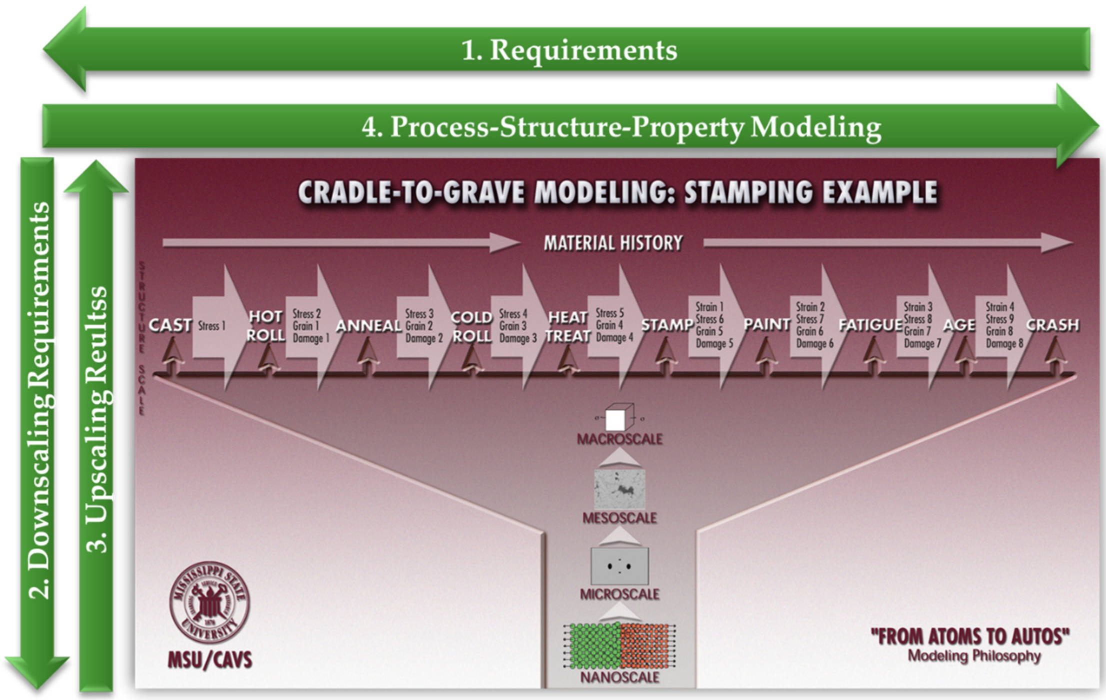


Figure 2.7: Vertical and horizontal integration as depicted by Horstemeyer (Horstemeyer 2012)

On analyzing the three definitions of vertical and horizontal integration, we understand that the vertical integration has been defined as the integration of models at multiple length and time scales by all the three authors. There is a slight variation in the definition of horizontal integration by these authors. In this dissertation, we accept the definition of vertical and horizontal integration by (Tennyson, Shukla and coauthors 2015) as it more closely relates to the problem at hand and the modeling approach followed in this dissertation - where we focus on the flow of information across models and systematically establishing linkages via workflows and provide design decision support. The focus in this dissertation in not on multi-scale modeling. Thus, to carry out design space exploration across the material processing-structure-property-performance spaces there should be flow of information via simulation models integrated across multiple scales and across multiple manufacturing processes – defined as the vertical and horizontal integration of models. We define *vertical integration* as the integration of models and simulations of different phenomenon that occur at multiple length scales for a specific manufacturing process so as to generate information that can be passed to other manufacturing processes that follow. We define *horizontal integration* as the integration of different such manufacturing processes using simulation models ensuring proper flow of the information generated through vertical integration at each manufacturing process thereby establishing the processing-structure-property-performance route to realize an end product. This will be addressed in detail in Chapter 6 of this dissertation using the hot rolling process chain problem.

2.4 Verification and Validation in Materials Design

Verification and validation were addressed from the perspective of dissertation chapters in Chapter 1. In the context of integrated materials, products and process design, verification and validation (V&V) consists of the following activities (Panchal, Kalidindi and coauthors 2013):

1. Individual Model V&V – a single model focusing on single length and/or time scales.

2. Multiscale Model V&V – single model or coupled set of models spanning multiple length and/or time scales in an integrated manner.
3. Multi-physics Model V&V – ensuring the mathematical and physical consistency of modeling framework spanning multiple phenomena.
4. Design Process V&V – ensuring that the design process in its configured form will yield a solution that satisfies design requirements.
5. Design (outcome) V&V – comparing design outcomes to system-level requirements.

2.4.1 Individual Model Verification and Validation

Model verification and validation has received significant attention in the past years due to advent in simulation-based design technologies. The following tasks are associated with model verification and validation (Sargent 2009, Panchal, Kalidindi and coauthors 2013); the process of V&V is illustrated in Figure 2.8:

- *Conceptual model verification and validation*: process of validating whether the theories and assumptions underlying a model and its sub-models are correct and that the representation of the system including models and sub-models are correct and reasonable for the intended study.
- *Model verification*: Process of assuring that the computer model is "good enough" in terms of accuracy of representation of a conceptual model.
- *Operational validation*: Process of determining whether the computerized model is sufficiently accurate for the needs of the simulation study.
- *Data validation*: Checking the accuracy and consistency of the numerical data used to support the models in the simulation study.

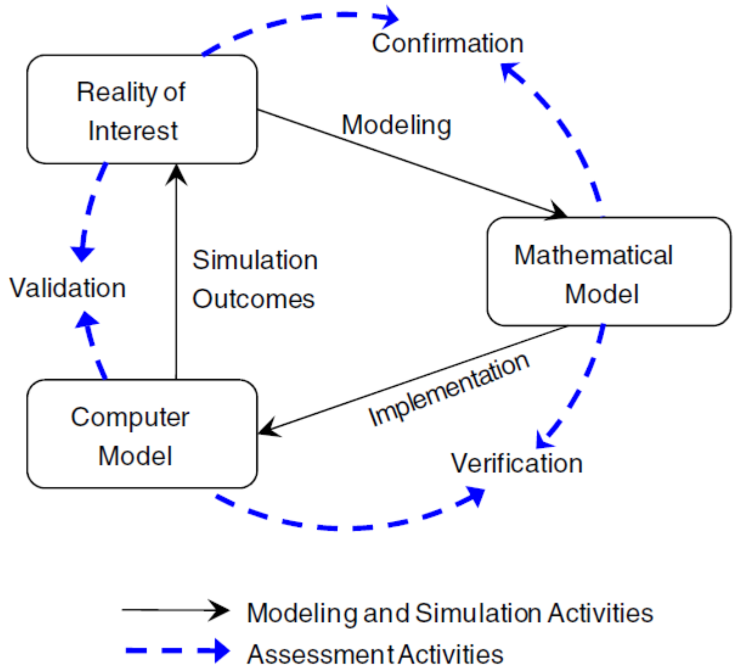


Figure 2.8: Model Verification and Validation Process (Sargent 2009, Panchal, Kalidindi and coauthors 2013)

2.4.2 Multiscale Model Verification and Validation

Multiscale model V&V is very important because valid individual models for specific length and time scales won't necessarily result in valid multiscale models across scales. The following tasks are involved with multiscale model V&V:

- *Compatibility validity*: Compatibility validity is the process of determining whether the input ranges of an upper-level model is consistent with the domain of outputs of a lower-level model. This ensures whether the output domain of the lower level model is a subset of the valid input domain of the upper-level model.
- *Uncertainty propagation check*: The goal here is to check that the effects of uncertainty at lower length scales do not amplify beyond the desired uncertainty bounds or limits set for which the design decisions are to be made. This can be

viewed both from bottom-up and top-down perspectives. From a top-down perspective the uncertainty limits allowable for a system is used to determine the allowable uncertainty limits for lower scales and thereby manage the propagation across a chain of models.

2.4.3 Design Process Verification and Validation

The goal in design process V&V is to ensure that the design process will yield design solutions worthy of investigation satisfying the design requirements. In the simulation-based design of complex systems, design processes represent the manner in which design decision networks and simulation models are configured to achieve the design task. One approach to verify and validate a design process is with the help of the verification and validation square framework introduced in Chapter 1 of the dissertation. The V&V square consists of four quadrants, as shown in Figure 2.9:

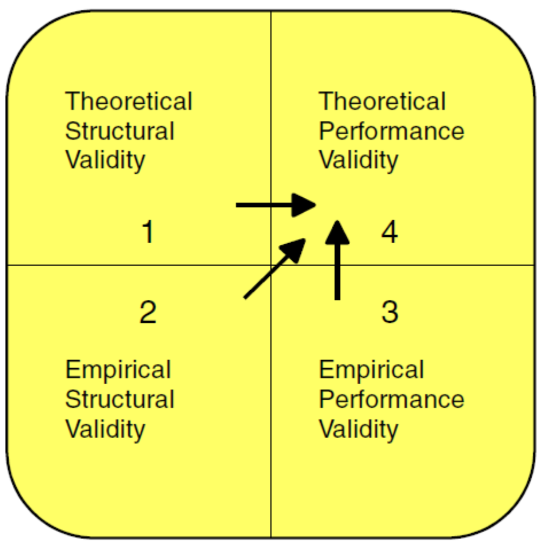


Figure 2.9: The verification and validation square framework (Pedersen, Emblemsvag and coauthors 2000, Seepersad, Pedersen and coauthors 2006)

1. *Theoretical Structural Validity*: *Is the design method internally consistent?*

   Internal consistency of the design method is checked – this includes, checking the logical soundness of the constructs used in the design method both individually and integrated.

2. *Empirical Structural Validity*: *Are the example problems appropriately chosen for testing the design method?* The appropriateness of the chosen example problems to test the efficacy of the design method is checked.
3. *Empirical Performance Validity*: *Does the application of method to the sample problems produce practical results?* Checking the ability of the design method to produce useful results worthy of investigation for the chosen example problems.
4. *Theoretical Performance Validity*: *Is the design method applicable for the other problem?* Here the ability of the design method to produce useful results beyond the chosen example problems is established. This requires the designer to take a "leap of faith" which is supported by the confidence gained by carrying out V&V process 1 – 3 in establishing the generic nature of the design method.

2.4.4 Design Outcome Verification and Validation

The goal here is to ensure the validity of the design outcome rather than the simulation models used for the design. The process involves gaining confidence in the resulting design of the material when compared with the system-level design requirements. Experiments are generally carried out to test the design outcomes. Li and co-authors propose an approach for design outcome validation. The approach is illustrated for a simple cantilever beam design subject to vibration.

2.4.5 Verification and Validation in this Dissertation

In this dissertation, the different verification and validation approaches described are used to verify and validate the design methods, simulation models, and design results. The verification and validation square framework is used to verify and validate the systems-based design architecture proposed in Chapter 4 of this dissertation. The systems-based design architecture is tested for the hot rod rolling process chain problem introduced in Chapter 1. Three example problems are used for achieving this. The first example involves macrostructural design of a hot rolling process chain involving the product. The horizontal integration of manufacturing processes is illustrated via this example. The second example involves designing the microstructure of a rod for target mechanical properties. Both these examples are discussed in Chapter 5 of the dissertation. The comprehensive example problem discussed in Chapter 6 involves the integrated design exploration of rod – product, steel – material, hot rolling and cooling processes – manufacturing processes. This comprehensive example is used to test the inverse design method developed in this dissertation and serves the Theoretical and Empirical Structural and Performance validations of the design method. Individual, multi-scale and multi-physics models used in the example problems are tested in terms of concept, accuracy, operation and data and will be discussed in detail in Chapters 5 and 6.

2.5 Remarks on the Current Status of Materials Design

A paradigm shift is happening from the classical material selection (Ashby and Johnson 2013), with a focus on designing the material by tailoring the chemical composition, constituent phases, microstructure, and processing paths of a material to obtain desired properties and performances at the product/system level, subject to the dynamic changes in customer requirements and market. Most efforts in this domain are focused on multi-scale modeling techniques that allow designers to come up with the material processing-microstructure-property-performance relationships. However, materials design is still addressed at the embodiment and detail design phases and does not support early stage conceptual design exploration.

The integration of design engineering and materials science is still limited to the selection of appropriate materials from a set of material databases. Product development cycles for new products and materials are still consuming huge time and resources and thus are highly expensive. Even now the performance of many systems and products are limited to the properties offered by the available set of materials from which a selection can be made. New materials development primarily has occurred via empirical, trial-and-error experiments that are usually time consuming and costly. Here material remains a black box that is subjected to repeated experiments resulting in the population of material databases for material selection. Methods to select materials by analysis, synthesis, similarity or inspiration are proposed by Ashby. These selection methods are useful for selecting material properties and mapping to the performance that is possible. However, these methods do not support tailoring the material microstructure or processing paths to satisfy certain end performance goals. The necessary combination of material properties needed to satisfy a performance requirement may not be available in the material database. There is enormous potential here, if material selection approaches are integrated with materials design techniques and methods that allow tailoring of material processing paths and microstructures to meet performance goals. This is an important research gap that is worthy of further investigation and this is addressed in **Research Gaps 1**, **2, 3** and **4** identified in Chapter 1 of this dissertation.

Multi-scale modeling efforts are the next class of research efforts focused on materials design. However, it can be said that multi-scale modeling efforts are simply a tool that may be used in materials design and does not comprise the whole of materials design and its goals. The objective in multi-scale modeling is to accurately predict the response of material microstructures with focus in specific applications. This usually corresponds to detail design of different scales associated with a material and generate information that can be passed to subsequent upper scales. Thus, as mentioned in Chapter 1, complex multiscale models might not be necessary in many materials design cases because the goal in materials design is to not accurately predict material properties but to satisfy a range of performance requirements. To this argument, we include the second fact that bottom-up modeling is not design but analysis. Thus, we believe that the key to materials design is an interplay of multiscale modeling and bottom-up analysis along with top-down, goal-oriented inverse design and human decision making. All these are investigated as **Research Gaps 3** and **4** in this dissertation. Research Gaps 1, 2, 3 and 4 identified in Chapter 1 are summarized below.

G1. Systematic approaches to identify and integrate material, process and product models based on their function structures to frame system-level structure

G2. Systematic approaches to define the forward processing-structure-property-performance relationships and develop material and product workflows

G3. Support systematic and rapid concept exploration of materials, products and processes to generate satisficing design specifications

G4. Systematic design methods to carry out inverse design exploration of materials, products and processes meeting end goals

To address these research gaps both deductive mapping and inductive design exploration are necessary to support materials design. In this dissertation, the challenge of incorporating the design of the material is addressed as part of a larger overall systems design process embodying the hierarchy of process-structure-property-performance set forth by Olson (Olson 1997) with consideration on supporting coordination of information and human decision making as illustrated in Figure 2.10.

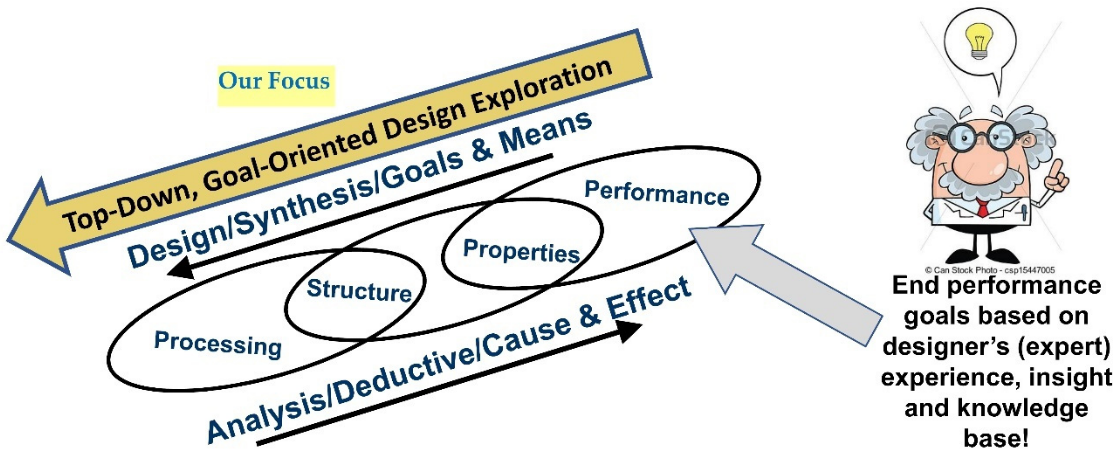


Figure 2.10: The focus in this dissertation founded on Olson's Materials-by-Design

Olson's hierarchy includes as shown in Figure 2.6:

- Processing-structure mapping: This includes relationships that can map the way a material is processed from the manufacturing process side to the corresponding microstructures, composition and phases that can be generated;
- Structure-property mapping: This includes relationships that can map the composition, phases, microstructures of the material to the properties of relevance to achieve desired performance attributes; and
- Property-performance mapping: This includes relationships between properties and the specific performance requirements that are desired for the end product/system.

However, our major focus in this dissertation is to use this foundational philosophy to support systematic goal-oriented materials design for a designer (who is considered an expert in the domain) based on the his/her experience, insight and knowledge base. Foundational to the work in this dissertation is the decision-based design philosophy of finding "satisficing" and robust solutions based on work of Mistree and co-authors (Mistree, Hughes and coauthors 1993), Chen and co-authors (Chen, Allen and coauthors 1997), Seepersad and co-authors (Seepersad, Allen and coauthors 2005) and Choi and co-authors (Choi, Austin and coauthors 2005). However, the work in decision-based design carried out till now fail to address the need for a goal-oriented, inverse design exploration of materials, products and processes and identification robust "satisficing" solutions for multiple conflicting goals. These research gaps are addressed in this dissertation and will be explained in detail in Chapters 4, 5, 6 and 7. An overview of the research efforts discussed in Chapter 2 is provided in Table 2.1.

Table 2.1: Limitations and use of existing materials design research efforts

Research Effort	Limitations	Use in Dissertation
Material Selection (Ashby and Cebon 1993, Ashby and Johnson 2013)	• Lacks ability to tailor material microstructures and processing paths for defined property or performance requirements; • Choice of only selecting from a set of material databases to identify the achievable performances for the material.	Used as a theoretical foundation to develop the systems-based design architecture for integrated materials, product and process design

Multi-scale Modeling (Khaleel 2004, Horstemeyer 2012, Horstemeyer 2018)	• Focus on bottom-up modeling spanning different material scales to predict responses of structure and properties. • Highly focused on detailed design of materials and in accurately predicting the behavior • The focus here is not in achieving system-level design objectives and inverse design exploration.	Used as theoretical foundations for establishing processing-structure-property-performance relationships that are further explored using goal-oriented inverse design exploration.
Microstructure Design using Invertible Linkages (Kalidindi, Niezgoda and coauthors 2010, Kalidindi, Niezgoda and coauthors 2011, Adams, Kalidindi	• Focused only on design of those microstructures for which invertible linkages between property and structure can be established; • Focus is on detail design and not on early stages of design;	Used as theoretical foundations for establishing inverse mapping.

and coauthors 2013)		
Material Informatics (Rajan 2005, Rajan 2013)	• Focused only on data-driven formulation of surrogate PSP linkages ("soft" computing); • Not possible if sufficient data to establish linkages are not present; • Need to be configured with "hard" computing practices to address materials design challenges.	Used as a theoretical foundation – need for databases and models.
Systems-based Materials Design (Olson 1997, Olson 2000, Panchal, Choi and coauthors 2005)	• Require systematic methods to carry out inverse, goal-oriented design to tailor microstructure and processing paths for specified performances; • Require approaches to manage uncertainty across material process chains; and • Require efficient ways to merge product design and	Philosophy used to address the research gaps 1, 2, 3 and 4 identified in this dissertation.

	materials design in an integrated fashion.	
Robust Materials Design under Uncertainty (Chen, Simpson and coauthors 1999, Choi, Austin and coauthors 2005, Seepersad, Allen and coauthors 2005, Choi, McDowell and coauthors 2008)	• Current focus is in embodiment and detail design stages – Require methods for early stages of design; • Focus on mitigating uncertainty rather than managing it; • Limited methods to address propagation of uncertainty and management of uncertainty across process chains; and • Current practices do not address situations where multiple conflicting goals are present.	Philosophy used to address the research gaps 5 identified in this dissertation (Chapter 7).

2.6 Role of Chapter 2 in this Dissertation

In Chapter 2, a review of the existing efforts associated with materials and product design is carried out. Several critical issues associated with the current capabilities of materials design is discussed in this chapter. Some of the major elements of modern materials design like material selection, multi-scale modeling, microstructure design using invertible linkages, systems-based materials design, material informatics, uncertainty management, verification and validation in materials design are discussed in this chapter. Based on the review carried out limitations of the existing capabilities are identified and reported in Table 2.1. The research gaps that are worthy of investigation are identified based on this review for further exploration. In next chapter, the design foundations for addressing some of the research gaps identified in this chapter are reviewed and limitations that exist in the current capabilities are identified.

Chapter 3: Design Foundations - State of the Art in Decision-Based Design, Robust Design Approaches and Platform for Decision Support

The objective in this chapter is to introduce and review the design foundations based on which the systems-based design architecture for integrated design of materials, products and manufacturing processes design is developed. Besides the underlying decision-based design, systems design, and robust design approaches, methods and tools reviewed are classified in terms of concept, application to design process and value in design. The relationship of these research efforts reviewed in this Chapter with the constructs of the systematic approach developed in this dissertation is highlighted in Figure 3.1.

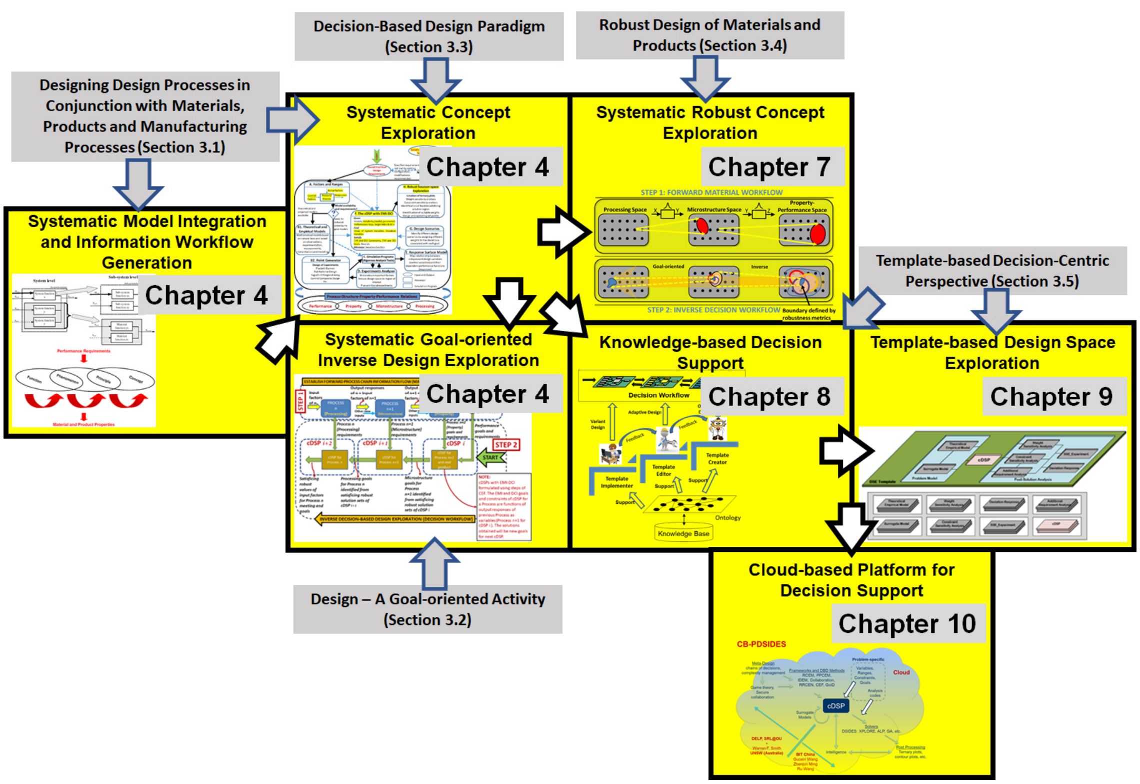


Figure 3.1: Relationship of research efforts discussed in this chapter with the constructs of the systems-based design architecture developed in this dissertation

In Section 3.1, the need for the systems-based design architecture is emphasized from the perspective of materials and product design. In Section 3.2, the perspective with which design is viewed in this dissertation is defined with a review on the different design paradigms that exists. In Section 3.3, the Decision-Based Design paradigm adopted in this dissertation is reviewed. This is followed by a review of robust design and design under uncertainty in Section 3.4. In Section 3.5, the foundations for a platform for decision support is reviewed and discussed.

3.1 Designing Design Processes in Conjunction with Materials, Products and Manufacturing Processes

In Chapter 2, we had emphasized the point that "*Materials Design goes beyond Materials Selection*". The goal in integrated design of materials, products and processes is to tailor material microstructures and processing paths to satisfy specific system-level (material, product or assembly) properties and performances. In accordance with the above point, the fundamentals of engineering design are introduced in this chapter. The concepts, tools and constructs reviewed in this chapter are used in the rest of the chapters of the dissertation to develop the systems-based design architecture for integrated material, product and process design. We begin this section with the goal-oriented nature of design processes. There are several schools of thought for engineering design. One school of thought is Decision-Based Design (DBD). Two different perspectives are popularly identified within DBD: one articulated by Hazelrigg (Hazelrigg 1996, Hazelrigg 1998) and the other by Mistree and co-authors (Mistree, Smith and coauthors 1990, Mistree, Smith and coauthors 1991, Mistree, Smith and coauthors 1993). In this dissertation, we follow the perspective of Mistree and co-authors; the details of which will be discussed in later sections. In next section, we discuss design as a goal-oriented activity and its implications in materials and product design.

3.2 Design – A Goal-Oriented Synthesis Activity

The following conversation takes place between Alice and The Cheshire Cat in Lewis Carroll's 'Alice's Adventures in Wonderland' (Carroll and Tenniel 1865):

"Cheshire Puss, would you tell me, please, which way I ought to go from here?"

*`**That depends a good deal on where you want to get to**,' said the Cat.*

"I don't much care where—" said Alice.

*`**Then it doesn't matter which way you go**,' said the Cat.*

"–so long as I get SOMEWHERE," Alice added as an explanation.

*`**Oh, you're sure to do that**,' said the Cat, `**if you only walk long enough.**'*

Figure 3.2: Image depicting conversation between Alice and Cheshire Cat in Lewis Carroll's 'Alice's Adventures in Wonderland' (Image source: Internet)

Charles Lutwidge Dodgson (better known by his pen name Lewis Carroll), an English writer and mathematician, presents a fundamental aspect of design decision making in *Alice's Adventures in Wonderland* (Carroll and Tenniel 1865). Alice, comes to a fork after walking through the wonderland forest. She stands pondering about the decision she should make, not knowing which way to go. This is when the Cheshire Cat appears on the tree above her.

Alice asks the Cheshire Cat to make a decision for her, *"Cheshire Puss, would you tell me, please, which way I ought to go from here?"*. The Cat instead of offering a decision responds `***That depends a good deal on where you want to get to,'***. The Cat here recognizes the fact that it cannot make the choice for Alice. It is completely upon the person actually taking the action resulting directly from the decision can make the decision (Hazelrigg 1996). The Cat instead offers a piece of advice in general which is foundational to design decision making: `***That depends a good deal on where you want to get to,'***. The choice of taken by the decision maker should be based on namely the decision maker's preference over the outcome of the decision (Hazelrigg 1996). This is a very powerful statement and has wide implications across design and decision making.

A very important implication that can be derived here is that the decision maker should have a preference on the outcomes (or a goal that he/she wants to achieve/satisfy) and only the decision maker's preference matters here. Here the Cat makes it clear to Alice that the preferences are on the outcome and not on the choices of decisions as to which path to take.

Alice then responds, *"I don't much care where—"*. Alice suggests that she doesn't have a preference over the outcomes. To this the Cat responds, `***Then it doesn't matter***

which way you go,'. The Cat basically is saying that: *'If you don't know where you are going ... any road will take you there.'*. The implication that can be derived from this statement is that unless the decision maker has a preference over the outcomes, any choice can be accepted equally. The Cat here reminds that one choice is better than the other only because we have a preference over the outcomes (Hazelrigg 1996); this is the perspective of modern normative decision theory.

From the standpoint of this dissertation, an important implication that we derive out of this conversation is that every designer (or decision-maker) should have a goal that he/she wants to satisfy, and that the designer should start the path that he/she wants to traverse with this goal in mind. If there is no such goal that the designer wants to satisfy, then the designer is free to choose any path that he/she wishes to traverse. This idea is very relevant to decision-based design and forms the foundational research philosophy for this dissertation from the context of integrated materials and product design.

"*While natural sciences are concerned with how things are, an engineer, and more generally a designer is concerned with* ***how things ought to be in order to attain goals and to function****"* (Simon 1996). The distinction between natural science and engineering science is pointed out by Braha and Maimon (Braha and Maimon 1997). Natural science is theory oriented and focuses on analysis. Engineering science is result oriented and focuses on synthesis. This difference reflects in the definitions of 'design' by many researchers.

3.2.1 Some Background on Models for Design

Descriptive and Prescriptive Models of Design

Research in engineering design can be categorized as design philosophies, models and methods. **We believe that the term "Design Theory" is an oxymoron**. This is because there cannot be a unique theory in design that proposes how design must be carried out. However, we review design theory in the way it has been defined in past. Design theory as per popular belief is a collection of principles that are useful for explaining a design process and provide a foundation for basic understanding required to propose useful methodologies (Panchal 2005). An explanation of what design is provided by design theory. Design methodology on the other hand is a collection of procedures, tools and techniques for designers to use when designing. **Again, we also believe the term "Design Methodology" is an oxymoron.** Methodology is the systematic, theoretical analysis of the methods applied to a field of study and use of the term in the context of design as collection of procedures, tools and techniques is an oxymoron. This also holds for the term "**Design Research**" as discussed by Krippendorff (Krippendorff 2007). Krippendorff in his essay makes the point that design research is an oxymoron whose contradictions, because they are not obvious to everyone, can lead its naïve users into thinking of it as a kind of research similar to what reputable scientists do. Ignoring the issue of the usage of terms being an oxymoron, design methodology is prescriptive, while design theory is descriptive (Finger and Dixon 1989, Finger and Dixon 1989, Evbuomwan, Sivaloganathan and coauthors 1996).

Design methods are developed from different viewpoints emphasizing various facets of overall design process. An ideal design method supports all the following viewpoints of design as (Evbuomwan, Sivaloganathan and coauthors 1996):

- a top-down and bottom-up process;
- a incremental activity (evolutionary);
- a knowledge based exploratory activity;
- an investigative process (research);
- a creative process (art);
- a rational process;
- a decision making process;
- an iterative process; and
- an interactive process.

Design methods are usually developed with some of these viewpoints in mind. An ideal design, however should support all of these.

Pahl and Beitz Design Process

Pahl and Beitz (Beitz, Pahl and coauthors 1996, Pahl and Beitz 1996) define four phases of design. These four phases are common to any prescriptive model of design. These phases include planning and clarification of task, conceptual design, embodiment design and detail design. In planning and clarification, the designer identifies requirements that the outcome of design should fulfill. From these requirements a problem statement is formulated. Conceptual design includes generation of solution principles to satisfy the problem statement. In embodiment design, these solution principles are refined until the final solution remains. In detail design, all the details of the final design are specified, and manufacturing drawings and documentation are produced. Steps of the Pahl and Beitz approach are shown in Figure 3.3.

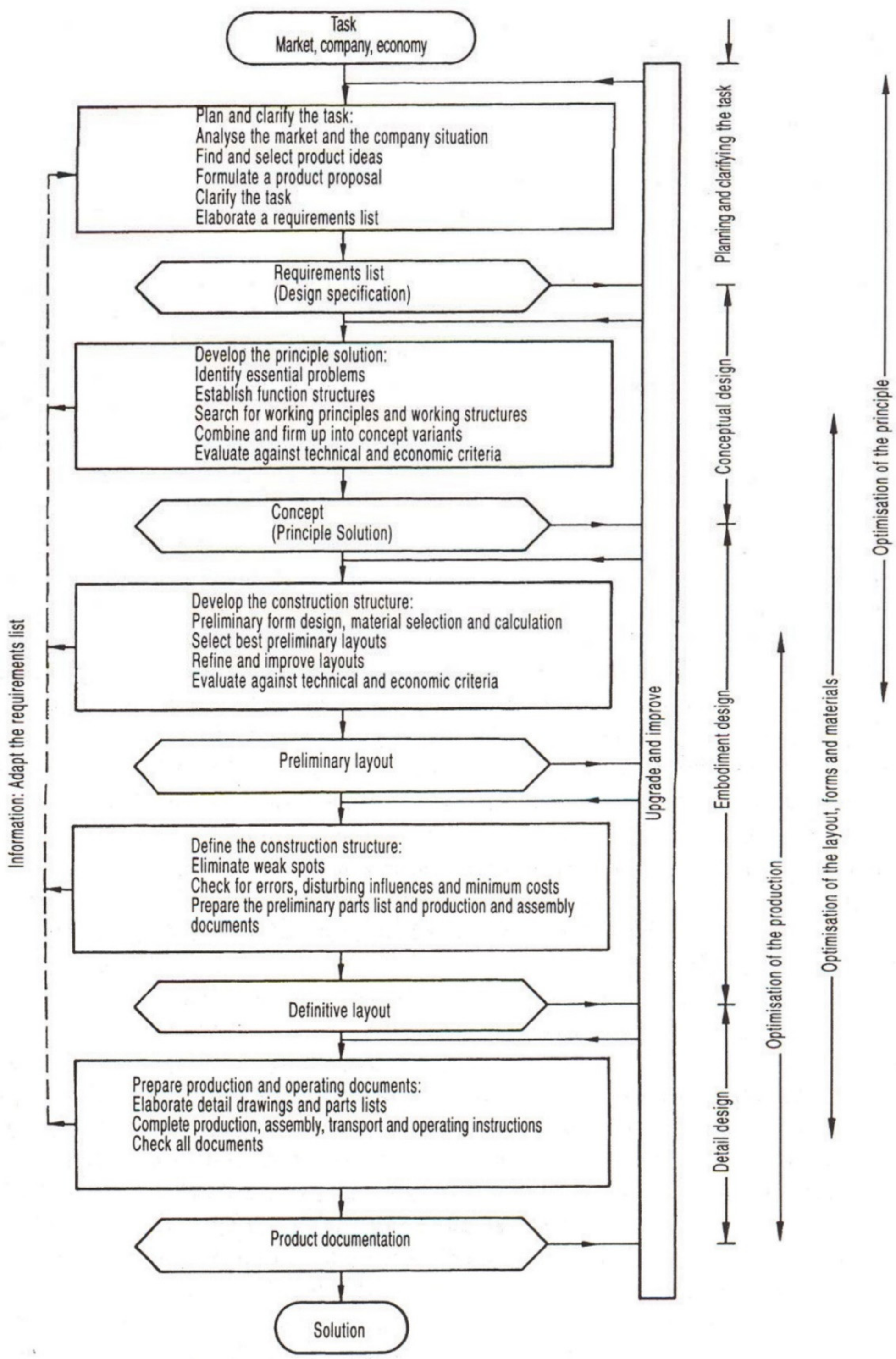


Figure 3.3: Pahl and Beitz design process (Pahl and Beitz 1996)

Pahl and Beitz design process is a systematic design process and is based on ***discursive thinking*** and ***intuitive thinking***. We believe that for systematic design to happen both discursive thinking and intuitive thinking are needed. Discursive thinking is a conscious process in which scientific knowledge and relationships are consciously analyzed, varied, combined in new ways, logically checked, rejected and considered further to come up with reasonings or conclusions (Pahl and Beitz 1996). In this systematic process **information is transformed successively** via successive steps – which helps in making problem solving systematic. Intuitive thinking is strongly associated with flashes of inspiration required to fulfill various information transformation in systematic design; see Figure 3.4 (adopted from (Messer 2008)) for illustrations on discursive thinking and intuitive thinking for systematic design.

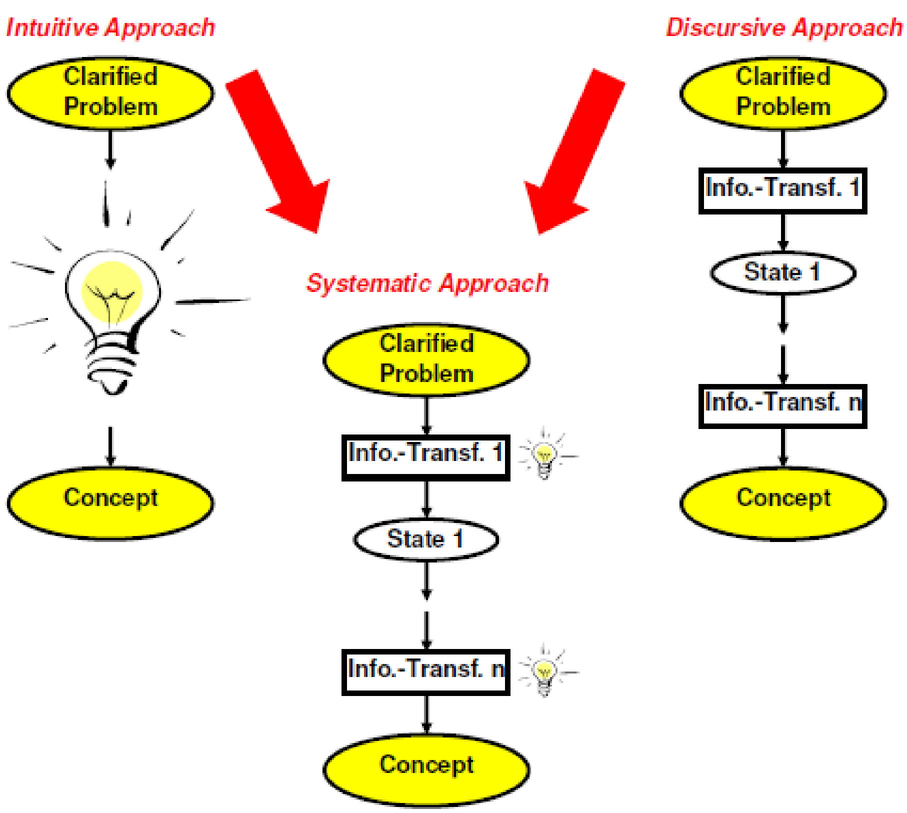


Figure 3.4: Systematic design (Messer 2008)

After the planning and clarification of the task phase of Pahl and Beitz design process, the designer comes up with a requirements list and starts the conceptual design phase. In the conceptual design phase, the designer determines a principal solution or a concept. This is achieved by abstracting the essence of the problem, establishing ***function structures***, searching suitable ***working interrelationships*** (working principles, phenomenon, etc.) and then combining those (integration of information) to develop a **system-level function structure** or working structure or a **workflow** – from the context of this dissertation. The working structure is then transformed into a more comprehensive representation so as to evaluate the essentials of the principal solution and review constraints, goals and other design objectives. Once the specification of concepts is done at conceptual design stage, the design process re-starts at a much more concrete level in embodiment and detail design phases.

Gero's Model of Design as a Process

The prescriptive models of design are mostly based on the assumption that a design activity consists of three core activities – **Analysis**, **Synthesis**, and **Evaluation** (**ASE**). Analysis is defined as the resolution of anything complex into its elements and the study of these elements and of their relationships. Synthesis is putting together of parts or elements to produce new effects and to demonstrate that these parts create an order (Pahl and Beitz 1996). Design can be visualized as an iterative feedback loop of synthesis, analysis and evaluation. Gero (Gero 1990) describes the ideas of analysis, synthesis and evaluation as a **series of information transformation** starting with requirements and ending with descriptions of design that satisfies those requirements.

Gero's view of design is foundational for many research efforts focused on product design.

Gero defines the key aspects of product information as Function (F), Structure (S), Expected Behavior (Be), Achieved Behavior (Bs), and Product Descriptions (D), see Figure 3.5.

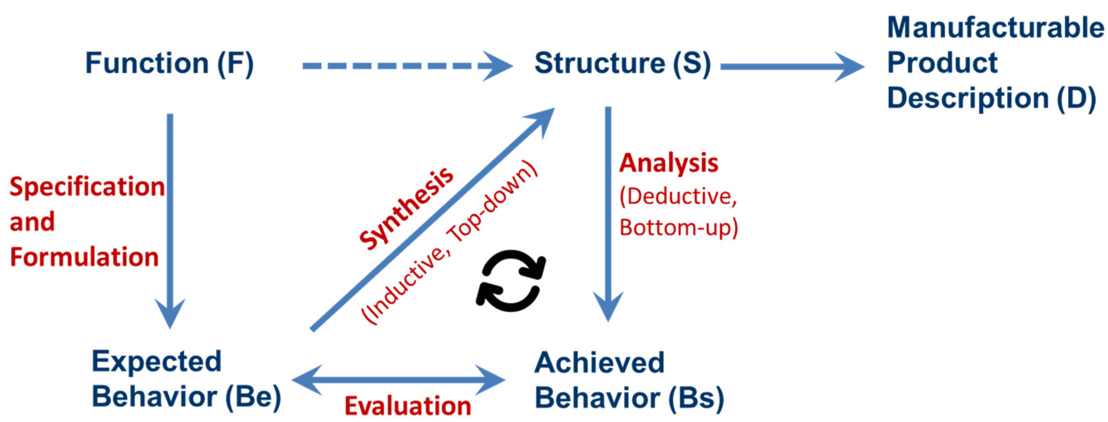


Figure 3.5: Gero's model of design as a process (Gero 1990)

- **Function (F):** Function F is the relation between the goal of a human designer and the behavior of the system. It specifies a relation between input and output in terms of material (matter), energy and signal (information).
- **Expected Behavior (Be):** Expected Behavior (Be) represents the physical behavior that the artifact being designed should have in order to satisfy the functional requirements (F).
- **Structure (S):** Structure (S) represents the artifact's elements and its relationships. It is also called the form of the artifact. It represents the proposed design solutions – information about geometry, material, configurations, etc.

- **Achieved Behavior (Bs):** Behavior of the structure derived directly using engineering principles
- **The manufacturable product descriptions** are derived from the product structure.

Connecting Gero's Model of Design with Olson's Materials-By-Design

The process of designing a material starts with customer needs and requirements for the end product. These customer needs are captured as functional requirements or functions. Using engineering parameters, these functional requirements are mapped into the expected behavior. Based on the expected behavior formulated, the structure of the material is synthesized (synthesis transformation). The synthesis here may be using expert's knowledge, previous designs or through computations and is a top-down inductive approach. Simulation models may be used to predict/analyze the achieved behavior from the structure synthesized from expected behavior. This refers to analysis and is a bottom-up deductive approach. The expected behavior is then evaluated with the achieved behavior. This is referred to as evaluation. This whole cycle of synthesis, analysis and evaluation is repeated, and the structure is refined until the required performance is satisfied. From the final structure identified the manufacturable product descriptions are derived. This model of design usually applies to product design. However, it has strong ties to the systems-based materials design proposed by Olson. In terms of Olson's processing-structure-property-performance relationships, the function (F) corresponds to the performance of the system/product/material. Behavior (B) corresponds to the properties of the material system. The specification and formulation step in the process is equivalent to performance to property mapping. The design synthesis step involves mapping from property to microstructure. The Structure (S) in Gero's model corresponds to the structure domain in Olson. The design synthesis is a top-down, inductive process. The microstructure obtained is then analyzed by mapping structure to properties. This is bottom-up, deductive process of predicting properties from structure. Finally, the product descriptions correspond to the processing information of the product/material. This whole scheme is depicted in Figure 3.6.

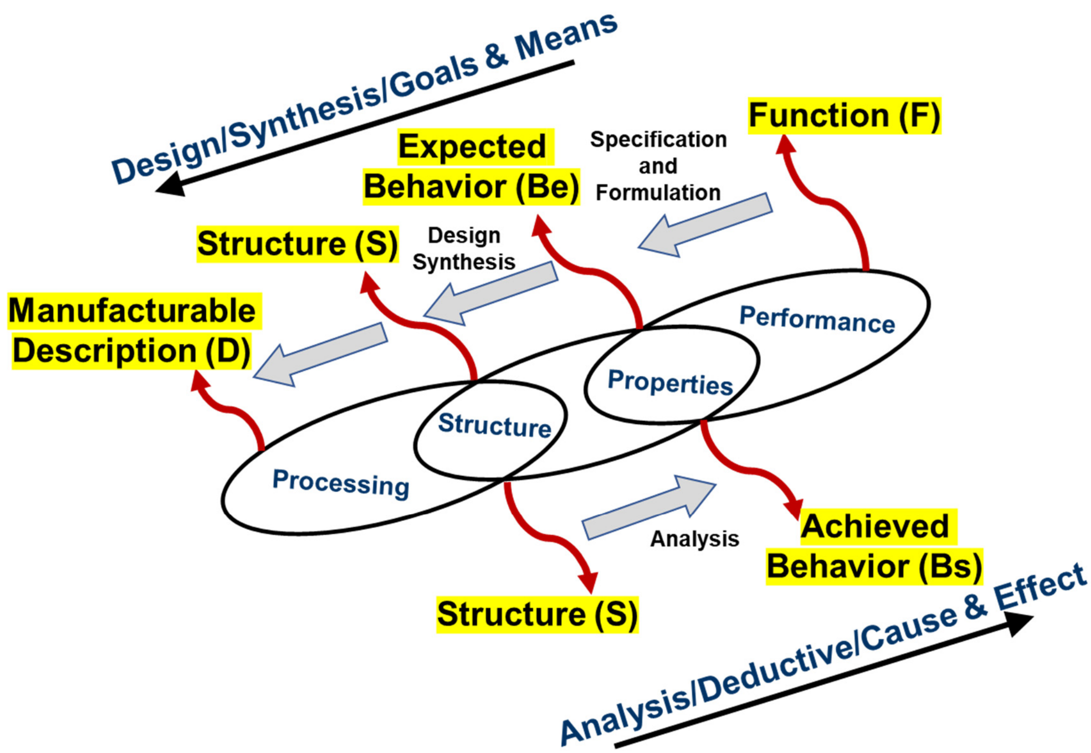


Figure 3.6: Connecting Gero's model (Gero 1990) of design with Olson's (Olson 1997) diagram

The design model by Gero is foundational for function-based design and will be discussed in detail in later sections. In the last chapter, Gero's model will be addressed from the perspective of robust product design.

3.2.2 Suh's Axiomatic Design

Suh defines design as an **interplay** between "**what we want to achieve**" and "**how we want to achieve it**" (Suh 1990). Here what we want to achieve is the goal, and how we want to achieve is the path that needs to be taken to reach/satisfy that goal. Suh proposes the engineering sequence in which this happens via four design domains – the four domains of design world. This includes Customer Attributes (CAs) – Customer Domain, Functional Requirements (FRs) – Functional Domain, Design Parameters (DPs) – Physical Domain, Process Variables (PVs) – Process Domain, as shown in Figure 3.7. CAs are the customer needs. CAs are transformed into functional requirements FRs. This is equivalent to "what we want to achieve" or the goals identified by the designer. FRs are satisfied by identifying appropriate design parameters (DPs) in the physical domain. In a similar manner process variables (PRs) are identified from the DPs. All this process is carried out by effectively mapping from one domain to another. A good design process here is defined by means of the efficiency of mapping process.

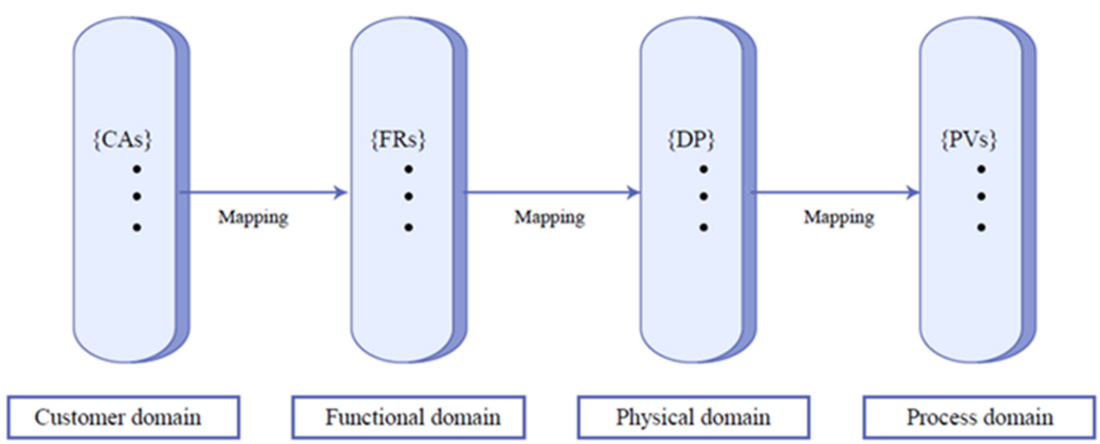


Figure 3.7: Relationship of domains, mapping and design spaces in Suh's Axiomatic Design (Suh 1990)

Suh proposes two design axioms that forms basic principles that govern design decision making. The two axioms are (Suh 1990):

- "The Independence Axiom" (maintain independence of functional requirements); and
- "The Information Axiom" (minimize the information necessary to meet the functional requirements).

The two axioms can be interpreted as follows (Park 2007):

- A good design according to Suh's Axiom 1 always maintains the independence of functional requirements (FRs). This means that in an acceptable design, DPs and FRs are related in such a way that a specific DP can be adjusted to satisfy its corresponding FR without affecting other functional requirements.
- A good design according to Suh's Axiom 2 is a functionally uncoupled design (satisfying Axiom 1) that has minimum information content.

The axioms help designers to structure and understand design problems, thereby facilitating the synthesis and analysis (interplay) of suitable design requirements, solutions, and processes. However, the axiomatic character of these two design axioms is found to be flawed, as discussed by (Olewnik and Lewis 2005). From a validation perspective, the issue with Suh's Axiomatic Design is that it forces the designer to conform to a particular preference structure, thereby biasing the designer (Olewnik and Lewis 2005). Even though Suh's axioms are flawed, the four domains and the way mappings are carried out across these domains to satisfy customer attributes finds application in Olson's process-structure-property-performance mapping from top-down design perspective. Suh's axiomatic design domain mappings can be translated to Olson's

Materials-by-Design as shown in Figure 3.8. This relationship will be explored further in the last Chapter, Chapter 10 in terms of robust product design.

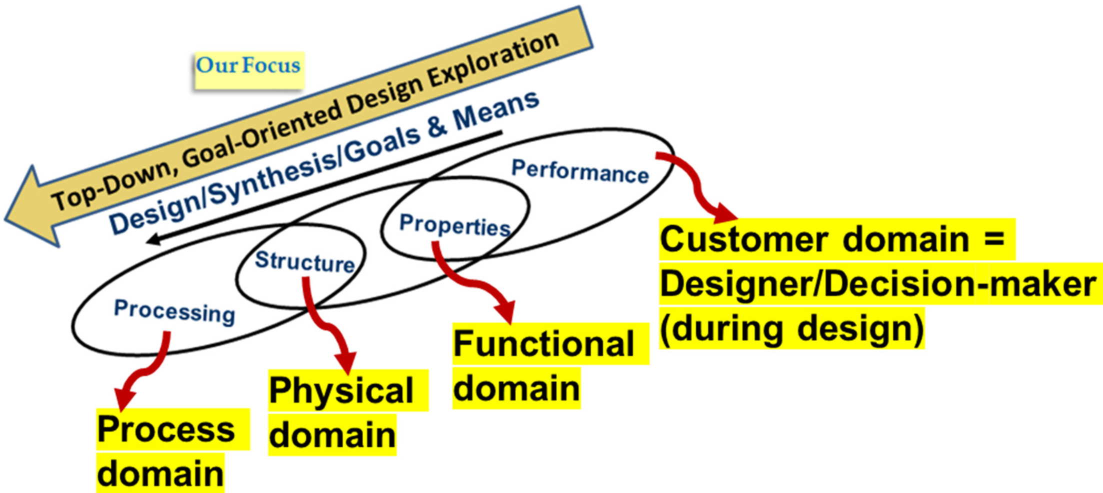


Figure 3.8: Translation of Suh's Axiomatic Design Domain mappings to Olson's Materials-by-Design

Suh (Suh 1990) presents a design equation to mathematically represent design process in terms of design equations. The design equation follows:

$$\{FR\} = [A]\{DP\} \qquad \textbf{Equation 3.1}$$

Using the equation, Suh represents the mapping between functional domain and physical domain. Here functional domain refers to "what we want" and physical domain refers to the means for satisfying what we want. Functional requirements in Suh's design equation refers to the "minimum" (Axiom 2) set of "independent" (Axiom 1) requirements that completely characterize the functional needs of the product in the functional domain that is translated from the customer attributes. Design parameters (DP) are the "key" (Axiom 2) design variables that characterize the physical domain that can satisfy the FRs. The matrix [A] is called the design matrix. A similar vector equation can be written for the mapping from physical domain to process domain.

FR-DP relationships could be uncoupled (diagonal A matrix), decoupled (triangular A matrix), or coupled (neither diagonal nor triangular) designs. The Independence Axiom is satisfied only by uncoupled or a decoupled design; while the coupled design does not satisfy Axiom 1. Thus, Suh's design equation has the following drawbacks:

- Inability to capture complex relationships: For complex problems and relationships, there does not exist an information model associated with Suh's design equation to represent FRs and DPs. Thus, relationships between functional requirements and design parameters is not captured following the axioms.
- Inability to capture design activities other than mapping: In Suh's design equation the only transformation of information captured is the mapping from one domain to another. Other activities associated with design such as decomposition, abstraction, evaluation etc., are unable to be modeled using the design equation.
- Computational implementation of a design process is not easy using Suh's design equation.
- The design equation serves as a guideline for what a good design is but does not provide guidelines for designing design processes or meta-design.
- Evolution of product information along the design process cannot be understood via Suh's design equation.
- Reusability of design process related information is also not addressed in Suh's design equation.
- Suh's design equation forces the designer to conform to a particular preference structure, thereby biasing the designer.

3.3 The Decision-Based Design Paradigm – Our Frame of Reference

Mistree and co-authors (Mistree, Smith and coauthors 1990) define design as the conversion of information that characterizes the needs and requirements for a product into knowledge about the product. **The underlying philosophy in the definition of design by Mistree and co-authors (Mistree, Smith and coauthors 1990) is that the designer starting with the functional requirements that is desired (the goal that designer wishes to achieve), should be able to work backwards to explore effective design solutions.** This philosophy is adopted in this dissertation for design – as a goal-oriented activity. As noted by Gero (Gero 1990), the goal of design is to transform requirements – generally termed *functions* – into design descriptions.

The work on Decision-Based Design by Mistree and co-authors (Mistree, Smith and coauthors 1990) is anchored in the works of Herbert Simon and James Miller. Simon (Simon 1969), in his book suggests that design is decision-based and one of the sciences of the artificial. The development of any science is anchored on a body of beliefs, hypothesis and knowledge. In the case of Mistree and co-authors, this is anchored in the exposition of Living Systems Theory by James Miller (Miller 1978).

Decision-Based Design (Shupe 1988, Mistree, Smith and coauthors 1990) is a term coined to emphasize a different perspective to develop methods for design. The principal role of a human designer in Decision-Based Design (DBD), is to make decisions given the information available. Now how do we define a decision here? From an engineering perspective, decisions exclusively deal with allocation of resources in some form, usually as capital expenditures. Thus, the definition of a decision here is as "an irrevocable allocation of resources" (Hazelrigg 1996).

"There are two important characteristics of a decision:

- A decision is made at an instant in time.
- A decision must be made based on the information available at the time it is made." (Hazelrigg 1996)

In this definition of design and decision, the term product is used in its most general sense; it may include processes as well (Mistree and Allen 1997). Through a process of decision making, there occurs the conversion of information into knowledge. Several characteristics associated with design decisions are identified and are summarized as descriptive sentences (Mistree, Smith and coauthors 1990):

- Decisions in design are invariably multileveled and multidimensional in nature.
- Decisions involve information that comes from different sources and disciplines.
- Decisions are governed by multiple measures of merit and performance.
- All the information required to make a decision may not be available.
- Some of the information used in making a decision may be hard, that is, based on scientific principles and some information may be soft, that is, based on the designer's judgment and experience.
- The problem for which a decision is being made is invariably loosely defined and open and is characterized by the lack of a singular, unique solution. The decisions are less than optimal and represent ***satisficing solutions***.

3.3.1 The Design Equation (The Decision-Based Design Equation)

Bras (Bras 1993) developed a generalization of Suh's design equation. Design is viewed as a process of converting information that characterizes the needs and requirements of products into knowledge about a product. Knowledge is derived by human beings from information by reasoning, discussion and other mind-involving processes. Thus, knowledge here is specific information. Data is the simple form here and is characterized by a sense of hardness. Information is data, but not all data is information. In the design equation by Bras, a single transformation in design process is represented as an algebraic design equation, as shown in Equation 3.2, Figure 3.9.

$$\mathbf{K} = \mathbf{T}(\mathbf{I}) \qquad \textbf{Equation 3.2}$$

where,

I is a vector with *n* components representing the information,

K is a vector with m components representing the knowledge,

T() is a function to transform the vector **I** into vector **K**; the transformation function **T()** comprises a set of *m* functions, that is, **T()** = (T_1(), T_2(),….,T_m()).

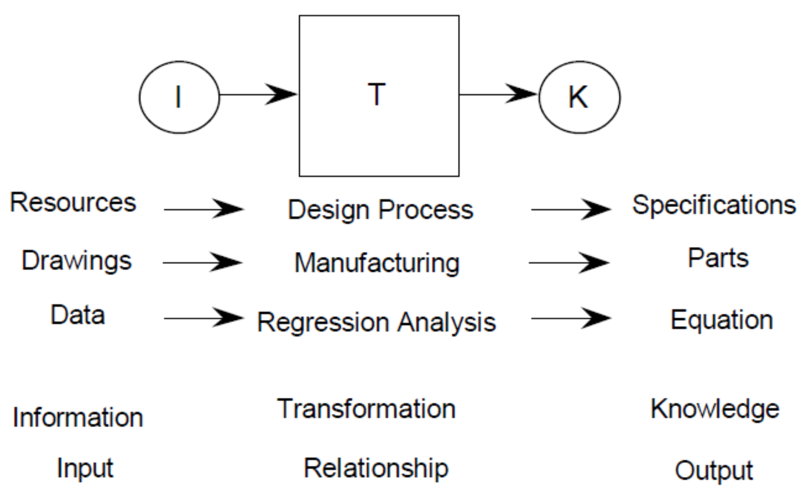


Figure 3.9: The design equation (Bras 1993)

The design equation by Suh can be viewed as a special case of the design equation developed by Bras and Mistree (Bras 1993). This is because of the ability of the design equation by Bras and Mistree to capture non-linear transformations unlike Suh's design equation which can capture only linear transformations.

A meta-design equation is also developed as an approximation of the design equation. The meta-design equation is represented as,

$$\mathbf{\Delta K} = [\mathbf{T}]\mathbf{\Delta I} \qquad \textbf{Equation 3.3}$$

where, $\mathbf{\Delta I}$ represent difference in information and $\mathbf{\Delta K}$ represent difference in knowledge respectively. The $[\mathbf{T}]$ is a *m* x *n* transformation matrix. The conversion of information to knowledge is embodied in the transformation matrix. The meta-design transformation matrix can be interpreted as an equivalent of Suh's axiomatic design matrix, [A], which converts design parameters (DPs) into functional requirements (FRs). However, the $[\mathbf{T}]$ matrix is not limited to functioning as an approximation to Suh's axiomatic design equation but has the capability to provide an approximate relationship between $\mathbf{\Delta K}$ and $\mathbf{\Delta I}$ for any design. The function T() in Equation 3.2 is satisfied by multiple Decision-Support Problems (DSPs). Hence, DSPs are the implementation of the design equations within DBD. Note – there is a difference between matrix [T] and function T(). DSP Technique uses function, whereas Suh uses matrix.

3.3.2 The DSP Technique

In this section, we discuss the DSP technique which is one of the implementation approaches for DBD. According to Muster and Mistree (Muster and Mistree 1988), the Decision Support Problem Technique support a human designer in making rational design decisions using human judgement. There are several methods/approaches to plan, establish goals and plan systems. However, independent of these approaches, designers are and will continue to be involved in two primary activities, namely, *processing symbols* and *making decisions* (Mistree, Smith and coauthors 1993). The assertion here is that the process of design is basically a network of decisions. Designers and engineers need an approach for negotiating ***satisficing solutions*** for their problems rather than optimal solutions due to increasing complexity and interactions of system with its environment resulting in more and more uncertainty within the system. The DSP technique supports a human designer in portioning and formulating the problems in simple terms so that it is possible to find satisficing solutions for it, while being close to the actual system without removing its sources of uncertainty.

Meta-Design and Design Phases in the DSP Technique

The DSP technique requires designers to implement two phases: a) *meta-design* and b) *design phase*. The meta-design phase consists of planning and structuring of decision support problems. Meta-design phase is accomplished via problem partitioning into its elemental DSPs and devising a plan of action. In this phase, there is no attempt to make or pursue product specific decisions. The goal in this phase is to ***design the design process*** (meta-design) to be implemented. The base entities used to specify a design process are phases, events, decisions, tasks, etc. The information generation comes from input-output relationships. The base entities are used to model the design process as a network that can be managed. In the design phase, the decision support problem is actually solved, and post-solution analysis is carried out. In this phase, the solutions to the design process is sought and these solutions are further verified and validated. Decision Support Problems provide a means for modeling decisions encountered in design and the domain specific mathematical models so built are called ***templates*** or Decision Support Problem templates (Mistree and Allen 1997).

The two phases of DSP Technique can be represented as shown in Table 3.1.

Table 3.1: The phases of DSP Technique (Mistree and Muster 1990)

<table>
<tr><th>Phase I: Meta-Design</th><th>Phase II: Design</th></tr>
<tr><td rowspan="2">STEP 1: IDENTIFY/CLARIFY PROBLEM
(Characteristics and design type)
Problem story
↓
Technical brief
↓
Abstracts</td><td>STEP 3 & 4: STRUCTURE
• Organize domain-dependent information and formulate DSP templates
• Develop DSP word formulations.
• Develop DSP mathematical formulations.</td></tr>
<tr><td>STEP 5: SOLVE
• Obtain solutions.
• Solve the DSPs using appropriate means.</td></tr>
<tr><td>STEP 2: PARTITION AND PLAN
• Partition each abstract into problem statements and identify decisions associated with each problem statement.
• Devise plan for solution in terms of DSPs corresponding to decisions.</td><td>STEP 5: POST-SOLUTION ANALYSIS
• Verify and validate solutions
• Sensitivity analysis.
• Check for consistency.
• Check for need for iteration.
• Make design decisions.</td></tr>
</table>

Design Process Modeling using DSP Technique Palette

In DSP Technique, the entities for carrying out meta-design are contained in a DSP Palette. These entities are domain independent and supports hierarchical modeling of design processes. There are three classes of entities – ***potential support problem entities***, ***base entities*** and ***transmission entities***. The *potential support problem entities* include phases, events, tasks, decisions and system, as shown in Figure 3.10.

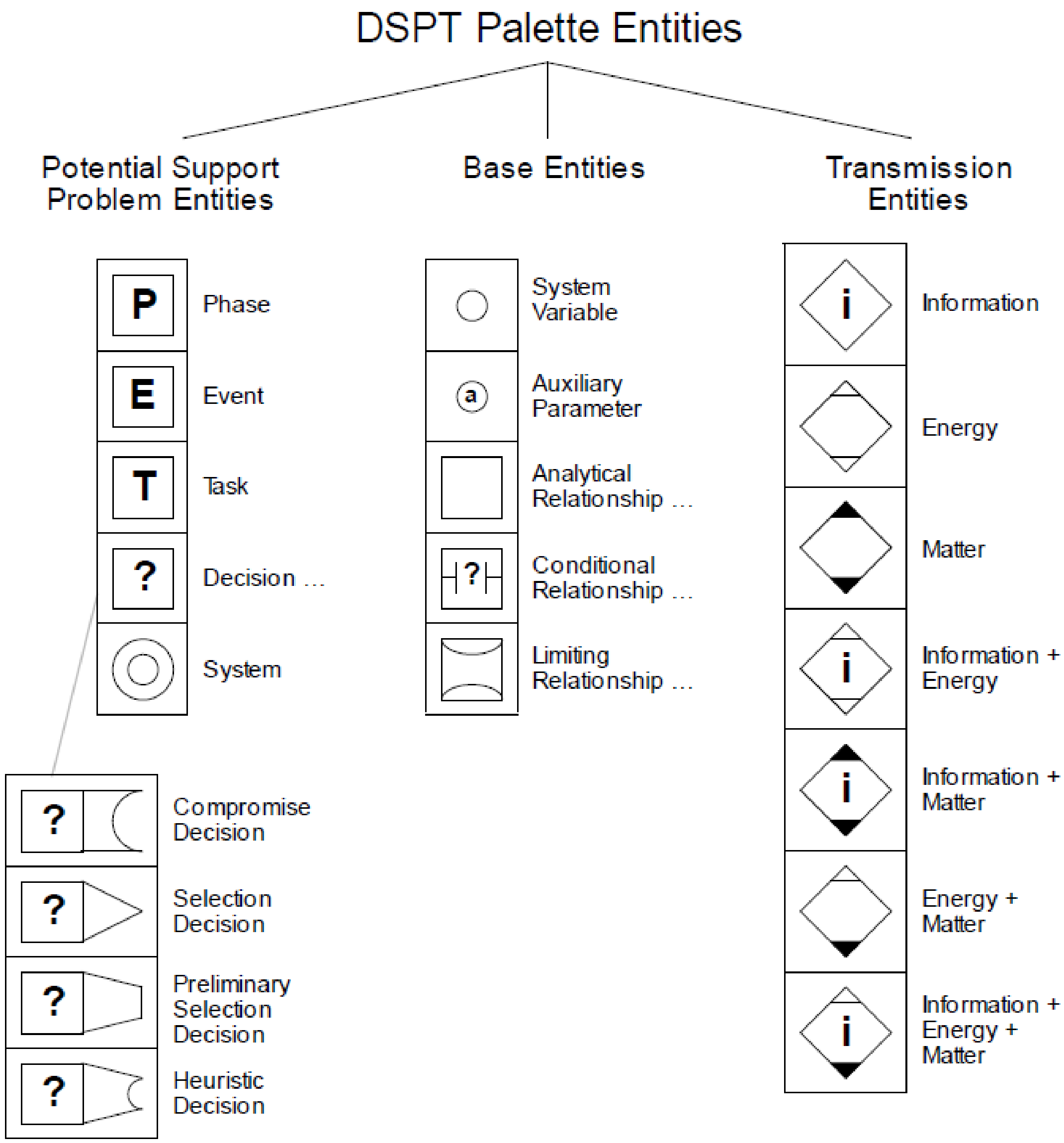


Figure 3.10: Decision Support Problem Technique Palette entities (Mistree, Smith and coauthors 1993)

Phases, denoted by the icon "P" are used to represent elements of partitioned process. An example of phases are the different phases of design in Pahl and Beitz design process like conceptual design, embodiment design, detail design, etc. Events, denoted by "E" occur within a phase. An example of an event is - "check for system feasibility". Accomplishments of phases and events occur by tasks and decisions for which a human designer is required. A task here refers to any activity that needs to be accomplished. According to Mistree and co-authors (Mistree, Smith and coauthors 1991, Kamal, Garson and coauthors 1992), all decisions identified in the DSP technique are categorized as ***selection, compromise***, or a ***combination*** of these. The selection and compromise decisions are considered as ***primary decisions*** and others as **derived decisions**.

Base entities are the most elementary entities in the DSP technique. They can be implemented on a computer and are used to describe constraints, bounds, relationships between design variables, etc. Base entities are shown in Figure 3.10.

Transmission entities are used to define the connections between various other entities used to model the design process and include three types of basic transmissions – mass, energy, information and their combinations. These entities are based on Miller's Living Systems Theory. Transmissions entities are shown in Figure 3.10.

3.3.3 Decision-Making in Decision-Based Design

According to the types of decisions, there are the following types of DSPs, see Figure 3.11.

- ***Selection DSP*** – a primary DSP - making a choice between a number of possibilities taking into account a number of measures of merit or attributes

(Kuppuraju, Ittimakin and coauthors 1985, Mistree, Marinopoulos and coauthors 1988, Vadde, Allen and coauthors 1995). The emphasis in selection is on the acceptance of certain alternatives through the rejection of others based on different measures of merit, called attributes, which represent the functional requirements.

- ***Compromise DSP*** – a primary DSP - the determination of the "right" values (or combination) of design variables to describe the ***best satisficing*** system design with respect to constraints and multiple goals (Mistree, Hughes and coauthors 1993). The cDSP is discussed in greater details in the Section 3.3.4 and is the foundational mathematical construct used in this dissertation.
- ***Derived DSPs*** – combination of primary DSPs to model a complex decision, e.g., selection/selection, compromise/compromise and selection/compromise decisions (Bascaran, Bannerot and coauthors 1989, Karandikar and Mistree 1993, Mistree, Smith and coauthors 1993, Vadde, Allen and coauthors 1994).

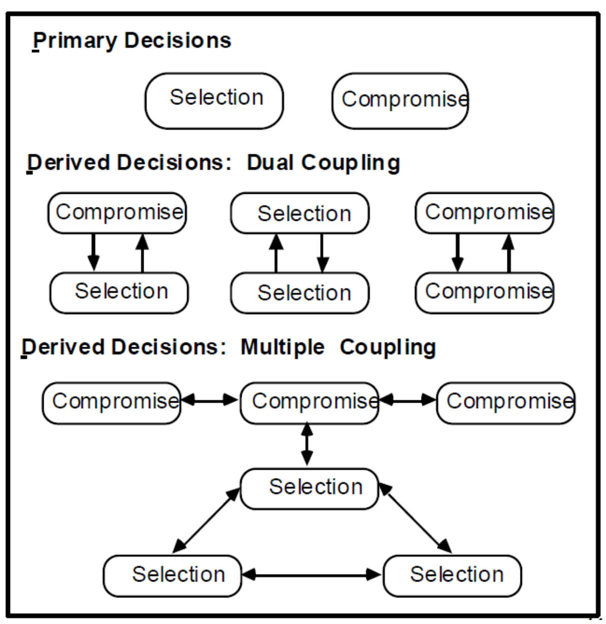


Figure 3.11: Primary and derived decisions (Mistree and Allen 1997)

In the DSP technique, the selection and compromise DSPs are used to address independent decisions. Coupled DSPs are used to model hierarchies of decisions, thus forming a network of decisions (Bascaran 1991). Given a network and its information interactions, two types of modeling of decisions relationship is possible – hierarchical and heterarchical (Mistree, Smith and coauthors 1990), see Figure 3.12. Heterarchical decision relationships are unordered and it is difficult for designers to define precedence in such decision networks. Hierarchical decisions, on the other hand are clear in terms of information flow and the sequence of decisions are well defined. Coupled DSPs can be used to implement such hierarchical decisions.

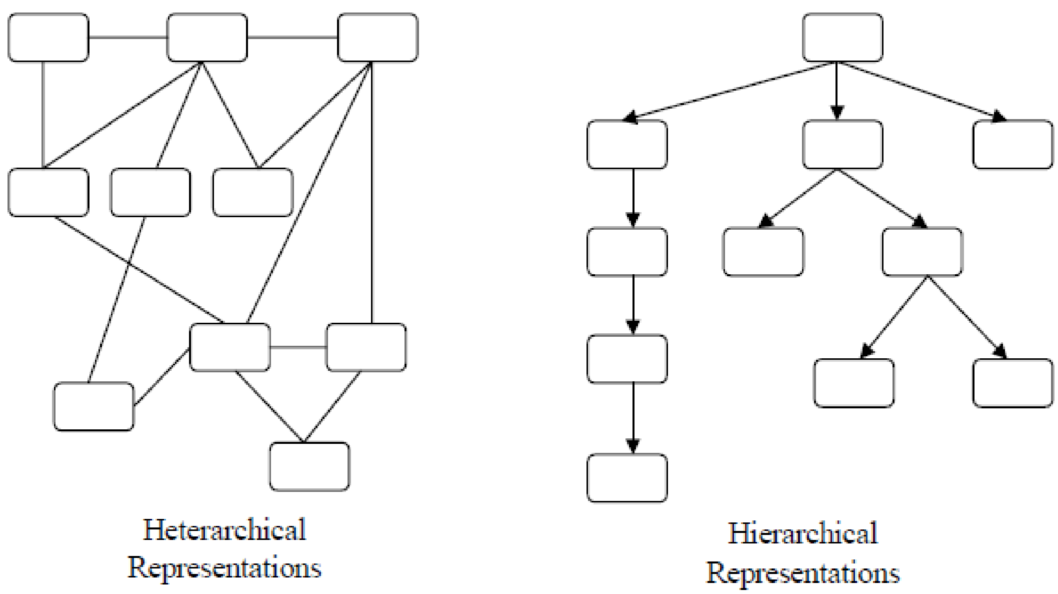


Figure 3.12: Heterarchical and hierarchical representations (Mistree, Smith and coauthors 1990)

Coupled decisions occur during collaborative design scenarios. One example will be the design of a product with coupling between design engineer and materials engineer. Such coupled decision support problems are applied in various problems like design of composite material structures (Karandikar and Mistree 1993).

3.3.4 The Compromise Decision Support Problem Construct

In the model-based realization of complex systems, we have to deal with models that are typically incomplete, inaccurate and not of equal fidelity. This brings into the design process different types of uncertainties associated with the system, the parameters considered, the models considered and the uncertainties due to their interactions (McDowell, Panchal and coauthors 2009). From the decision-based design perspective, the fundamental role of a human designer is to make decisions given the uncertainties associated. In this regard, we define robust design as design that is relatively insensitive to changes. This involves achieving a desired performance for the system while the sensitivity of the performance objectives with respect to the system variables are minimized (Ebro and Howard 2016). Thus, the designer's objective here is to find '*satisficing'* solutions that showcase good performance given the presence of uncertainties and not optimum solutions that are valid for narrow range of conditions while performing poorly when the conditions are changed slightly. The cDSP is proposed by Mistree and coauthors for robust design with multiple goals (Bras and Mistree 1993, Mistree, Hughes and coauthors 1993). The fundamental assumption here is that the models are not complete and accurate; opposed to the fundamental assumption in optimization where the models are complete and accurate, and the objective function can be modeled accurately so that solution obtained is implementable. Hence the cDSP construct is anchored in the robust design paradigm first proposed by Taguchi (Taguchi). Using the cDSP construct several solutions are identified by carrying out trade-offs among multiple conflicting goals. The obtained solutions are then evaluated by carrying out solution space exploration in order to identify the best solutions that satisfy the specific requirements identified. The cDSP is a hybrid formulation based on mathematical programming and goal programming. It also makes use of some new features. In goal programming (GP), the target values for each goal are defined and the emphasis is on achieving the target for each goal as close as possible (Ignizio 1976, Ignizio 1978, Ignizio 1983, Ignizio 1985). In cDSP, different weights are assigned to these goals and the compromised solutions obtained for different appropriate weights are explored. The obtained solutions are further evaluated by carrying out solution space exploration to identify solution regions that best satisfy the requirements identified. The generic formulation of cDSP is shown in Table 3.2.

The cDSP is similar to GP in that the multiple objectives are formulated as system goals, involving both system and deviation variables and that the deviation function is solely a function of the deviation variables. However, this is in contrast to traditional mathematical programming where multiple objectives are modeled as a weighted function of the system variables associated with the problem. From the traditional constrained optimization formulation, the cDSP retains the concept of system constraints. The cDSP places a special emphasis on the bounds of a system variable which is unlike traditional mathematical programming and GP. Contrary to GP formulation, the cDSP constraints and bounds are handled separately from system goals. In the cDSP, the feasible design space is defined by the set of system constraints and bounds. The aspiration space is defined by the set of system goals, see Figure 3.13. For feasibility the system constraints and bounds must be satisfied. A satisficing solution then is that feasible point which achieves the system goals as far as possible. The solution to this problem represents a tradeoff between that which is desired (as modeled by the aspiration space) and that which can be achieved (as modeled by the design space) (Mistree, Smith and coauthors 1993).

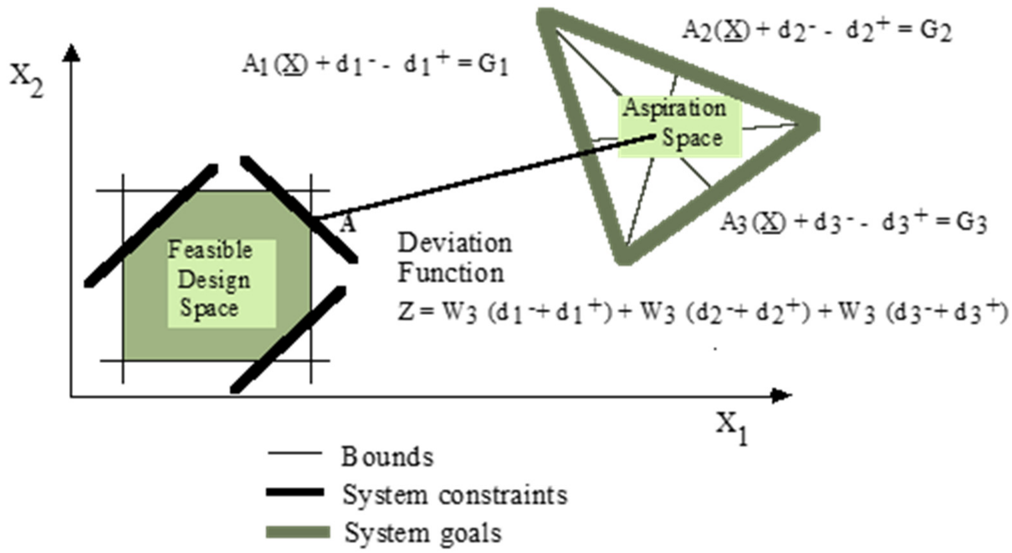


Figure 3.13: Graphical representation of a two-dimensional compromise DSP, Archimedean formulation (Mistree, Smith and coauthors 1993)

There are four keywords in the cDSP formulation. All the information that are available for the designer to formulate the cDSP so as to make effective decisions are captured by the "Given" keyword. In the cDSP, for each objective an achievement function A_i(X) is formulated and represents the achieved value of the i^{th} objective as a function of a set of system variables, X. The deviation variables, d_i^- and d_i^+ represents the extent to which the goal target G_i is underachieved or overachieved with respect to the value of A_i(X). The information regarding the system variables and the deviation variables are embodied in the "Find" keyword. The information regarding system constraints, variable bounds and system goals are captured by the "Satisfy" keyword to determine the feasible design space and the aspiration space. The "Minimize" keyword embodies the objective function which is formulated as a function of the deviation variables. The overall goal of the designer using the cDSP construct is to minimize the deviation function so that the target values specified for the system goals are attained as closely as possible by identifying the combination of design/system variables that best satisfy the conflicting requirements. The formulation of the deviation function is done in two ways – a) as a Preemptive (lexicographic) formulation or b) as an Archimedean formulation - based on the manner in which importance is assigned to satisficing the goals. The most general form of the deviation function for "m" goals in the Archimedean formulation is:

$$\mathbf{Z} = \sum_{i=1}^{m} W_i(d_i^- + d_i^+); \ \sum_{i=1}^{m} W_i = 1 \qquad \textbf{Equation 3.4}$$

where the weights W_i reflect the level of desire to achieve each of the goals.

The details regarding formulating the cDSP and the associated rules are provided by Bras and Mistree (Bras and Mistree 1993); and Mistree, Hughes and Bras (Mistree, Hughes and coauthors 1993).

Table 3.2: The cDSP formulation (Mistree, Hughes and coauthors 1993)

GIVEN
An alternative to be improved, domain dependent assumptions
The system parameters:
n number of system variables,
q inequality constraints,
$p + q$ number of system constraints,
m number of system goals,
$g_i(\mathbf{X})$ system constrain functions

$f_k(d_i)$ function of deviation variables to be minimized at priority level k for the preemptive case

FIND

System variables: The values of the independent *system* variables.

X_i $i = 1, 2, \ldots, n$ (They describe the physical attributes of an artifact.)

Deviation variables: The values of the deviation variables.

d_i^-, d_i^+ $i = 1, 2, \ldots, m$ (They indicate the extent to which the goals are achieved)

SATISFY

System constraints: These must be satisfied for the solution to be feasible (linear, non-linear)

$g_i(\mathbf{X}) = 0; i = 1 \ldots. p$

$g_i(\mathbf{X}) \geq 0; i = p+1 \ldots.. p+q$

System goals: These need to achieve a specified target value as far as possible (linear, non-linear)

$A_i(X) + d_i^- - d_i^+ = G_i; \; i = 1 \ldots m$

Bounds: Lower and upper limits on the system variables.

$X_i^{min} \leq X_i \leq X_i^{max}; i = 1 \ldots n$

$d_i^-, d_i^+ \geq 0, d_i^- * d_i^+ = 0; i = 1 \ldots m$

MINIMIZE

A deviation function: A function that quantifies the deviation of the system performance from that implied by the set of goals and their associated priority levels or relative weights.

Case a: Preemptive formulation (lexicographic minimum)

$$\mathbf{Z} = [f_1(d_i^-, d_i^+), \dots\dots, f_k(d_i^-, d_i^+)]$$

Case b: Archimedean

$$\mathbf{Z} = \sum_{i=1}^{m} W_i(d_i^- + d_i^+); \sum_{i=1}^{m} W_i = 1$$

The cDSP can be reformulated to carry out selection decisions also. Hence it is the principal mathematical DSPT formulation (Bascaran, Bannerot and coauthors 1989). The cDSP is used in this dissertation and is the foundational mathematical construct to provide design decision support in identifying satisficing design solutions. In the next section, we discuss the philosophies of an "optimizer" and that of a "satisficer" (the designer's philosophy in this dissertation).

3.3.5 Optimizing vs Satisficing Philosophy in this Dissertation

We believe there are two schools of thought for modeling design decisions – i) that of an optimizer and ii) that of a satisficer. The focus in this dissertation is to share the observations with respect to modeling such decisions from the perspective of a satisficer and not that of an optimizer. The difference here is as follows. Consider a haystack with a number of needles hidden in it. An optimizer will continue searching the haystack until the last needle has been found. A satisficer, on the other hand, stops when he/she has found enough needles to proceed to the next step. We capture the perspective of the satisficer by using the compromise DSP. Our intention in solving the compromise DSP is to satisfice a set of goals. In our formulation the satisficing of goals solves the mathematical problem at hand; optimizing the numerical value of a goal function is not an issue. Let's discuss this in detail from the perspective of integrated materials and product design.

For complex systems design problems like the problem discussed in this dissertation on the integrated realization of materials, products and associated manufacturing processes, the following characteristics can be observed about the design problem and the information available (McDowell, Panchal and coauthors 2009):

- Design problem could be loosely defined and open;
- Design information comes from different sources and disciplines;
- There will be multi-functional requirements in design and they are governed by multiple measures of merits and performances;
- All information required for design may not be available and thus the designer may have to work with incomplete, inaccurate and infidel models and information;
- Design information may be hard (quantifiable) and some may be soft (qualitative).

Thus, such complex design problems are not characterized by utopian single point unique solutions. The solutions due to these characteristics of complex design problems are less than optimal and therefore seek for satisficing solutions. Simon (Simon 1996)coined the term "satisficing" to describe solutions that are "good enough to be acceptable but are neither exact nor optimal”. Designer/decision-maker has two choices while formulating and solving such complex design problems:

- Solve the exact problem approximately, and
- Solve an approximation of the problem exactly.

In the first choice, the designer seeks an optimal solution using algorithms that are based on relatively simple models, by means of which an exact optimal solution can be found provided the assumptions on which the model is based can be satisfied exactly. However, only rarely does a solution that is optimal for a simple model is optimal in reality.

In the second choice, an approximate algorithm or heuristic, based on relatively complex model that can capture the reality more closely than a simple model is used. The solutions thus obtained using an approximate algorithm are satisficing. The sequential linear programming approach is used for solving cDSP formulations because it has the highest potential for being used to develop a single algorithm for solving a range of DSPs in engineering design, as described by Mistree and co-authors (Mistree, Hughes and coauthors 1993). Refinements to Sequential Linear Programming (SLIP) and its Multi-Level version (SLIPML) have resulted in the Adaptive Linear Programming (ALP) algorithm. The ALP algorithm with its multilevel, multigoal feature is incorporated in DSIDES (Decision Support In the Design of Engineering Systems), a tailored computational infrastructure for formulating, solving and analyzing Decision Support Problems (Mistree and Kamal 1985, Reddy, Smith and coauthors 1996). Mistree and co-authors believe three important features contribute to the success of the ALP algorithm, namely (Mistree, Hughes and coauthors 1993),

- the use of second-order terms in linearization;

- the normalization of the constraints and goals and their transformation into generally well-behaved convex functions in the region of interest;
- an "intelligent" constraint suppression and accumulation scheme.

The approach followed in this dissertation is based on the ***satisficing view of design*** embodied in the Decision Support Problem technique proposed by Mistree and co-authors.

3.3.6 Use of DBD and cDSP in this dissertation – Architecting Robust Materials, Product and Manufacturing Process Networks

The primary goal in this dissertation is to develop a systems-based design architecture for the integrated realization of materials, products and processes and contribute the knowledge generated to advance the field of systems-based materials design. We adopt a decision-centric approach in this dissertation because our end goal is to carry out decision-based meta-design and design of complex material and product systems. In this dissertation, meta-design involves partitioning the complex material-product system based on functions into system-level function structures, partitioning the design process into decisions, and planning the sequence in which decisions are most appropriately made, following the procedures of DBD proposed by (Mistree, Smith and coauthors 1990). A decision-centric view accommodates easily the other views of design processes like model-centric and tool-centric views, which is an added advantage. It also supports domain-independent representation of design processes. Decision-based design is described as the seed that glues together the heretofore disparate engineering disciplines as well as economics, marketing, business, operations research, probability theory, optimization and others (Hazelrigg 1998). Hazelrigg therefore describes DBD as omnidisciplinary. In the case of integrated materials and product design, we are dealing with multiple disciplines and a network of decisions to develop a product. The information flowing through the process chain serves as the source of the knowledge about the product which is captured in DBD.

In this dissertation, ***decision-based design is used as a philosophical foundation for the systems-based design architecture for the integrated design of materials, products and associated manufacturing processes***. Hence, the focus in this dissertation is on making decisions that ***supports architecting networked material-product systems***. The second, third and fourth research questions (**RQ 2, 3 and 4**) addressed in the dissertation are answered from a decision-based design perspective. The design of design processes (***designing design methods in this dissertation***), hence, is equivalent to the configuration of **networked design decisions** – related to both materials/products and design processes. The **idea of robustness** in the network is key here and is reviewed in next section and will be discussed in detail in Chapter 7. This leads to the key outcome in this dissertation - ***Architecting Robust Materials, Product and Manufacturing Process Networks***.

3.4 Robust Design of Materials and Products

In the design of complex networked systems, a very important factor that needs to be taken into account is uncertainty. As discussed in previous sections, in the model-based realization of complex systems designers have to deal with models that are typically incomplete, inaccurate and not of equal fidelity leading into uncertainty. The presence of uncertainty may lead to wrong decisions during the design of such networked systems.

Now, the perfect approach will be to eliminate or mitigate this uncertainty. However, eliminating the uncertainty present in a system and its models is practically infeasible, time consuming and expensive. To address this challenge, a robust design paradigm was proposed where the focus is to **design systems to be insensitive to these uncertainties without removing their sources**. In this section, we carry out a review of robust design and investigate the progress made and their limitations in achieving robustness in design.

3.4.1 Uncertainty Classification

Uncertainty classification was discussed in brief in Chapter 1. In this section, we look at it in much greater details. There are different views to the types of uncertainty that is present in engineering systems involving materials and products. From the ICME perspective the types of uncertainties are classified based on experimental (extrinsic) and modeling perspectives (intrinsic) (Horstemeyer 2012), see Figure 3.14. The extrinsic uncertainty includes errors due to experimental setup, sensors, surroundings etc. Intrinsic uncertainty includes uncertainty due to modeling (model related) and parametric (due to parameters involved in model).

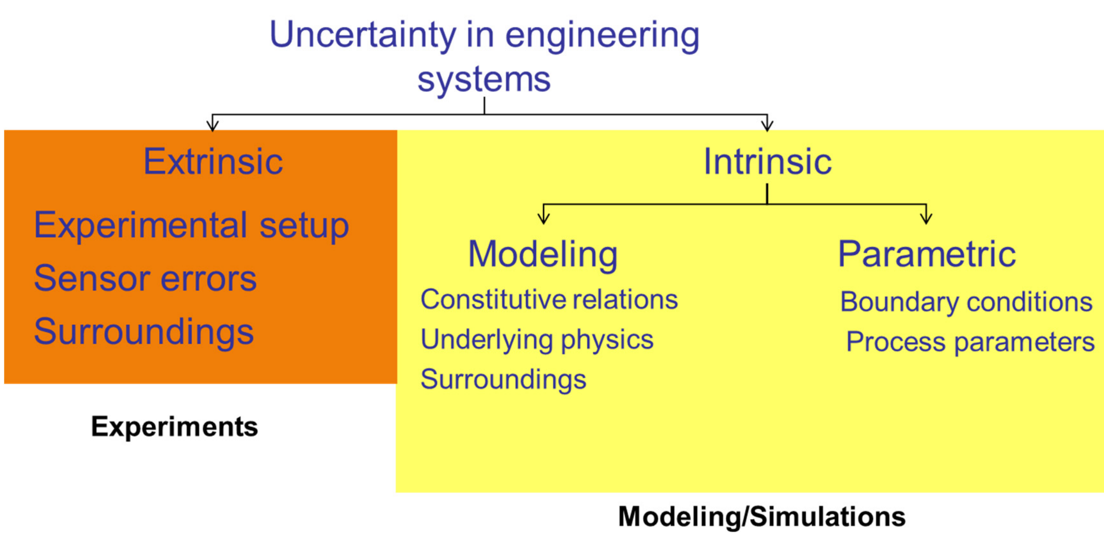


Figure 3.14: Types of uncertainty from ICME perspective (Horstemeyer 2012)

The different sources of uncertainty that arises in multi-scale modeling hierarchy both at a given scale and scales linking different algorithms is summarized by McDowell, see Figure 3.15. McDowell (McDowell 2018) observes that quantifying uncertainty in schemes for linking models at different length and time scale is still an immature field and formal mathematical approaches for doing this are largely undeveloped. The uncertainty in the coupling of models across length and time scales can compound different other sources of uncertainty that are related to material model or material hierarchy at each scale, as summarized by McDowell in Figure 3.15.

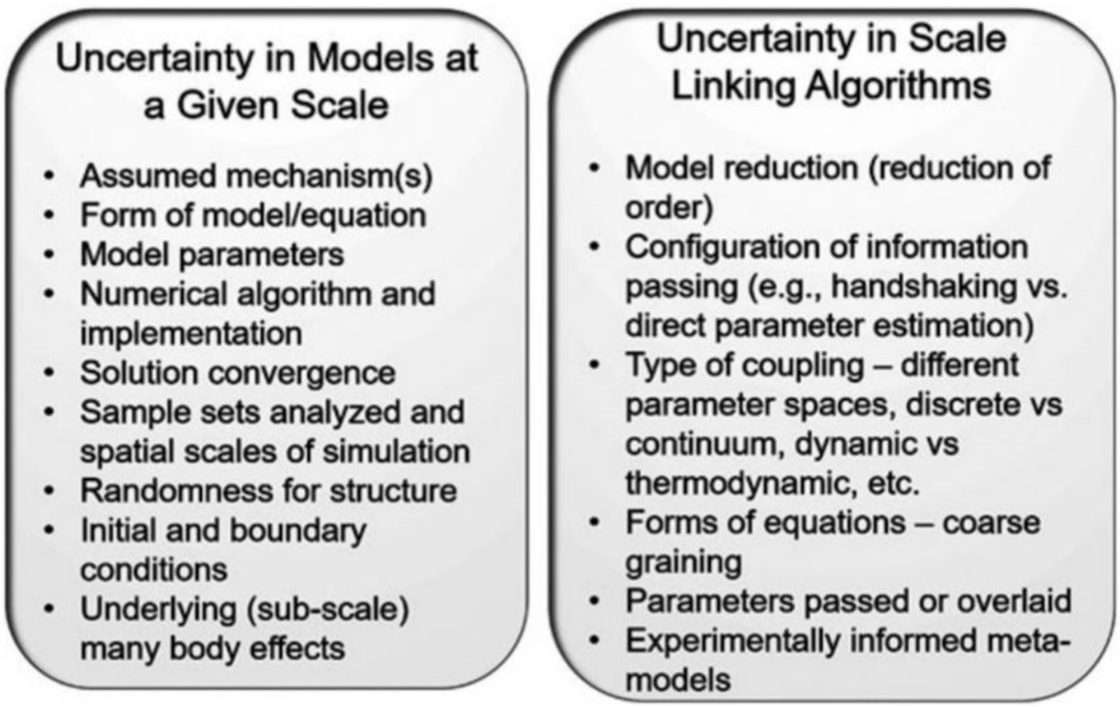


Figure 3.15: Sources of uncertainty in models at a given scale in material structure hierarchy (left) and in scale linking or scale transition algorithms (right) (McDowell 2018)

Since it's impractical to quantify uncertainty accurately in such multi-scale models and systems, the recommendation made for simulation-assisted materials design is to focus on understanding the sensitivity of material properties to material microstructure and to capture dominant mechanisms and transitions that affect material responses or properties instead of focusing on accurately predict mean properties at higher scales. This is the philosophy of managing uncertainty. Sensitivity analysis of responses is important because of several reasons (McDowell 2018):

- It is challenging to isolate response sensitivity experimentally at specific scales in the material hierarchy,
- The identification of key design variables across material structure hierarchy is possible via sensitivity analysis, and
- Core to the concept of robust design is the sensitivity of process-structure and structure-property relations, where the focus is to explore a range of solutions that meet conflicting response requirements and identify satisficing design solution that are relatively insensitive to uncertainty (McDowell, Panchal and coauthors 2009).

Uncertainty Classification Adopted in this Dissertation

In this dissertation, we adopt a more general classification of uncertainty. We are not focused on the uncertainty due to experiments in this dissertation. Uncertainty could be either *Aleatory* (irreducible) or *Epistemic* (reducible), depending on their causes. Improving the measurements and/or model formulation and/or increasing the accuracy are ways to diminish Epistemic uncertainty. Aleatory uncertainty, however is inherent in the physical system and can only be quantified in a statistical sense. Extending the classification by Isukapalli and coauthors (Isukapalli, Roy and coauthors 1998), the types of uncertainty in simulation-based integrated design of material, product and processes are classified as (Choi, Austin and coauthors 2005, McDowell, Panchal and coauthors 2009), see Figure 3.16:

- *Natural Uncertainty* (NU): uncertainty due to the inherent randomness or unpredictability of a physical system; Aleatory in nature.
- *Model Parameter Uncertainty* (MPU): incomplete knowledge of model parameters/inputs due to insufficient or inaccurate data; reducible by sufficient data or accurate measurements; uncertainty in design variables or control factors.
- *Model Structure Uncertainty* (MSU): uncertain model formulation due to approximations in a model; reducible by improving model formulation; uncertainty in function relationship between control/noise and response.
- *Propagated Uncertainty* (PU): uncertainty compounded by the combination of all the above three types of uncertainty in a chain of models that are connected through input output relations; interdependent responses and shared control/noise factors as one model interacts with another (Allen, Seepersad and coauthors 2006).

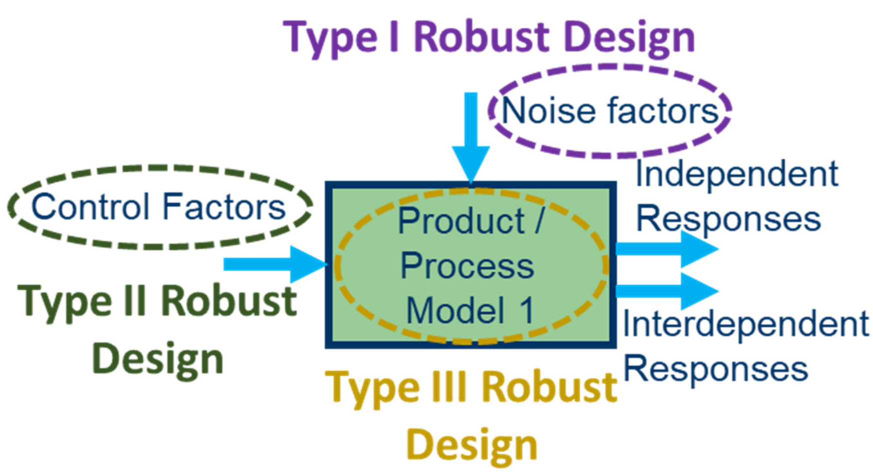


Figure 3.16: A P-diagram showing the input and response in a design product or process. Robust design is classified based on the source of variability.

All these types of uncertainty can exist in a system and it is very difficult to differentiate out which is dominant among them. It is not possible to eliminate all uncertainty. The possibility here is to manage them. The focus therefore is to manage uncertainty by designing the system to be insensitive to the sources without reducing or eliminating them. This is done by exploring the solution space and studying the sensitivity of responses to variations in noise, control factors and models themselves and understanding the tradeoffs required with various compromises; this is called robust design (Chen, Allen and coauthors 1996, Choi, Austin and coauthors 2005, Murphy, Tsui and coauthors 2005, Allen, Seepersad and coauthors 2006, Choi, McDowell and coauthors 2008, Nellippallil, Allen and coauthors 2017). There are several practical implications with this approach. Robust solutions are not focused on extensive optimization searches at individual levels and do not necessarily involve large number of iterations (McDowell and Olson 2008). The practical interest here is for ranged set of solutions that showcase good performance under variability rather than single-point solutions that are valid for narrow range of conditions, while performing poorly when the conditions are changed slightly. The human designer plays the role of an interpreter of value of information in this approach. Concepts and mathematical constructs from information economics (Howard 1966, Panchal, Paredis and coauthors 2006, Sinha, Bera and coauthors 2013) are used to manage uncertainty by studying the value of information for cost/benefit tradeoff to make design decisions in the presence of uncertainty. In next sections, we review the robust design types and methods, frameworks that allow

3.4.2 Robust Design Type I – Taguchi Method

In robust design (RD), the quality of products and processes are improved by reducing their sensitivity to variations without eliminating the sources (Taguchi 1986, Taguchi and Clausing 1990, Nair, Abraham and coauthors 1992, Tsui 1992). The robust design principles and methods are founded on the philosophy of Genichi Taguchi (Taguchi 1986). Three categories of information interact with the system model in robust design (McDowell, Panchal and coauthors 2009): i) control factors, also known as design variables are parameters that the designer adjusts to move towards a desired product, ii) noise factors, are exogenous parameters that affect the performance of product/process but cannot be controlled by the designer, iii) responses are performance measures for the product or process. These categories of information are captured in Figure 3.16.

As briefly described in Chapter 1, Type I robust design is to identify control factor (design variable) values that satisfy a set of performance requirement despite variations in noise factors. Type I robust design was first proposed by Genichi Taguchi (Taguchi , Taguchi 1986, Taguchi and Clausing 1990, Taguchi 1993). Taguchi's robust design principles and approach are focused on reducing the effects of variability without removing its sources and were foundational for product and process design in Japanese industries. Taguchi's robust design approach uses experimental design (orthogonal arrays), quality loss function and signal-to-noise (S/N) ratio. Taguchi proposed a Quality Loss Function and the objective here is to quantify the loss that is imparted by the product to the society from the time the product is shipped. In Taguchi's approach the quality of the product is maximum when the loss imparted is minimum. Taguchi's Quality Loss Function is specified as:

$$L = k(y - T)^2 \qquad \textbf{Equation 3.5}$$

where, L is the loss in dollars, k is the cost coefficient, y is the value of quality characteristic and T is the target value. The Quality Loss Function is illustrated in Figure 3.17.

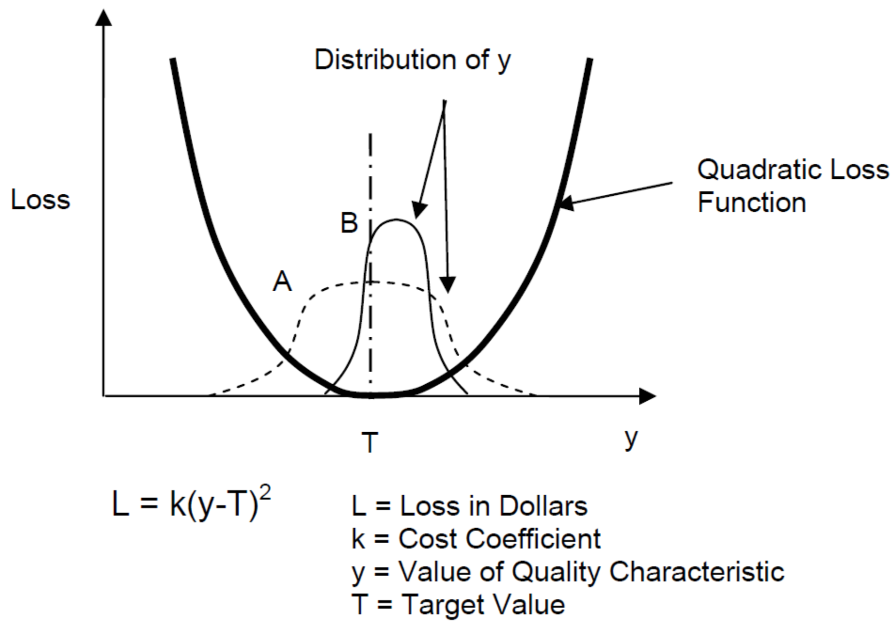


Figure 3.17: Taguchi's Quality Loss Function (adopted from (Choi 2005)

In Figure 3.17, the two probability distributions A and B denote product outputs. The average loss of quality of B is smaller than that of A. This is predicted based on the deviation of the average value of y from the target, T and the mean squared deviation of y around its own mean, as described by Phadke (Phadke 1995). Taguchi proposes three stages for engineering design and asserts that all the three stages are important for achieving robust design. The three stages are: system design, parameter design, and tolerance design. Taguchi specifically highlights the importance of parameter design stage to identify desirable parameters so as to minimize quality loss. The parameter design stage in Taguchi's robust design approach starts with clearly classifying parameters into control factors and noise factors. Control factors are design parameters that can be controlled while noise factors are uncontrollable or expensive to control. An orthogonal array as the experimental design is recommended. The control factors reside in an orthogonal array and the noise factors in an outer array. All combinations of control and noise factors are recorded in the experiment. Nominal responses are evaluated by identifying an average response by varying the noise factors for fixed control factor conditions. Signal-to-noise ratio proposed by Taguchi captures the sensitivity of responses to variations in noise factors. Based on the mean response and the signal-to-noise ratio, the best combination level of each control factor is selected by designers.

The approach by Taguchi are widely accepted in industry and academia. Many industrial problems are addressed from the perspective of robust design using Taguchi's approach. Though Type I robust design principles as proposed by Taguchi are advocated widely, his statistical techniques that includes orthogonal arrays and signal-to-noise ratio are widely criticized. Many researchers (Box 1988, Vining and Myers 1990, Welch, Yu and coauthors 1990, Shoemaker, Tsui and coauthors 1991, Tsui 1992, Parkinson, Sorensen and coauthors 1993, Sundaresan, Ishii and coauthors 1995, Chen, Allen and coauthors 1996) have actively worked on improving the statistical techniques in robust design and thus have over the years developed mathematical constructs that bring in robust design into a systematic framework. We discuss some of the criticisms about the Taguchi approach next.

Criticisms on the Taguchi Approach

Taguchi's experimental design and orthogonal arrays are widely criticized as computationally costly and inefficient as the approach requires large number of experiments which are mostly unnecessary. There have been efforts to minimize the computational burden associated with this approach. Welch and coauthors (Welch, Yu and coauthors 1990) and Shoemaker and coauthors (Shoemaker, Tsui and coauthors 1991) address this issue and presents a combined single array for both control and noise factors and thereby reducing the computational cost associated. Also, approximations of the mean and variance using response surface method was developed by Vining and Myer (Vining and Myers 1990) and Shoemaker and co-authors (Shoemaker, Tsui and coauthors 1991).

The second major criticism on Taguchi's robust design is on the signal-to-noise ratio. This is criticized because there is high chance for designers to miss useful information since the S/N ratio includes both mean and variance in its formulation. Since the effects on the mean are confounded with the effects on the variance, then the true factors affecting the mean cannot be separated. An alternative proposed here by statisticians (Box 1988, Vining and Myers 1990, Tsui 1992) is to model both the mean and variance directly instead of combining them into one signal-to-noise ratio function.

Another criticism is regarding the usage of Taguchi's robust design approach for only unconstrained problem. Parkinson and co-authors (Parkinson, Sorensen and coauthors 1993) address this issue by proposing "feasibility robustness" for design. Feasibility robustness is considered by using first order Taylor series expansion to calculate the amount of variation that needs to be considered in constraint function for variations in control and noise factors.

Even though the Taguchi method has been criticized and many researchers have developed alternatives for robust design, the philosophy of robust design by Taguchi has found lot of applications in industry leading to successful outcomes. Achieving design insensitive to the surroundings (noises) is a significant achievement by Taguchi's robust design approach. Taguchi's approach is invalid in situations where noise factors cannot be quantified as numeric parameters – a situation that can happen in integrated materials and product design.

3.4.3 Suh's Axiomatic Design and Shannon's Information Theory in Robust Design

Suh's Axiomatic Design facilitates robust design at the conceptual design phase, unlike Taguchi's robust design that is employed at embodiment or detail design phase. Suh's Axiomatic Design is discussed in detail in Section 3.2.2. The two axioms by Suh, 'The Independence Axiom' and 'The Information Axiom' can be used to support robust design. As per Suh, a good design is one that satisfies both the axioms. Three types of designs are possible: a) uncoupled design, b) decoupled design and c) coupled design following the design equation matrix by Suh. The corresponding design equations following $\{\mathrm{FR}\} = [\mathrm{A}]\{\mathrm{DP}\}$ (Equation 3.1) are shown below.

$$\begin{bmatrix} FR_1 \\ FR_2 \\ FR_3 \end{bmatrix} = \begin{bmatrix} X & 0 & 0 \\ 0 & X & 0 \\ 0 & 0 & X \end{bmatrix} \begin{bmatrix} DP_1 \\ DP_2 \\ DP_3 \end{bmatrix} \text{ Uncoupled Design} \qquad \textbf{Equation 3.6}$$

$$\begin{bmatrix} FR_1 \\ FR_2 \\ FR_3 \end{bmatrix} = \begin{bmatrix} X & 0 & 0 \\ X & X & 0 \\ X & X & X \end{bmatrix} \begin{bmatrix} DP_1 \\ DP_2 \\ DP_3 \end{bmatrix} \text{ Decoupled Design} \qquad \textbf{Equation 3.7}$$

$$\begin{bmatrix} FR_1 \\ FR_2 \\ FR_3 \end{bmatrix} = \begin{bmatrix} X & X & X \\ X & X & X \\ X & X & X \end{bmatrix} \begin{bmatrix} DP_1 \\ DP_2 \\ DP_3 \end{bmatrix} \text{ Coupled Design} \qquad \textbf{Equation 3.8}$$

In Suh's axiomatic design, the uncoupled design is always considered the best design because it satisfies the independence axiom. The decoupled design follows the uncoupled design in terms of preference because it satisfies independence axiom by sequentially selecting design parameter values thereby ensuring that the functional requirements are independent with each other with respect to the design parameters. However, the coupled design is not acceptable as per Suh's axiomatic design as it does not satisfy the independence axiom. Suh's suggestion to designers is to use the independence axiom first to select the best functional configuration of the system among all available design candidates.

Once the independence axiom is followed to select the system's functional configuration, the next step is to follow the information axiom and select design parameters so as to minimize information content. The axiom may look simple, and something that all designers understand – "that is keep everything simple". However, this has significant meanings in engineering design. After finding multiple designs using Axiom 1, the best one can be chosen based on Axiom 2. The best design has minimum information content that is usually quantified by the probability of success. Now how can we quantitatively measure information? Usually information is related to the complexity. Then how is it possible to measure complexity? This leads us to definition of information content and Shannon's Information Theory (Shannon 1949, Shannon and Weaver 1963, Shannon 1997).

In 1948, Claude Shannon published a paper called "A Mathematical Theory of Communication" (Shannon 1948). James V Stone (Stone 2015) reports "*This paper heralded a transformation in our understanding of information. Before Shannon's paper,* *information had been viewed as a kind of poorly defined miasmic fluid. But after Shannon's paper, it became apparent that information is a well-defined and, above all, measurable quantity.*"

The key point in Shannon's information is that ***Shannon information is a measure of surprise***. One way to express this is to define the amount of surprise of an outcome value x to be the 1/(the probability of x) or $1/p(x)$, so that the amount of surprise associated with the outcome value x increases as the probability of x decreases. Since information associated with a set of outcomes is obtained by adding the information of individual outcomes (Shannon's additivity condition), Shannon define surprise as the logarithm of $1/p(x)$, see Figure 3.18.

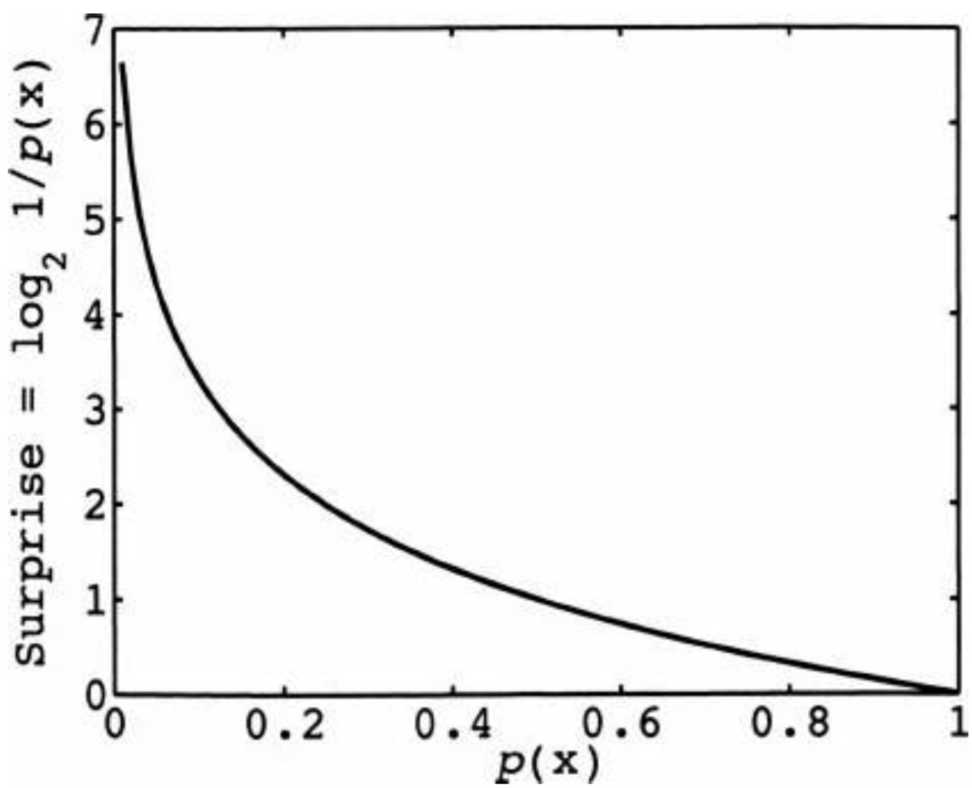


Figure 3.18: Shannon information as surprise. Values of *x* that are less probable have larger values of surprise. (Stone 2015)

Using logarithms to the base 2, the Shannon information of a particular outcome measured in bits is written as

$$h(x) = \log_2 \frac{1}{p(x)} \text{ bits}$$ **Equation 3.9**

where h stands for Shannon information. The average surprise is defined by the probability distribution of a random variable. The average surprise of a variable *X* which has probability distribution *p*(*X*) is called the entropy of *p*(*X*), represented as *H*(*X*).

Now how does Shannon's information relate to Suh's axioms and robust design?

Let us look at a case of uniform probability distribution of a design range. Let I be the information content measured in terms of entropy. The above equation can be rewritten as

$$I = \log_2 \frac{System\ Range}{Common\ Range}$$ **Equation 3.10**

In Figure 3.19, the desirable system range for meeting functional requirements is the design range, the system range defines the deviation of functional requirement of a candidate, and common range is the overlap between design range and system range. Now, the information content (*I*) is minimum when the probability of success is maximum. We achieve maximum probability of success when the common range is maximized and/or when the system range is minimized. Therefore, in the perspective of Suh's information axiom, the designer should select a design candidate that has minimum information content based on the calculation of probability of success.

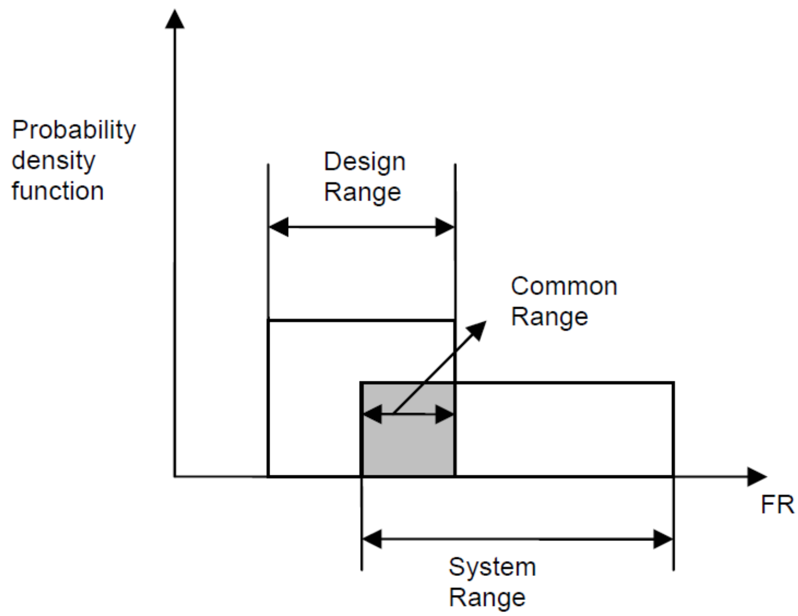


Figure 3.19: Design, system, and common range for calculating probability of success (Choi 2005)

The philosophies in Taguchi's approach and Suh's axiomatic design on robust design are different. This can be illustrated using Figure 3.20.

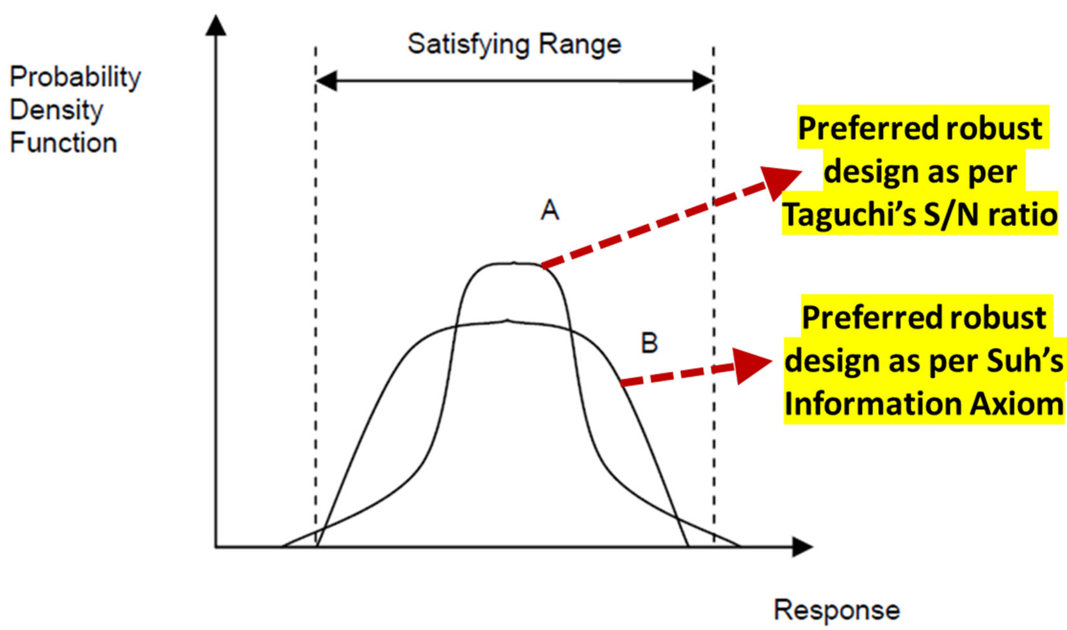


Figure 3.20: Robust designs from the perspective of Taguchi and Suh

In Taguchi's method, a designer will select design A in Figure 3.20 as design A results in minimum loss and maximum quality measured in terms of the signal to noise ratio. However, in Suh's axiomatic design, a designer will prefer design B as it results in minimizing of information content thereby satisfying the information axiom. Now, this cannot let us conclude that one method is better than the other. The selection of these approaches should depend on the problem type and the requirement of the designer. The axiomatic design is preferred if the boundary of the satisfying range is strict. However, if the goal of the designer is to hit a target value and minimize the variation with respect to noise factors, then Taguchi method has to be preferred. One remark that can be made based on this discussion is that the Taguchi's approach is clearly a parametric design method meant for detail design phase while Suh's axiomatic design is more like a decision-making tool that is more suited for the conceptual design stage.

One major drawback of Suh's axiomatic design for robust design is that it lacks a procedure to analyze the sensitivity of performance due to variations associated with the factors – control and noise factors. The information axiom can capture designer's specific preference but is not a systematic procedure or method to be adopted for robust design. Also similar to Taguchi method, Suh's axiomatic design cannot be applied to systems where we have unparameterizable variability - a situation that can happen in integrated materials and product design. Next, we discuss the robust concept exploration method for Type I and II robust design and the approaches followed in decision-based design (DBD) in accounting for robustness and managing uncertainty in the realization of complex systems.

3.4.4 Robust Design Type II – The Robust Concept Exploration Method (RCEM)

The focus of most of work carried out on robust design is on the detailed design stage. The assumption in most of the work is that a preliminary design has already been established with concrete layout and design specifications which is mostly not the case. Some researchers have focused on infusing robustness at early stages of design especially at the conceptual design stage. The decisions usually made at this stage has long lasting and profound impact on the final product performance and quality. Now while exploring concepts designers are required to work with continuous design spaces. The efficacy of Taguchi's robust design method and Suh's axiomatic design is limited mostly to discrete design spaces or when we have a number of discrete design alternatives (for Suh's axiomatic design) and cannot be used to actively search a continuous design space. Along with this requirement, there is also need for achieving designs insensitive to variations in not just the noise factors, but also the control factors. To address these needs, Chen and co-authors propose Type II robust design along with Type I for managing variations in control and noise factors (Chen, Allen and coauthors 1996) and propose the Robust Concept Exploration Method (RCEM) to systematically explore robust solutions insensitive to variations in control and noise factors at the early stages of design (Chen, Allen and coauthors 1997).

Chen and co-authors categorize problems associated with simultaneously minimizing performance variations and bringing the mean on target based on their source of variation as (Chen, Allen and coauthors 1996):

- Type I – minimizing variations in performance caused by variations in noise factors (uncontrollable parameters)

- Type II – minimizing variations in performance caused by variations in control factors (design variables).

The schematic of the concepts behind the two types of robust design is provided by Chen and co-authors in Figure 3.21.

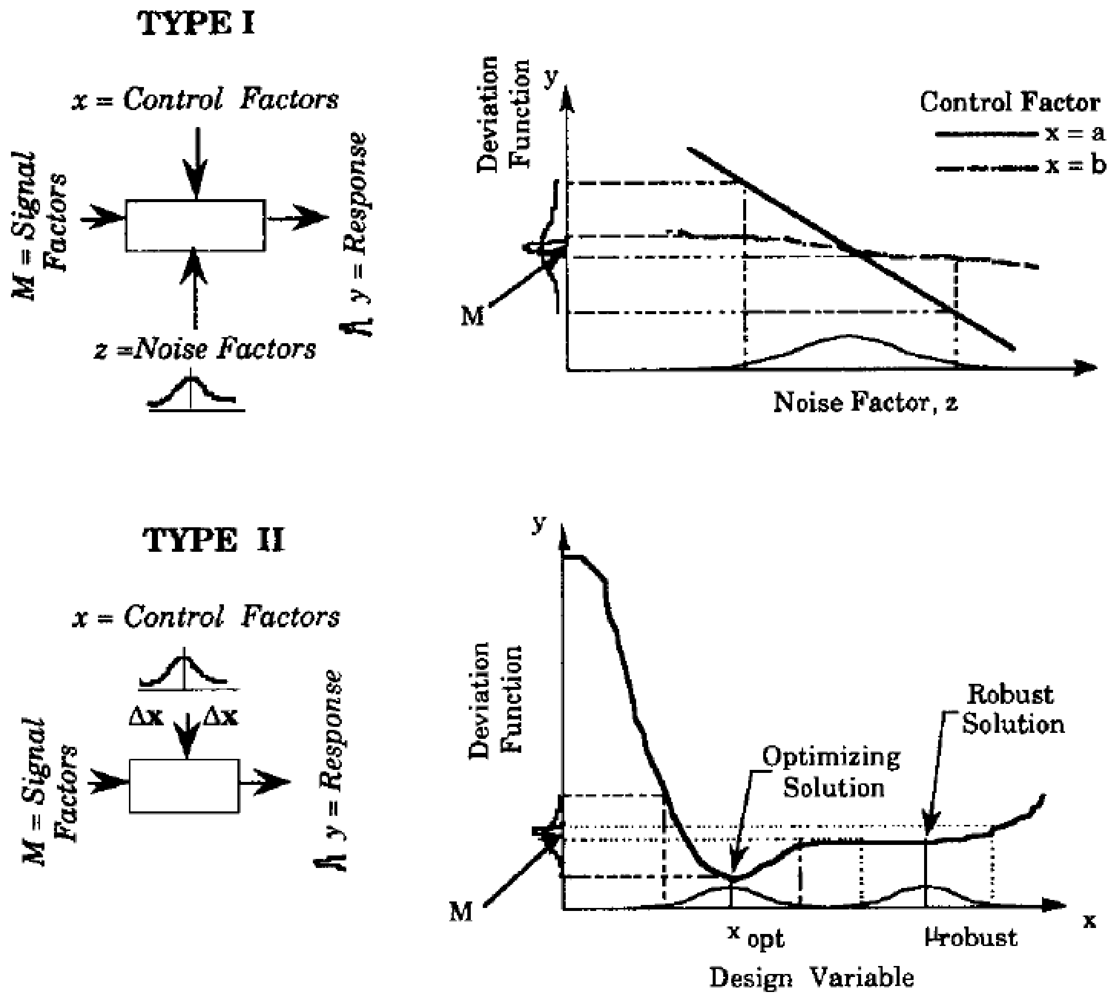


Figure 3.21: Robust design for variations in noise factors (Type I) and control factors (Type II) (Chen, Allen and coauthors 1996)

In Figure 3.21, right hand side Chen and co-authors show the variation that happens in the performance function when there is variation in noise factors and control factors. In

Type II robust design, we seek solutions in the nearly flat region where the variation in system performance is less for variation in control factors rather than the optimal solution point where even for a small variation in control factor, the system performance degrades significantly.

Chen and co-authors propose Robust Concept Exploration Method (RCEM) which is a domain-independent, systematic, method that integrates statistical experimentation, approximate models (metamodels/response surface models), multiobjective decisions and multidisciplinary analyses, to carry out robust design at early stages of design. The computing of RCEM is shown in Figure 3.22.

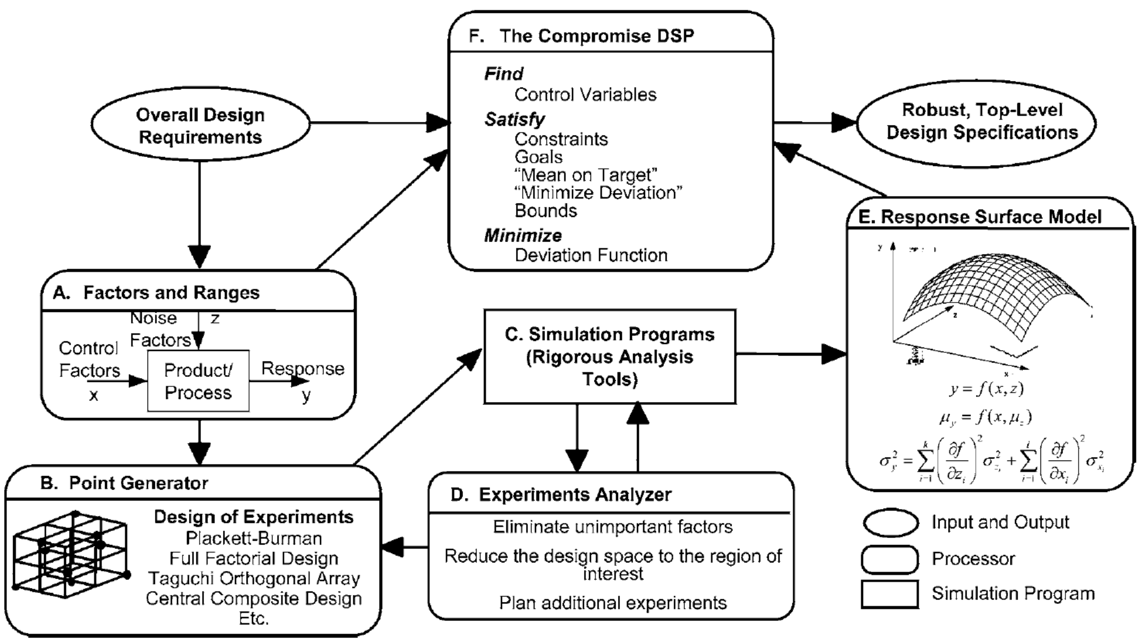


Figure 3.22: Computational infrastructure of RCEM developed by Chen and co-authors (Chen, Allen and coauthors 1997). In this figure, a modified version of the RCEM is shown; adopted from (Allen, Seepersad and coauthors 2006).

In the RCEM, design parameters are categorized as noise factors and control factors in Processor A – Factors and Ranges. Simulation experiments are designed in Processor B – Point Generator to develop response surface models that capture the problem specifications. Using Simulation Program C, experiments that are designed are carried out, results are generated which are further analyzed and screened in Processor D – Experimental Analyzer. The unimportant factors are removed based on statistical analysis. The stages C and D are repeated sequentially until the best set of data is generated to build the response surface model (RCEM uses Response Surface Method to develop meta models). The response surface models are build using Processor E. In Processor F, the cDSP construct is used to formulate the design problem and find ranged set of design specifications that are robust against the variations associated with noise and control factors. The RCEM uses specific goals in cDSP formulation that are meant to bring the mean on performance target and minimize performance variation. The RCEM has been used for variety of applications to design robust systems. This includes structural problem and design of a solar powered irrigation system (Chen, Allen and coauthors 1996), a High Speed Civil Transport (Chen, Tsui and coauthors 1995), a General Aviation Aircraft (Chen, Allen and coauthors 1996), product platforms (Simpson, Chen and coauthors 1996), and other applications (e.g., (Chen, Garimella and coauthors 2001)). The RCEM finds applications in most common class of materials and product design problems. Using RCEM designers can formulate design problems to find ranges of material structure and processing paths that satisfy specific material property or performance requirements. A schematic illustrating the application of RCEM in materials design is shown in Figure 3.23

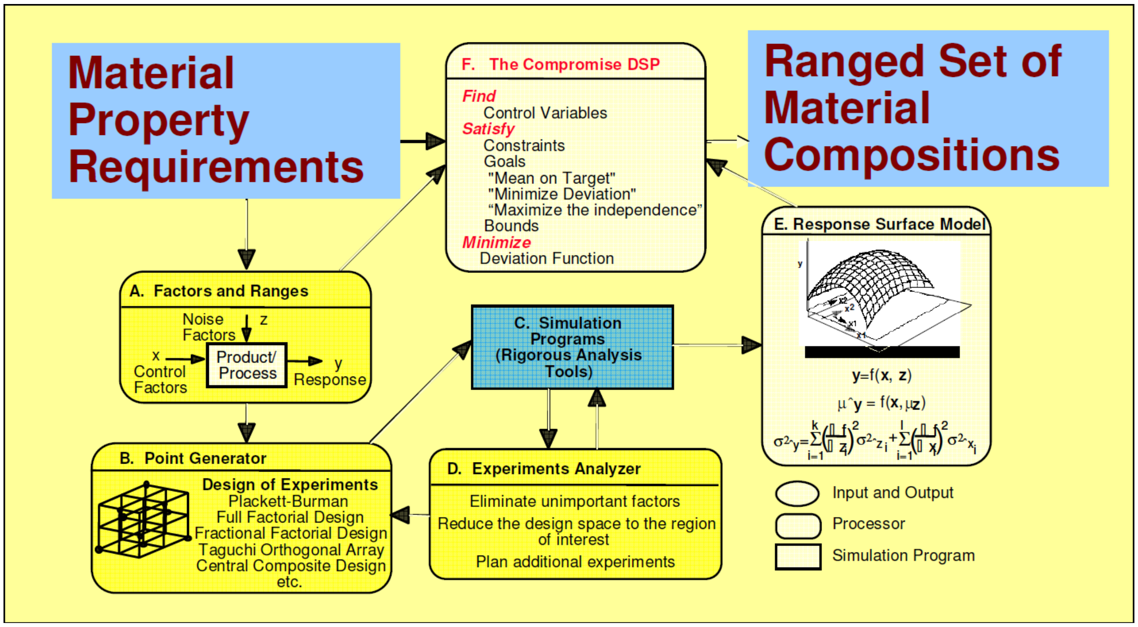


Figure 3.23: Schematic showing application of RCEM to materials design problems; adopted from (Messer 2008).

RCEM therefore offers major advantages over other robust design approaches. It can be used to find ranged set of robust design specification especially at early stages of design like the conceptual design stage. It also offers the ability to explore the entire continuous design space for finding robust solutions that are relatively insensitive to variations in noise as well as control factors. This is unlike other approaches like Taguchi approach and Suh's axiomatic design. RCEM facilitates fast evaluation and reduces computational complexity by using approximate models after several rounds of experimental screening. This is a huge benefit as usually complex system simulations or analysis models consume time and are thus computationally expensive to perform. Another unique feature about RCEM is the fact that it uses the compromise Decision Support Problem (cDSP) construct to formulate the design problem in terms of multiple goals that are meant to achieve a target mean and minimize performance variations with respect to control and noise factors.

There are also some limitations to RCEM and we discuss them here. The function evaluation in RCEM is not as accurate as actual analysis models or simulations due to the approximations. Thus, we have to deal with models that are incomplete, and inaccurate. The performance variation estimation in RCEM is carried out using first order Taylor series expansion, which could also add to the inaccuracy as we neglect the higher orders and also when we have problems with high order of non-linearity. Also, RCEM in the form discussed in this section does not address robustness as a metric. The situation of having multiple conflicting goals that require different types of robust design is also not addressed in RCEM as presented by Chen and co-authors.

The Robust Concept Exploration Method with Design Capability Indices (RCEM-DCI)

The RCEM with DCI is proposed by Chen and co-authors (Chen, Simpson and coauthors 1999) to determine whether a ranged set of design specifications satisfies a ranged set of design requirements. This is needed because there will be cases in the early stages of design when design requirements themselves are uncertain and are mostly expressed in terms of ranges rather than a target value. Design Capability Indices (DCIs) are introduced by Chen and co-authors as a measure of system performance and robustness. The DCIs address the limitation in RCEM by quantifying robustness in terms of a metric. The DCIs are used as goal formulations in the cDSP formulation instead of directly using the mean on target and variances of system performances. The DCIs are essentially mathematical constructs meant for efficiently capturing whether a ranged set of design specifications are capable of satisfying a ranged set of design requirements. The procedure includes calculation of the following indices, see Figure 3.24.

$$C_{dl} = \frac{\mu - LRL}{3\sigma}\ ;\ C_{du} = \frac{URL - \mu}{3\sigma}; \qquad \textbf{Equation 3.11}$$

$$C_{dk} = \min\{C_{dl}, C_{du}\}$$

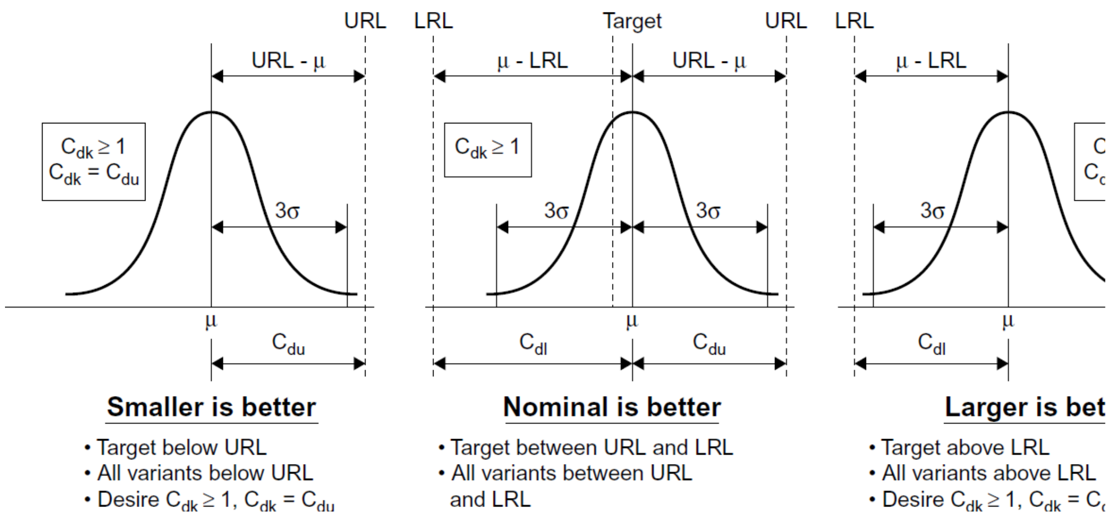


Figure 3.24: Design Capability Indices (Chen, Simpson and coauthors 1999)

A negative value of DCI means that the system performance is currently outside of the system requirement range. A DCI value greater than unity means that the system is satisfying its requirement on the system performance. This is achieved by moving the mean of the performance away from the requirements limits and/or by reducing the deviation associated with the performance function. The designer's goal in a cDSP formulated using RCEM-DCI is to force the index to greater than or equal to one so that performance requirement lies within the required performance range. This is achieved by formulating DCI goals in the cDSP formulation. The mathematical aspects of DCI are fairly simple and easy to understand and compute for designers. A major assumption, however made in RCEM-DCI is that the performance function is modeled accurately and that it has no uncertainty. This assumption is not valid for most complex problems as the models are typically incomplete and inaccurate and will have uncertainty associated with them.

3.4.5 Robust Design Type III

Another source of uncertainty that was not addressed by any of the methods discussed in previous sections is the uncertainty associated with models. Uncertainty in models is different from the uncertainty in control factors or noise factors. This uncertainty may be due to different reasons that include uncertain parameters (control and/or noise), model constraints, metamodels, approximations, model assumptions, functional relations, simulations, or analysis models. The presence of this uncertainty is high in materials and product design. This is due to the fact that material models are often non-linear and include history effects associated with the processing of material resulting in uncertainty. Also, the assumptions made at different length and time scales; the boundary conditions used, etc. will all contribute to model uncertainty in material models. Therefore, Robust Design Type III is proposed to manage the uncertainty embedded within a model. In Figure 3.25, a visual representation of robust design solutions for Type I and II and Types I, II, III together, along with optimal solution are shown. The system response is shown by the solid curve. The two dotted curves represent the uncertainty limits for the system response. The Type I, II, III robust solution identified has the least deviation in performance compared to Type I and II robust solution and optimal solution. Thus the aim in Type III robust design is to identify adjustable ranges for control factors (design variable), that satisfy a set of performance requirement targets and/or performance requirement ranges and are insensitive to the variability within the model.

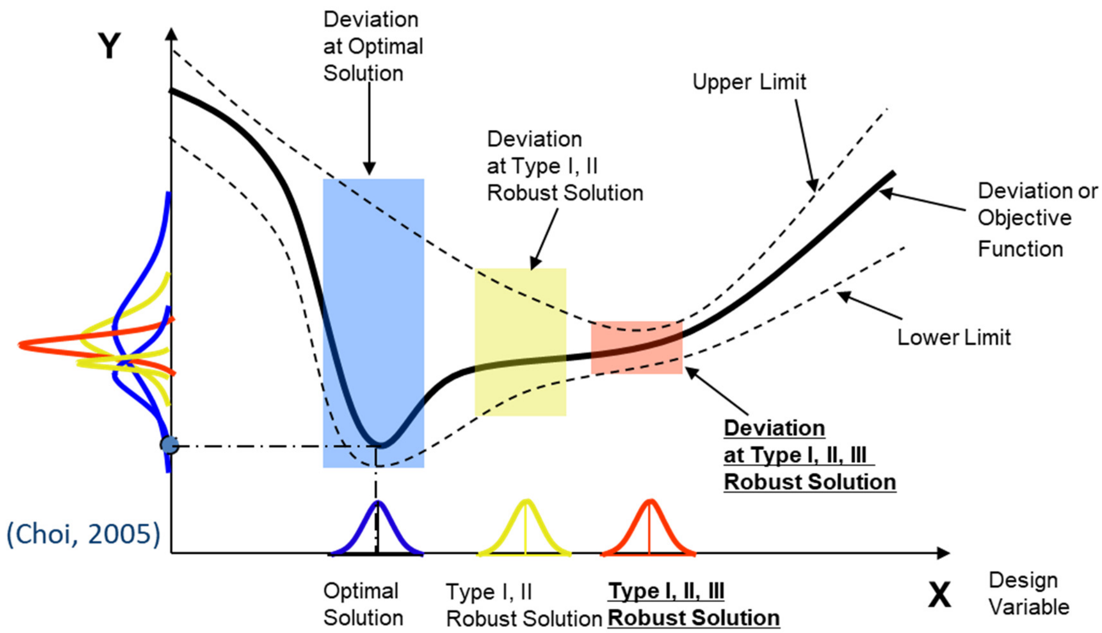


Figure 3.25: Robust Designs Type I, II and III

Choi and coauthors (Choi, Austin and coauthors 2005) propose the robust concept exploration method with error margin indices (RCEM-EMI) for Type I, II and III robust designs. Error margin indices are mathematical constructs that indicates the location of the mean response and the spread of the response considering the variability associated with design variables and system models. EMIs represent the margin against failure due to uncertainty in both model and design variables. It is dimensionless just like DCI. The EMIs support Type I, II and III robust designs. These are then incorporated as goals in the cDSP formulation to design the system under model structure and model parameter uncertainty. The RCEM-EMI procedure consists of (Choi, Austin and coauthors 2005): (a) clarification of the design task, (b) DOE and simulation, (c) integrated metamodel and prediction interval estimation, and (d) design space search using the cDSP for the RCEM-EMI. In the RCEM-EMI, the Error Margin Indices (EMI) are metrics indicating the degree of reliability of a decision that satisfies system constraints and bounds. The entire procedure involved in RCEM-EMI is depicted in Figure 3.26. The calculation of EMIs will be discussed in greater detail in Chapter 7.

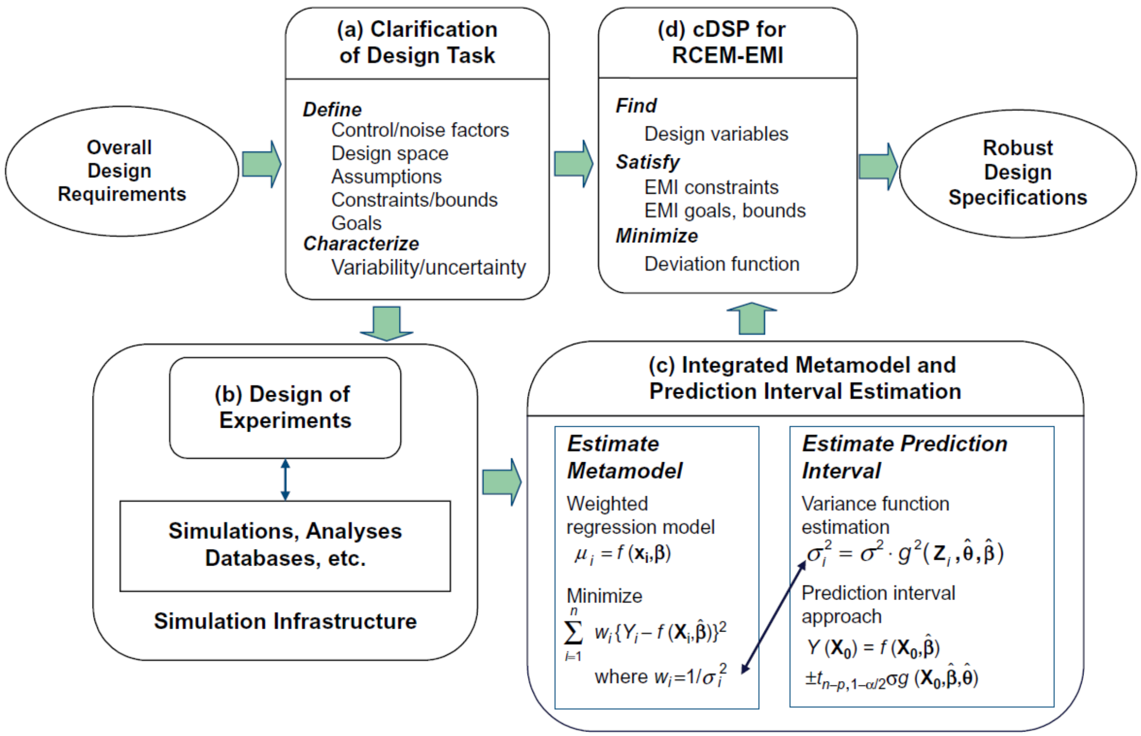


Figure 3.26: The RCEM-EMI procedure (Choi, Austin and coauthors 2005)

The major advantage of RCEM-EMI over other approaches is that it can produce accurate results in design exploration. This is because the RCEM-EMI takes into consideration the uncertainty associated with noise factors, control factors and the model itself. The RCEM-EMI helps a designer make decisions under a system's random variability and/or model parameter uncertainty in a model.

Some limitations associated with RCEM-EMI as presented by Choi and co-authors include the inability of RCEM-EMI to address multiple goals/performances that require different types of robust design. The RCEM-EMI in the form presented does not support management of propagation of all types uncertainty across process chains. It also requires large number of experiments for uncertainty analysis even in a single evaluation during design exploration and thus is highly computationally expensive.

3.4.6 Managing Uncertainty Propagation across Process Chains

Another challenge that need to be addressed in materials and product design is the propagation of uncertainty across process chains. This is the uncertainty compounded by the combination of all the three types of uncertainty (natural, model parameter, and model structure) in a chain of models that are connected through input output relations; interdependent responses and shared control/noise factors as one model interacts with another, see Figure 3.27 for the mode of interaction.

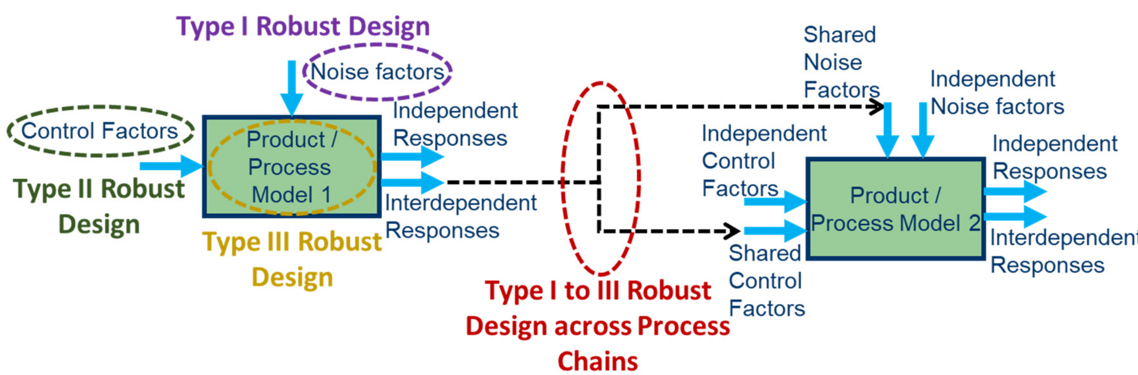


Figure 3.27: Propagation of uncertainty and need for Type I to III robust design across process chains

This model process chain could be sequence of manufacturing processes or the processing-structure-property-performance mapping or even a multi-scale model chain. In Figure 3.27, as models interact, uncertainty may be accumulated and amplified through this sequential chain, resulting in large variance of the final response (response of

Product/Process Model 2 of Figure 3.27). This is an important issue and it leads to high levels of variability in the system response.

The Inductive Design Exploration Method (IDEM)

Choi (Choi 2005) developed the Inductive Design Exploration Method (IDEM) to achieve Type IV Robust Design specifically for the integrated multiscale design of material and product. Hierarchical design of multiscale systems is facilitated by IDEM and accounts for NU, MPU and MSU and the propagation of uncertainty (PU) through the scales (Choi, Mcdowell and coauthors 2008). IDEM facilitates the exploration of robust solution and uses a metric known as Hyper-Dimensional Error Margin Index (HD_EMI) to assess the mapping across scales (Choi 2005). The higher HD_EMI value indicates that the mapped region is away from the boundary of the feasible region of interest and is less sensitive to any change. Thus, the HD_EMI value denotes the reliability of a chosen design variable that it satisfies the constraints and bounds.

IDEM is designed to provide ranged set of robust solutions against propagated uncertainty (PU) and under model structure uncertainty (MSU) by passing feasible solution range in an inductive manner from the desired given performance range to the design space. The IDEM involves three steps as shown in Figure 3.28. They are (Choi, Mcdowell and coauthors 2008, Panchal, Kalidindi and coauthors 2013):

(i) Parallel discrete function evaluation at each level of design process. This step includes bottom-up simulations and experiments (STEPS 1 and 2 in Figure 3.27).

(ii) Inductive Discrete Constraints Evaluation (IDCE) is carried out in step where top-down feasible design space exploration is carried out using metamodels. This exploration uses the Hyper-Dimensional Error Margin Index (HD_EMI) metric to assess mapping from higher space to lower space and to identify robust solution ranges from the feasible space (STEP 3 in Figure 3.27).

(iii) The compromise decision support problem (cDSP) for finding the best solution under MSU. The cDSP facilitates the designer to identify the most desirable robust solution among the feasible range set of solution obtained. This is achieved by carrying out a trade-off among the obtained HD_EMI values. The cDSP is the foundational computational construct in IDEM to carry out design decision making (This step is not depicted in Figure 3.27.).

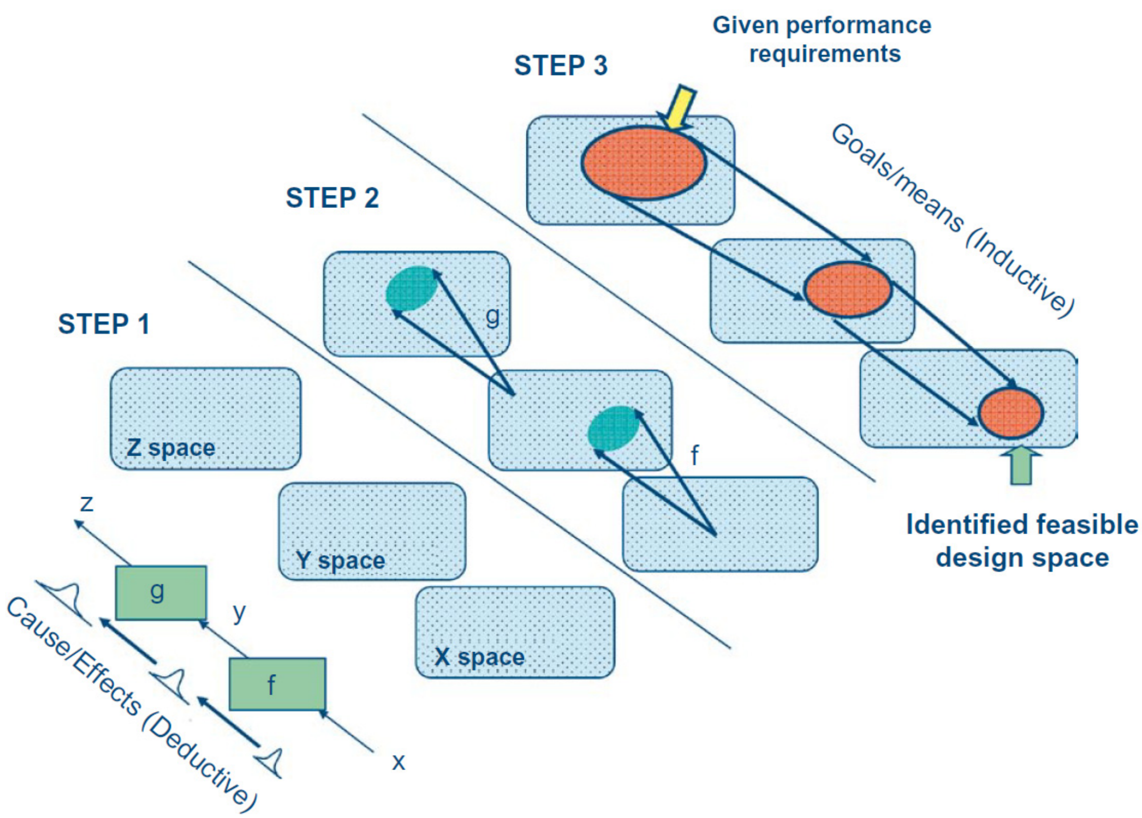


Figure 3.28: Solution search procedure in IDEM (Choi, Mcdowell and coauthors 2008, Choi, McDowell and coauthors 2008)

IDEM offers the following capabilities:

- Designers are able to identify robust solution ranges (multiple feasible solution ranges) with the consideration of uncertainty that is propagated across a process chain.
- None of the robust design approaches reviewed in the previous sections provided range set of solutions – a characteristic specialty of IDEM. This can lead to reduction of design iterations.
- The sequential uncertainty propagation analyses necessary to estimate final performance deviation are decoupled in IDEM ad individual uncertainty analyses at each step.
- Designers can easily modify/change analysis models as there is no computational interfaces between models. Designer only need to reevaluate based on the altered model.

In this dissertation, the use of IDEM is explored and tested for robust design of process chains and the associated limitations are identified (see Appendix B). Some of these limitations are highlighted in this section (details in Appendix B). This will be addressed in greater details in Chapter 7. The limitations of IDEM include:

- Error due to discretization of design space – IDEM uses discretization of design space and further inductive discrete constraints evaluation for mapping from one space to another – this leads to discretization errors and also inability to capture the feasible boundary accurately – resulting in loss of information affecting system performance.

- Increasing accuracy by increasing the resolution of discrete points results in highly computationally expensive IDEM runs for evaluating feasible spaces.
- There is limitation in terms of the number of design variables that can be used in IDEM for a design problem under study. The number of design variables increases the discrete points to be evaluated in the order of power – virtually impossible to evaluate beyond 9 variables for an IDEM study.
- Limitation in terms of exploration and visualization – IDEM uses a three-dimensional visualization space using HD-EMI metric for exploration where only a maximum of 3 design variables can be studied at a time with the others variables taking defined values – this limits the scope of the simulation study and results.
- Issue of flexibility in design – IDEM do not allow designers to incorporate new goals or requirements at different levels during the process of design as the method is based on mapping to feasible spaces of 'Y' and 'X' for a given 'Z' space.

3.4.7 Use of Robust Design in this Dissertation

Robust design is used in this dissertation for making material and product related decisions. As discussed in the previous section, the decisions are formulated as compromise Decision Support Problems. The design problems discussed in this dissertation related to integrated design of materials, products and manufacturing processes are associated with different types of uncertainty that the system should be robust to. These include uncertainty inherent in the environment, uncertainty due to assumptions in the simulation models, uncertainty due to simplification of design processes (caused by ignoring dependencies in the design process), uncertainty propagated from one simulation model to another across process chains, etc. Some of these aspects of uncertainty in materials design from different perspectives are discussed in Section 3.4. The robust formulation of compromise DSP in association with an inverse, decision-based design method is used in this dissertation to make decisions that are robust to these uncertainties. The inverse decision-based design method developed in Chapter 4 is augmented to consider the different types of uncertainty across a process chain in Chapter 7 and consists of robust design techniques discussed in this section.

3.5 Foundations for a Platform for Decision Support - Template-Based Decision-Centric Perspective

In this dissertation, a template-based decision centric design is carried out to capture the knowledge associated with the design of a system. The fundamental assumption here as discussed in previous sections is that the role of a human designer is to make decisions given the information available and that decisions and information transformations are used to make satisficing decisions from a systems perspective. The need for a template-based approach modeling design decisions and interactions is to facilitate reusability, adaptability, extendibility, modularity of design decision knowledge and support collaboration between distributed designers. Three key ideas are leveraged to achieve this: i) hierarchical systems view of design processes as decision workflows, ii) separation of declarative and procedural information, and iii) design as decision-centric activity. We discuss in brief about this in this section.

3.5.1 Hierarchical Systems view of Design Processes as Decision Workflows

Design processes can be progressively broken down into sub-processes from a hierarchical perspective. Looking at design from a decision-centric perspective, we can model design processes as decision nodes interconnected with different other decision nodes forming a decision network or a workflow that support decision making and information transformations.

The transformations from the context of materials and product design involve an input material/product state, an output material/product state and a design sub-process for execution – which is also a network of information transformations. In Figure 3.29, we show the input, output, transformations, and design processes and their relations. These form the key elements of hierarchical systems view of design processes as decision workflows.

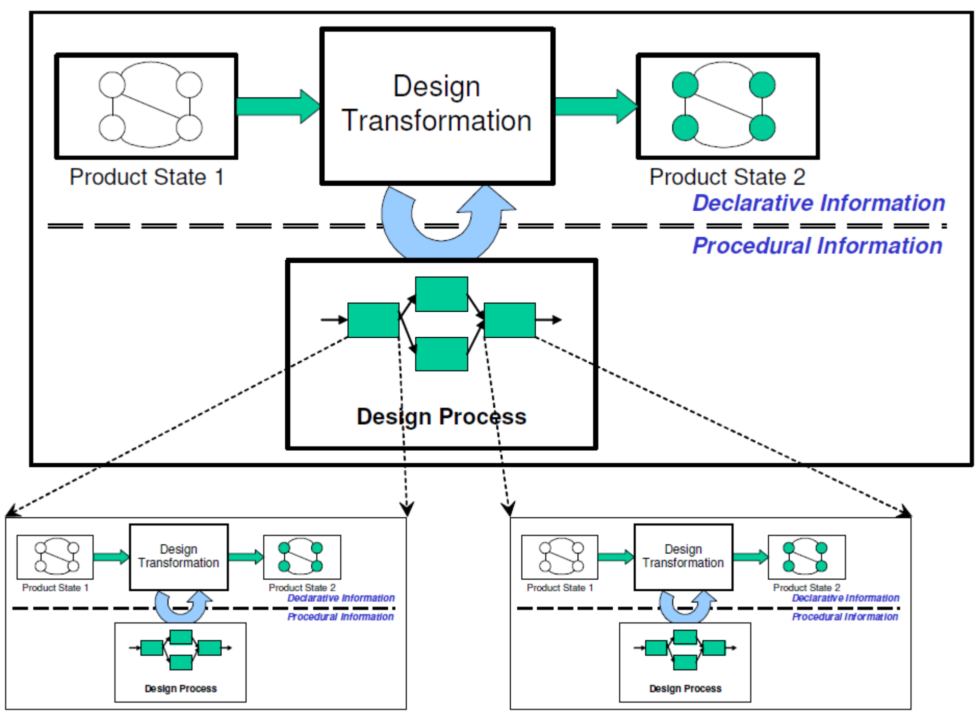


Figure 3.29: Hierarchical systems view of design processes (Panchal, Fernández and coauthors 2004)

The information related to the domain of the problem and the formulation of transformations, known as declarative information and the information associated with the domain-independent procedure of solving the problem (procedural information) are separated clearly.

Modeling Design Processes using Templates

The concept of modeling design processes using domain-independent decision templates is proposed by Panchal and co-authors (Panchal, Fernández and coauthors 2004) and is illustrated using Figure 3.30.

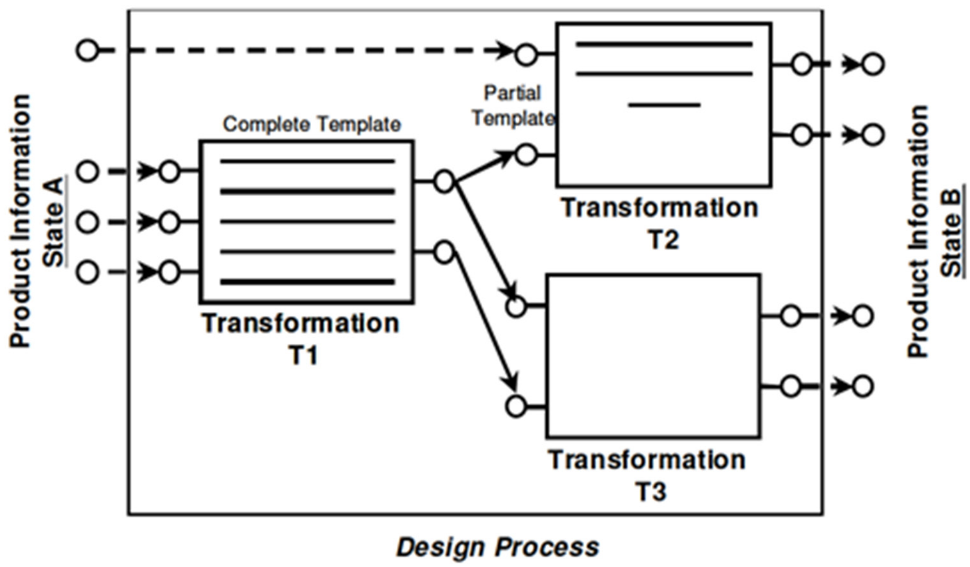


Figure 3.30: Design process modeling procedure using templates (Panchal, Fernández and coauthors 2005)

The design process shown in Figure 3.30 has three information transformations, T1, T2, and T3. Now depending on the level of information available for a problem, the templates can be instantiated to support design decision making. For example, in Figure 3.30, T1 is a complete template, i.e., it is completely instantiated as all the information available for executing it is available. T2 is a partially instantiated template and T3 is yet to be instantiated as the information on the problem for T3 may not be complete/available. However, the generic information transformation process remains the same as T1 or T2. This facilitates modular, reusable models for information transformation with a consistency in structure thereby providing the ability to capture, archive and reuse the design process knowledge at all levels of system hierarchy.

3.5.2 Separation of Declarative and Procedural Information and Knowledge

While developing templates, it is very important to separate the problem formulated related information (declarative) and the process execution specific information (procedural). The declarative information is associated with design transformation and the product states. It represents what the designer does via information transformation and will be domain specific. Procedural information is associated with how the information transformation is carried out and details how the transformation is executed via a decision workflow or decision network. It is domain-independent in nature. To separate out the declarative and procedural information, three levels are used – the product information level, the process information level (declarative), the process execution information level (procedural), as shown in Figure 3.31. More details on this are provided by (Panchal, Fernández and coauthors 2004, Panchal 2005, Panchal, Fernández and coauthors 2005, Messer 2008).

3.5.3 Design as a Decision-Centric Activity

From decision-centric perspective, design is the process of transforming information that characterizes the needs and requirements for a product into knowledge of the product – as discussed in previous sections. The decision-centric templates are rooted in the

Decision Support Problem Technique, specifically the compromise Decision Support Problem construct. This was covered in detail in Section 3.3 and are not repeated here.

In this dissertation, a Knowledge-Based Platform for Decision Support in the Design of Engineering Systems (PDSIDES) is proposed. In PDSIDES decision related knowledge is modeled with computational templates based on the Decision Support Problem constructs using ontology to facilitate reuse and execution. In order to provide appropriate decision support for users of different knowledge levels, we define three types of users, namely Template Creators, Template Editors, and Template Implementers, who perform Original Design, Adaptive Design, and Variant Design respectively. PDSIDES will be discussed in detail in Chapters 8 and 9 of this dissertation.

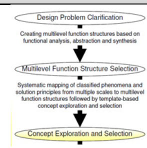
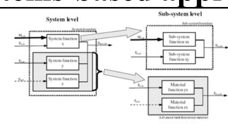
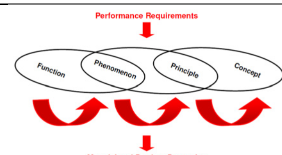
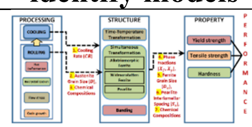
3.6 Role of Chapter 3 in this Dissertation

The objective in this chapter is to introduce the design foundations and the fundamental constructs based on which the systems-based design architecture proposed in this dissertation is developed. The design foundations reviewed and discussed in this dissertation include: i) Design as a goal-oriented activity, ii) Pahl and Bietz design method, iii) Suh's Axiomatic Design, iii) Gero's model of design as a process, iii) decision-based design paradigm and DSP Technique, iv) robust design, v) template-based decision-centric view of design. These foundations discussed in this chapter are used throughout this dissertation. In Figure 3.1, the utilization of these foundations in the development of the different components of the systems-based design architecture in the different chapters of this dissertation is shown.

Chapter 4: Systems-based Design Architecture for Integrated Design of Materials, Products and Associated Manufacturing Processes

In this chapter, the requirements for the systems-based design architecture for the integrated design of materials, products and associated manufacturing processes - “rendering conceptual materials design more systematic”, “providing systematic, domain-independent, goal-oriented and multi-objective decision support” – are addressed. All requirements for the systems-based design architecture are listed in Table 1.6. The constructs of the systems-based design architecture developed to address these requirements are highlighted in Table 1.6. A portion of Table 1.6 that is relevant to this chapter is reproduced in Table 4.1. The component of the systems-based design architecture developed in this chapter is a systematic, function-based approach for the integrated design of product and material concepts. The steel manufacturing process chain example is used in Chapters 5 and 6 for validation of this component of the systems-based design architecture. The systematic function-based approach is used for answering Research Question 1 posed in this dissertation. A Concept Exploration Framework is developed that supports a Goal-oriented Inverse Design (GoID) method developed to address Research Question 2. The relationship with the research questions and the supporting hypotheses is presented in Table 4.1.

Table 4.1: Requirements, constructs of the systematic approach, and associated hypothesis validated in Chapter 4

Requirements	Constructs of the Systems-based Design Architecture developed in this Dissertation	Research Hypotheses	Validation Examples
1.Systematically define the forward processing-structure-property-performance relationships 2.Systematic integration of material, process and product models	 **Systems-based approach**	**RH.1.** a systematic approach from a systems perspective, consisting of concept generation	1. Steel Manufacturing Process Chain Problem - Integrated design of steel (material), manufacturing processes (rolling and cooling) and hot rolled rods (product) for automotive gears 
	 **Systematic generation of multilevel function structures**	**RH1.1. a)** functional decomposition to generate multilevel function structures across the process chain for the end performance requirements,	
	 **Systematic design mappings to identify models**	**RH1.1. b)** identifying material and process phenomenon associated with function structures and systematically mapping them to solution principles (models identified from literature or developed through experiments)	
	 **Systematic integration of identified models to develop processing-structure-property-performance mapping (forward material workflow)**	framing the system structure for problem via, **R.H.1. c)** vertical integration of identified/developed material models and horizontal integration of identified/developed process models to systematically map material processing to material microstructure phenomena and next to macrolevel properties and performances	

4.1 Answering the Research Question 1

In this section, a function-based systematic approach to achieve the integrated design of materials, products and manufacturing process from a systems perspective is developed to answer Research Question 1. As discussed in Chapter 3, a systematic approach for the conceptual design of materials and products is not much addressed in literature. A systematic design method/approach that involve strategic and tactically placed successive steps of information transformation, supports designers to solve problems more efficiently and effectively. Since changes at the detail design stage and product develop change is highly expensive, designers are required to make right decisions at early stages of design without overlooking or ignoring anything essential. To achieve this a deliberate and systematic step-by-step procedure is required along with the designer's intuition and expertise supporting in the systematic approach.

As discussed in Chapter 3, after the planning and clarification of the task phase of a design process, the designer comes up with a requirements list and starts the conceptual design phase. In the conceptual design phase, the designer determines a principal solution or a concept. This is achieved by abstracting the essence of the problem, establishing function structures, searching suitable working interrelationships (working principles, phenomenon, etc.) and then combining those (integration of information) to develop a system-level function structure or working structure or a workflow – from the context of this dissertation. The working structure is then transformed into a more comprehensive representation so as to evaluate the essentials of the principal solution and review constraints, goals and other design objectives. By operating at the level of phenomena, and associated solution principles, the designer is able to go beyond a particular material/product system and will be able to adapt to changes, evolution and other market cycles – resulting in dynamic behavior/response to market shifts and ability to provide that knowledge in classified form for easy retrieval.

We revisit Secondary Research Question 1 and the Research Hypotheses in Table 4.2

Table 4.2: Research Question 1 and Research Hypotheses

Secondary Research Question 1	Research Hypothesis 1
RQ1. What are the foundations needed for ***systematically identifying*** and ***integrating*** material models with models of the rest of the system (product, manufacturing processes, and environment), so as to define the ***processing-structure-property-performance*** relationships and associated ***information workflow*** at early stages of design?	***H1.1.*** Through a systematic approach from a systems perspective, consisting of concept generation which includes, a) functional decomposition to generate multilevel function structures across the process chain for the end performance requirements, followed by b) identifying material and process phenomenon associated with function structures and systematically mapping them to solution principles (models identified from literature or developed through experiments), and framing the system structure for problem via, c) vertical integration of identified/developed material models and horizontal integration of identified/developed process models to systematically map material processing to material microstructure phenomena and next to macrolevel properties and performances, the design of product, process and material concepts are integrated, and conceptual materials design is rendered more systematic.

The research hypotheses (H1.1) is addressed in this chapter. To address this research question, the work carried out by Mathias Messer for his PhD on function-based systematic design is leveraged and applied in the context of integrated design of materials, products and manufacturing processes. An overview of the function-based approach to achieve systematic model integration and information workflow is presented in Figure 4.1.

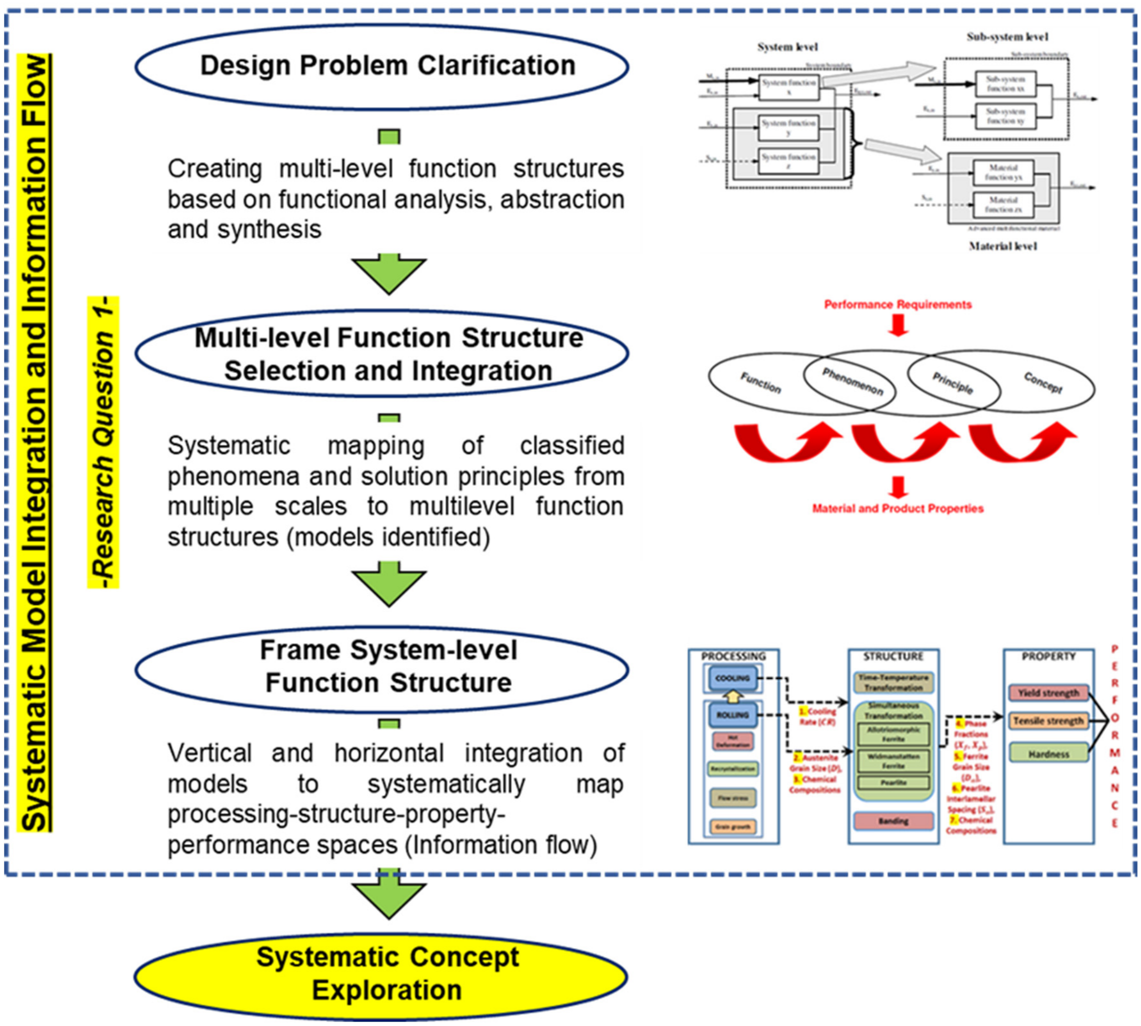


Figure 4.1: Overview of function-based approach to achieve systematic model integration and information workflow

4.2 Systematic Function-Based Conceptual Design

In Sections 4.2.1, 4.2.2 and 4.2.3, we discuss systematic function-based conceptual design is reviewed. We expand on some of the concepts on early stages of design discussed in Chapter 3 and address it from the perspective of the research questions and hypotheses.

4.2.1 Systematic Conceptual Design Exploration

Conceptual design is considered as the most demanding activity in a design process. Let us look at Figure 4.2. A change in design at later stages of design results in a cost of 1000x, while a design implemented at the conceptual level incurs only 1x. Traditionally, design is carried out using trial and errors and experiments resulting in design changes at later stages of design resulting in high design change cost at later stages as can be seen for the dotted blue curve in Figure 4.2.

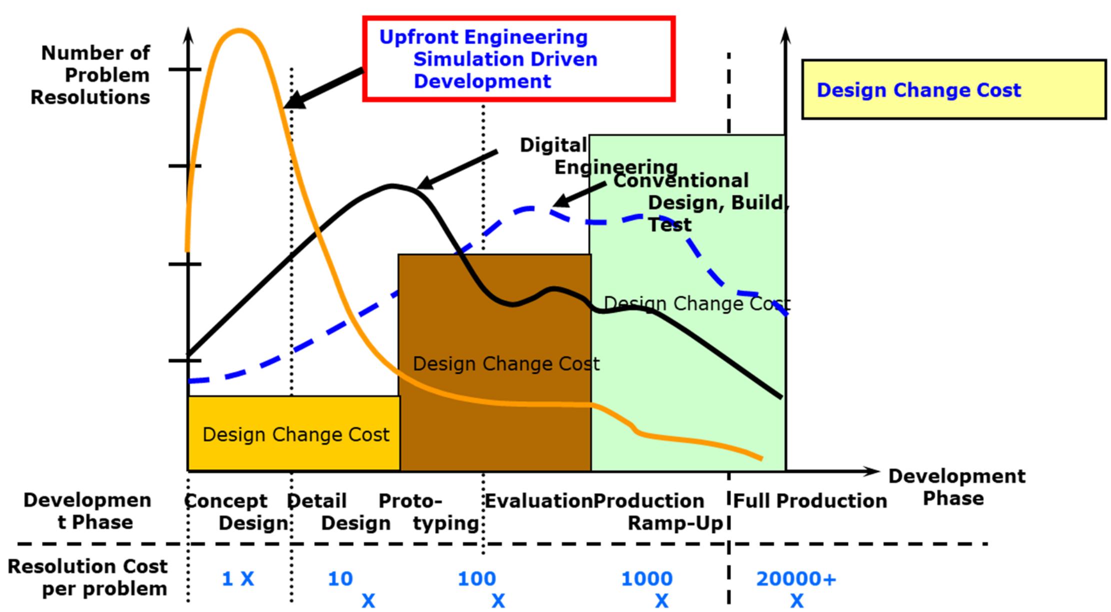


Figure 4.2: Cost timeline across various design phases. Source: ITI (GE Aircraft Engines)

Now, with the advent of simulations, digital twins, and digital threads there have been a shift in design changes to early stages of design and thus a fall in associated design change cost, see the black curve in Figure 4.2. What we intend to achieve in this dissertation, is to move all of this process to the conceptual design phase. Hence, all the major design decisions need to be systematically made at the conceptual design phase leading to "***satisficing design concepts***" that results in less resolution costs and less design change costs at later stages of design, see orange curve in Figure 4.2. Systematic design as discussed in Chapter 2 involves discursive and intuitive thinking. With both discursive thinking and intuitive thinking, a clarified problem and the associated information is systematically transferred from one state to the other to generate concepts.

4.2.2 Function-Based Design

Clarification of a design problem is followed by decomposing the system-level problem into sub-problems by defining a boundary. The aim in systematic conceptual design is to represent engineering systems in terms of their functions they must fulfill. Functional requirements are derived from customer needs and requirements in the case of Suh's Axiomatic Design or from desired product functions from the perspective of Gero's model of design as a process, as discussed in detail in Chapter 2. In this dissertation, we use the approach of functional decomposition or function-based approach for modeling the system structure. The sub-parts of a complex system will perform specific sub-functions that contribute to the overall system-level function structure. The strategy here involves functional decoupling of a coupled system so as to get the behavior of the system right and then focus on human decision making via decision workflows.

Key to function-based design is to develop functional relationships and interrelationships of a system. This was discussed in detail in Chapter 3 while reviewing Pahl and Beitz design process and Suh's axiomatic design. Pahl and Beitz (Pahl and Beitz 1996) specifies that the search for solutions is simplified and thus discovery of design solutions is facilitated by establishing functional interrelationships in a system. As per Suh (Suh 1990), the design process involves transforming customer needs into functional requirements and then interlinking the functional domain to physical domain at every hierarchy level of the design process.

Simon (Simon 2013) notes that discovering viable ways of decomposing a complex system into semi-independent parts corresponding to the system's many functional parts is a powerful and well-respected technique. In this dissertation, we focus on the use of functional decomposition of the design problem on multiple levels and scales for achieving systematic model integration and information flow.

The definition of function is different for different disciplines. The term function as defined by Pahl and Beitz is as the general input/output relationship of a system whose purpose is to perform a task. Here function is an abstract formulation of the task to be performed. The input and output here refer to energy, material or signals (information). A similar definition is proposed by Ullman (Ullman 1992) as "the logical flow of energy, material and information between objects or the change of state of an object caused by one or more of the flows". Both these definitions characterize function as involving certain transformation from an input to a system to an output of a system. In this dissertation, the word function is applied to the overall input/output relationship that is involved in the integrated material, product and manufacturing process system. Functions are represented in this dissertation by leveraging the work by Mathias Messer where solution-neutral natural language was used to represent functions by combining the nouns energy, material and signal while taking into account input and output flows. This allows for the representation of wider range of functions that can be used for functional representation in the materials and product domain. Thus, the advantages associated with function-based design are (Messer 2008):

- Domain-independent representation and solution exploration schemes;
- Generation of a broader solution filed;
- Abstraction of essential problem characteristics;
- Allows for defining a problem boundary and problem formulation;
- Designers are more likely to explore new solutions than known solutions;
- Easy to identify non-intuitive solutions;
- Supports systematic problem formulation, design space generation and expansion, and exploration of design and solution space;
- A foundation for modular and reconfigurable design
- Generation of rough idea of uncertainty and its propagation across process flow chain;
- Facilitation of planning and managing of design;
- Practical and easy to use for designers in any domain and can be interfaced with systems-based design exploration methods; and
- Emergence of innovative solutions and the logic underpinning the solutions can be clearly understood.

The major disadvantage associated with function-based design is that it does not provide systematic mappings to obtain concepts based on functional requirements.

4.2.3 Function-Based Systematic Conceptual Design – Pahl and Bietz Approach

The most well-known method for function-based systematic design is proposed by Pahl and Bietz (Pahl and Beitz 2013). The systematic approach proposed by Pahl and Bietz is based on best practices from industry and essentially includes the fundamentals of technical systems, systematic approach and general problem formulation and solving process. The whole planning and design process includes planning and clarification of the task, through the identification of the required function structures, the systematic elaboration of solution principles, the construction of modular structures to generate system-level function structures, to the detailed documentation of the complete product (Messer 2008). The four main phases of planning and design process as proposed by Pahl and Beitz is discussed in great detail in Section 3.2.1, Chapter 3, see Figure 3.3.

In this dissertation, we leverage the function-based systematic approach by Mathias Messer (Messer 2008) which is strongly related to the working steps in the conceptual design phase of the Pahl and Beitz (Pahl and Beitz 1996) design process. We start with clarification of the problem and identification and documentation of system-level requirements in a solution neutral form. The crux of the problem is then identified via analysis and further abstraction of problem specific information. The system and subsystem level function structures are developed by iteratively analyzing, abstracting and synthesizing. The individual sub-functions in the function structure are replaced by working solution principles. Working principles can be described quantitatively via physical laws governing the physical quantities involved. A functional relationship realized by the selected working principles and its characteristics results in a working interrelationship that fulfills the function in accordance with the task to be performed. Through combination of working interrelationships of the sub-functions into working structures, the solution principle for fulfilling the overall tasks for the system is established.

To summarize the steps involved in generating a concept within the conceptual design phase of the Pahl and Beitz design process involves (Messer 2008):

- Abstraction to identify essential problems,
- Generation of system function structures,
- Search for working interrelationships,
- Combination of working interrelationships into working structures,
- Selection of suitable combinations,
- Refinement into principal solution variants, and
- Evaluation against technical and economic criteria to determine a system concept.

In this dissertation, *functional decomposition, analysis, abstraction, synthesis and systematic variation* are leveraged from Pahl and Beitz design process as core transformations for the function-based systematic approach.

4.2.4 Analysis of Research Gap

The application of function-based systematic approaches is traditionally carried out for embodiment and detail design phases of design process and mostly for material selection. Generating concepts from a systems perspective so as to identify and integrate models and establish the information workflow that involves phenomena and associated solution principles for the integrated design of materials, products and manufacturing processes is not addressed in literature. The goal by addressing this research gap is to enhance the existing function-based design methods so as to increase design concept flexibility at conceptual design phase in realizing the design of materials and products.

Systematic conceptual design is not typically addressed by current materials design. The design decisions made at the conceptual design phase are the most crucial ones that allocate a vast majority of product's resources. A materials design revolution is underway in the recent past where the focus is to design the material microstructure and processing paths to satisfy multiple property or performance requirements. Recent advancements in computational modeling tools and frameworks that support simulation-based, integrated design exploration of materials, products, and the manufacturing processes through which they are made have resulted in the speeding up of the process of discovering new materials and has paved way for rapid assessment of process-structure-property-performance relationships of materials, products, and processes. This has led to the simulation-based design of material microstructure (microstructure-mediated design) to satisfy multiple property or performance goals of the product/process/system thereby replacing the classical material design and selection approaches. This has resulted in a need to move the focus from embodiment and detail design phases to early stages of design like the conceptual design phase. A function-based systematic approach for conceptual design of materials and products is therefore proposed. This enables designers to identify underlying phenomena and associated solution principles that embody the functional relationships. The limitations of existing approaches to conceptual design of materials and products is summarized in Table

Table 4.3: Conceptual design efforts, limitations and use in this dissertation

Research Effort	Limitations	Use in this Dissertation
Decision-based Design	• Systematic concept generation at early stages of design not supported for materials and products; • Limited to systematic selection at early stages and systematic design during embodiment and detail design.	Used as foundational design philosophy in this dissertation
Systems Design	• The integrated design of materials, products and associated manufacturing processes is not yet addressed from a systems perspective (goal-oriented).	The focus in this dissertation is to achieve the systems-based design of materials, products and manufacturing processes
Materials Design	• Focus on intuitive methods for concept generation, followed by rigorous domain-dependent analysis using multiscale modeling efforts or material selection approaches;	Research efforts used to develop models that establish information linkage and workflow.

	• Highly domain-dependent; • Systematic conceptual design at early stages of design not addressed.	
Function-based design	• Focus on functional modeling • Do not support systematic mappings that allow concept generation	Foundation for addressing research question 1.
Function-based systematic design	• Limited to material selection and not on early stage concept generation	Foundation for addressing research question 1.

An overview of the systematic function-based approach to the integrated design of materials, products and manufacturing processes concepts and their subsequent exploration using a concept exploration framework is illustrated in Figure 4.3. In Section 4.3, systematic function-based conceptual design is proposed. Limitations and opportunities for future work are discussed in Section 4.5 along with verification and validation in Section 4.6. The systematic approach described in this section is tested with the hot rod rolling example problem in Chapter 6.

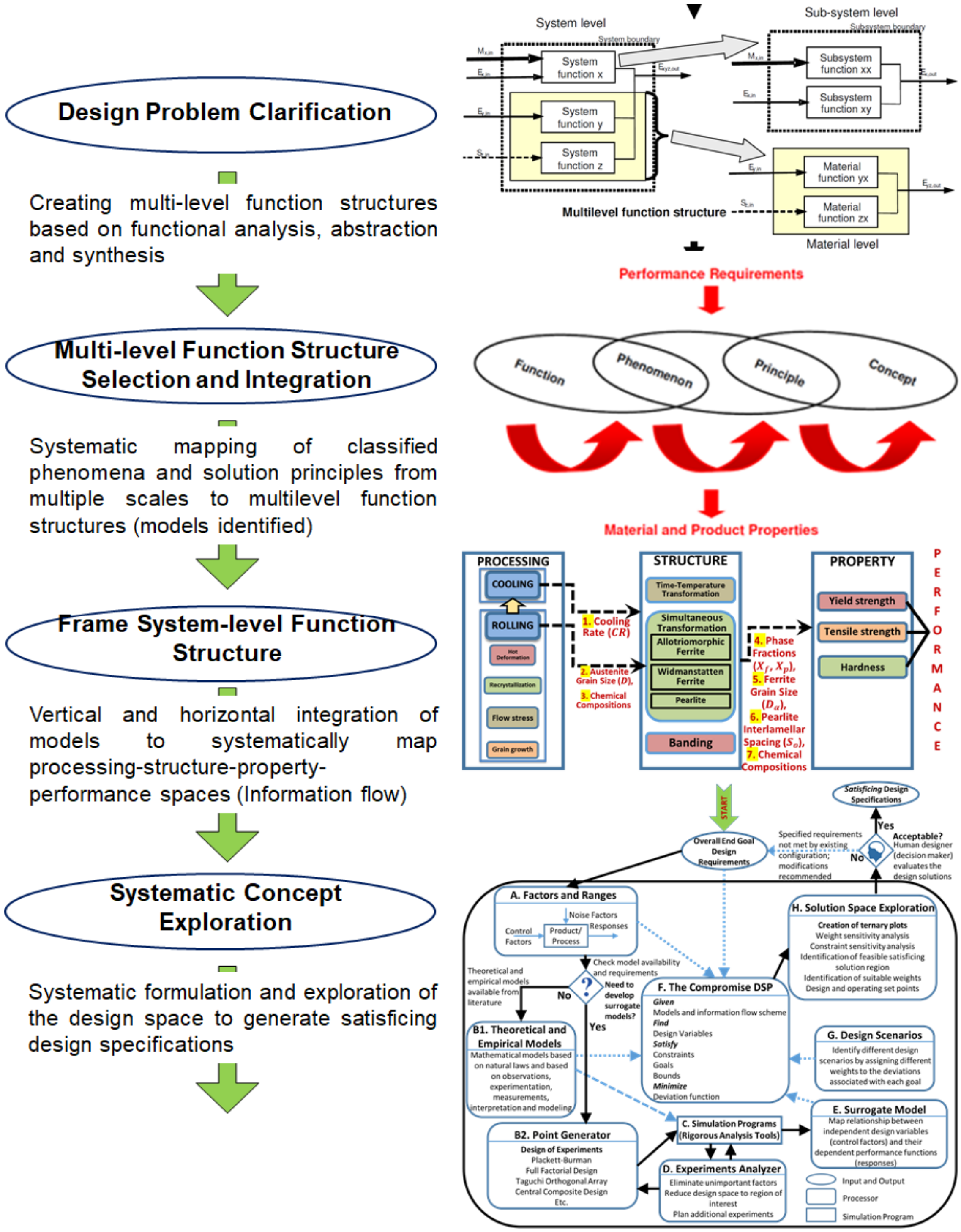


Figure 4.3: Overview of systematic generation and exploration of concepts for the integrated design of materials, products and manufacturing processes

4.3 Proposed Function-Based Approach for Systematic Conceptual Design

Leveraging from the work of Mathias Messer (Messer 2008) which is based on the Pahl and Bietz approach, the function-based approach for systematic conceptual design proposed in this dissertation for the integrated design of materials, products and associated manufacturing processes consists of (Messer 2008):

i) ***Functional decomposition*** of products and material systems into multilevel function structures through functional analysis, abstraction and synthesis, and;

ii) ***Systematic mapping*** of phenomena and associated solution principles from multiple disciplines to multilevel function structures in order to develop principal material and product system solution alternatives and concepts.

The mappings in the systematic approach is shown in Figure 4.4.

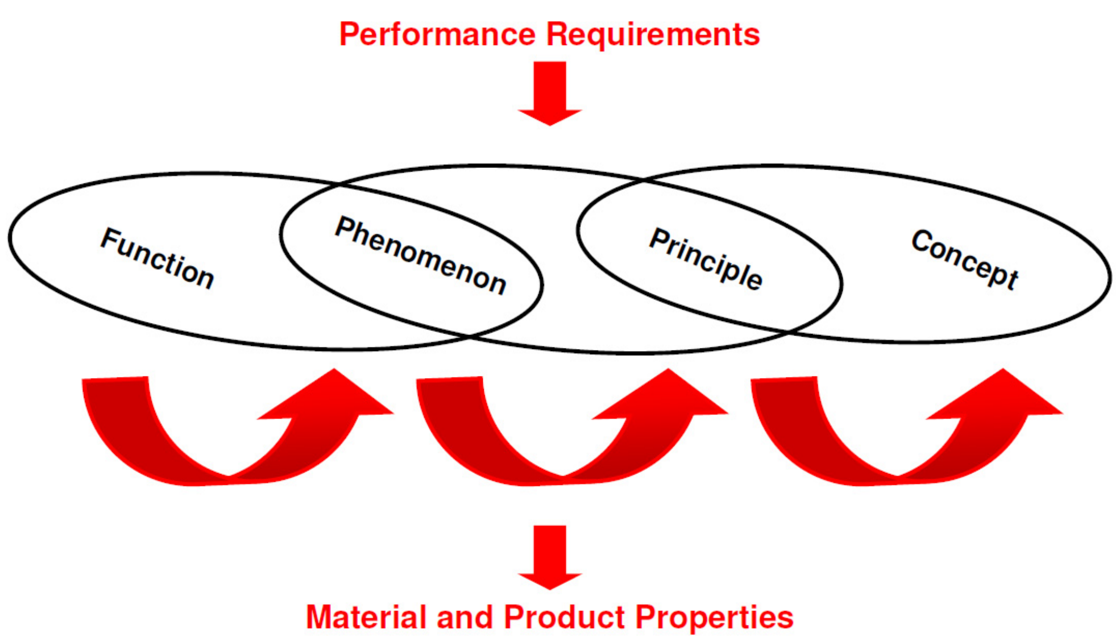


Figure 4.4: Key mappings in systematic conceptual design (Messer 2008)

The key mapping includes (see Figure 4.4):

Clarified Problem	➡	Functional relationships
Functional relationships	➡	Phenomena
Phenomena	➡	Associated solution principles
Functional relationships, phenomena and associated solution principles	➡	Principal solution alternatives characterized by specific properties

The key mappings are described in the following sections.

4.3.1 Formulating Multilevel Function Structures

For the integrated design of materials, products and manufacturing processes at the conceptual design phase, it is critical to take a systems perspective. This allows to carry out functional decomposition of the of products and material systems into multilevel function structures through functional analysis, abstraction and synthesis. Here function is defined as the overall input-output relationship in the integrated material and product system. To address this in a domain-independent manner, functions here are represented in solution neutral way. Having defined and clarified a problem in a solution neutral way, we specify an overall system function. Function structure here refers to a meaningful and compatible combination of sub-functions into the overall system function (Messer 2008). We create multi-level function structures by decomposing overall system level function into sub-functions on various levels of hierarchy like sub-system, assembly, component, part, materials, etc., see Figure 4.5.

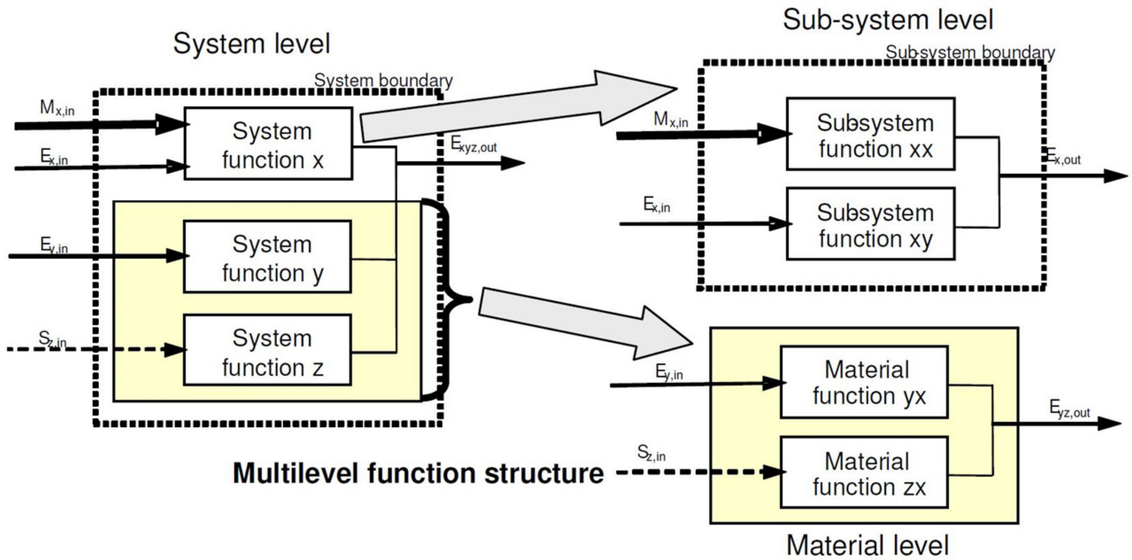


Figure 4.5: Multilevel function structures. Adopted from (Messer 2008).

In this dissertation, multi-level function structures are proposed to include the material level at the conceptual design stage that spans the processing paths and material microstructures which further allows to make system-level connections with the product properties and performances. The path in the system configuration space made up of input-output relationships and their links can be mathematically varied. The sub-functions present can be mathematically varied and combined into function structure alternatives. ***Multilevel function structures support a designer in framing the system level structure by identifying and combining functional relationships on different levels and scales.***

Function taxonomies are available for product domain in literature. A comprehensive list of function taxonomies is provided by Szykman and co-authors (Szykman, Racz and coauthors 1999). A collection of verbs well-suited for function based systematic conceptual design of materials is proposed by Mathias Messer (Messer 2008) and is reproduced in Table 4.4.

Table 4.4: Verbs frequently used to define functional relationships (Messer 2008)

Sink	Source	Store	Combine	Modify	Convey	Control
Absorb	Create	Accumulate	Mix	Amplify	Channel	Actuate
Dissipate	Emit	Deposit	Couple	Attenuate	Conduct	Detect
Receive	Supply	Record	Link (sequential)	Prepare	Direct	Sense
	Release		Constrain	Filter	Divert	Display
			Separate	Shape	Guide	Maintain
			Compare	Transform	Transmit	Resist (deformation)
				Change	Transport	Support (loading)
						Stabilize (buckling)

At the material level, commonly used verbs could be "change" and transform". "Change" refers to changing material/energy from one state to another while transform refers to transforming from one form to another.

The key to the systematic approach is function-based abstraction, through which the problem complexity is reduced, and essential characteristics of the problem are emphasized. This supports the discovery of non-intuitive solutions. The function structure thus developed consists of several linked sub-functions that represents the flow of information, energy and material. Individual sub-functions are first represented as "black boxes" and are further replaced by more concrete statements which are in mathematical form to allow for simulation-based material and product design. Phenomena and associated solution principles are identified to develop wide range of principal solution alternatives. Phenomena are described quantitatively by means of laws (laws of physics and mathematics) governing the quantities involved. Solution principles refers to means to embody phenomena. These means are physical, quantitative descriptions in terms of laws of physics and mathematics, to fulfill functional relationships. From the standpoint of integrated materials, product and manufacturing process design, the phenomena and associated solution principles for property-structure relationships and are not yet addressed.

It is very essential to identify phenomena and associated solution principles for property-structure relationships on multiple scales for effective and efficient integrated design of material and product concepts. To facilitate a function-based systematic approach to the integrated design of product and material concepts, design catalogs are proposed for phenomena and associated solution principles that represents property-structure relations on multiples scales. In this dissertation, we are interested in identifying material models and integrating them so that we can establish the process-structure-property-performance relationships given the performance requirements. For achieving that, we focus on identifying phenomena and corresponding solution principles (models in our case) that embody the phenomena. One approach to systematically identifying solution principles is by using design catalogs. We discuss the design catalogs and their application in next section.

4.3.2 Design Catalogs

Design catalogs are classification schemes that are used to provide a classified collection of known and proven solutions (knowledge) for easy retrieval. They are characterized by systematic presentation of information from which the required knowledge can be retrieved. It also facilitates identification and combination of essential solution characteristics that meets the requirements. Design catalogs are therefore knowledge base in a classified form. It provides the designers with an overview of a certain domain or subarea. Design catalogs are therefore intended to provide (Messer 2008):

- knowledge and experiences of different designers is captured in a single location,
- quicker, more problem-oriented access to the accumulated solutions or data,
- self-explanatory classification for easy retrieval,

- a comprehensive range of possible solutions or at the very least the most essential ones which can be extended later, and
- the greatest possible range of interdisciplinary applications.

From the perspective of integrated materials and product design, the requirement is a knowledge base (an open-ended map) that enables designers to identify the structure-property relationships – which in terms of systematic conceptual design is the identification of underlying phenomena and associated solution principles that cause a certain behavior and thereby provide solutions for a variety of problems or cases. An example of the mapping and the design catalog is adopted from Matthias Messer's doctoral dissertation (Messer 2008), see Figure 4.6. The system-level function is to dissipate energy. The identified phenomenon is "inelastic deformation" that embodies the system level function "dissipate energy". The most promising solution principles are selected and evaluated for feasibility based on the given performance requirements.

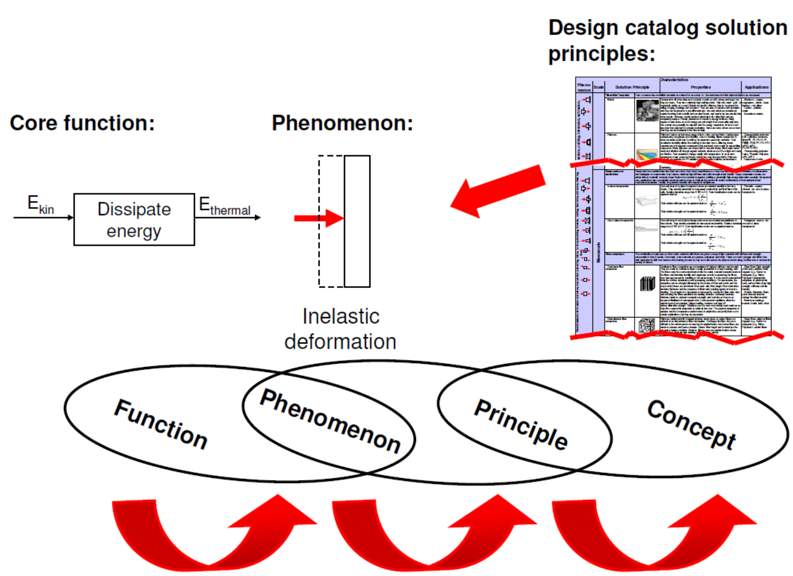


Figure 4.6: Mapping solution principles to phenomenon inelastic deformation to embody system level function "dissipate energy". Adopted from (Messer 2008).

A design catalog showing solution principles is adopted from Matthias Messer's dissertation (Messer 2008) and is shown in Figure 4.7.

Alternatives

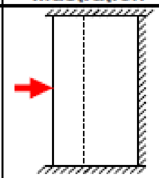
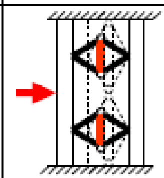
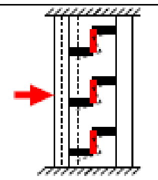
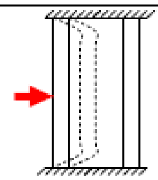
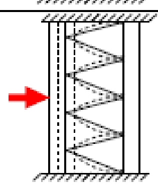
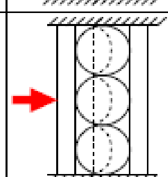
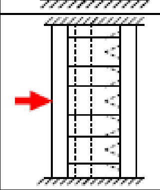
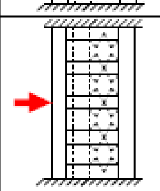
Solution Principles	Acronym	Illustration	Remarks	Feasibility
Compression of structures	C		Ultimate tensile strength is an excellent indicator of the ability of a material to absorb energy. The uniform elongation parameter is unimportant provided that the ductility is sufficient to allow the requisite plastic deformation. However, compression of structures usually suffers form the limited zone of plastic deformation and the unavailability of lightweight materials that combine high ultimate tensile strength and sufficient plastic deformation in this configuration.	⊘
Tension of structures / Nanotubes	T(N)		The maximum energy that can be absorbed per unit weight before tensile instability supervenes depends upon the ultimate tensile strength and strain. Structures with incorporated carbon nanotubes could be substantially stronger and lighter than conventional, but, besides the stroke (maximum displacement limitation), cost and manufacturability are still major problems with nantobes.	⊘
Torsion of structures	T		The maximum energy that can be absorbed per unit weight before torsional instability supervenes depends upon the ultimate torsional strength and strain. Besides the maximum stroke limitation, energy absorbers based on torsion suffers from the unavailability of lightweight materials that combine high ultimate torsional strength and strain.	⊘
Bending of Plate structures	BP		Kinetic energy of an incoming blast impinging on a plate can be dissipated by bending and stretching. The superior performance of sandwich plates relative to solid plates of equal mass for shock loading is due (i) the substantial bending strength of a sandwich plate as described above, and (ii) energy absorption by the sandwich core.	✓
Bending of Shell structures	BS		The failure mode of laterally loaded shell structures starts as local denting followed by global bending collapse. For shell structures such as tubes, the axial buckling mode has a specific energy absorption capacity which is approximately 10 times that of the same tube in lateral bending. Moreover, in the bending of shell structures, usually not all material participates in the absorption of energy by plastic work.	⊘
Inversion of structures	I		Inversion of structures involves for example the turning inside or outside in of a thin circular tube made of ductile material. Another example is the inversion of spherical shells where material passes into the central dimple region through a circular knuckle whose radius increases with deformation. In general, practical shortcomings, such as difficulties in securing axial loading, did not yet proove inversion to be a feasible energy dissipation mechanism.	⊘
Splitting of structures	S		Tube splitting is a special case of tube inversion where the die radius is large enough to cause splitting instead of inversion. Again, practical shortcomings, such as difficulties in securing axial loading, did not yet prove inversion to be a feasible energy dissipation mechanism.	⊘
Progressive Buckling of Open-top tubes and frustra	BO		Circular tubes under axial compression provide one of the best energy absorption devices since they feature "optimal" energy dissipation characteristics. They provide a high stroke length per unit mass and a reasonably constant operating force. Best energy dissipation is obtained through progressive plastic buckling via a series of ringlike folds which avoids overall elastic buckling.	✓

Figure 4.7: Evaluation of solution principles for the function "dissipate energy". Adopted from (Messer 2008).

4.4 Discussion on Function-Based Systematic Approach and Use of Design Catalogs to the Integrated Design of Materials, Products and Manufacturing Processes

Using the function-based systematic approach, an abstract solution to the given design problem is developed by representing systems (product and material systems) in terms of functions to be fulfilled. Functions are represented in this work as solution-neutral using taxonomies. Using functional representations at material level for structure-property relations will bridge the gap between product design and materials design and support the integrated design of materials and products. Design catalogs facilitate access to classified and reusable knowledge and expertise in both materials and products domains. Functional relationships are used as a common interface here and this leads to increased synergy between the two domains leading to integration, transparency, modularity and reconfigurability of design processes. This encourages designers to think more deeply about fundamental phenomena and solution principles. Phenomena are physical effects that can be described in terms of mathematical equations. Solution principles associated with certain phenomena are further embodying phenomena. The approach followed in this dissertation is based on systematic identification and variation of functional relationships, phenomena and associated solution principles. This leads to comprehensive design space exploration. It is reported that more innovative solutions emerge from function-based systematic approaches and the logic behind the solutions are clearly understood and evident. Thus the result of applying the function-based systematic approach to the integrated design of product and material concepts is (Messer 2008):

i) a more thorough search through,

ii) an informed decision making, as well as

iii) an expansion of the design space and hence increase in concept flexibility, which is crucial when facing dynamic demands in a global marketplace.

Discussion on Design Catalogs

Design catalogs support function-based systematic design and helps a rational designer by extending cognitive abilities and increasing the designer's concept flexibility. Design catalogs, however are not static. They must be considered as a living document that is updated continuously, extended and maintained to keep up with expanding body of knowledge. Design catalogs are intended for multidisciplinary exchange of knowledge, exploration of the relationships between phenomena and associated solution principles at multiple scales and their differing behaviors. Since designers are operating at the phenomenal level, it helps them to view the problem from a systems perspective. Once the specific phenomena and associated solution principle is decided, designers focus on material properties and start the design activities from there for conceptual design.

Design catalogs thus provide knowledge in a form classified for easy retrieval for different applications. They are essentially an open-ended map that enable a designer to identify underlying phenomena and associated solution principles. Focusing on phenomena and associated solution principles, i.e., property-structure relations a designer is able to step out of the technological cycle of obsolescence and evolution. To convert design catalogs into "living" documents, web-based tools can be used/developed that support live editing and updating of catalogs.

4.5 Answering Research Question 2

Having addressed research question 1 dealing with systematic function-based design of materials and products, Research Question 2 on systematic concept exploration and inverse design exploration is addressed next. In section 4.6, the Concept Exploration Framework (CEF) is presented and introduced as a step-by-step approach for formulating design problems and quickly evaluating design alternatives to generate satisficing design specifications. The CEF is developed to support systematic and rapid concept exploration of complex engineered systems involving the material, product and manufacturing processes. The CEF is presented in Section 4.6. In Section 4.7, we present the Goal-oriented Inverse Design (GoID) method that uses the Concept Exploration Framework to facilitate the systems-based inverse design exploration of material microstructures and processing paths to meet multiple product level performance/property requirements. Both CEF and GoID together addresses the requirements of Research Question 2. A portion of Table 1.6, that is relevant to this chapter is reproduced in Table 4.5. The relationship with the research questions and the supporting hypotheses is presented in Table 4.6.

In this chapter, the focus is to develop a concept exploration framework that is based on simulation-based design approach for designing complex systems. An ideal concept exploration framework should support both the activities of *a priori* analysis and *a posterior* evaluation/synthesis in concept exploration. The focus however in this dissertation is to use the concept exploration framework to support systems-based top-down design to generate "***satisficing design specifications***". The inverse method is supported by the CEF to systematically explore design alternatives and generate '***satisficing***' design solutions across process chains.

Table 4.5: Requirements, constructs of the systematic concept exploration and inverse design exploration, and associated hypothesis validated in Chapter 4

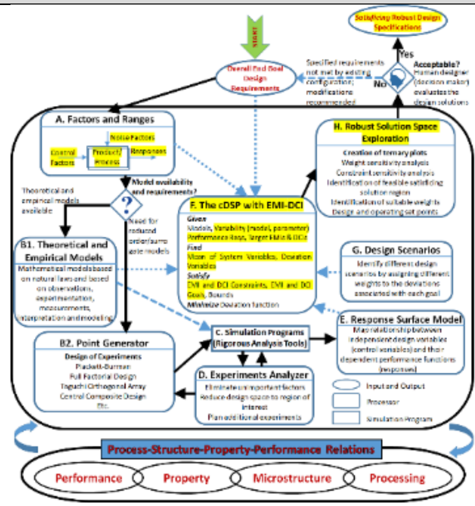
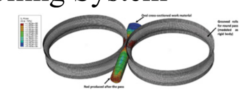
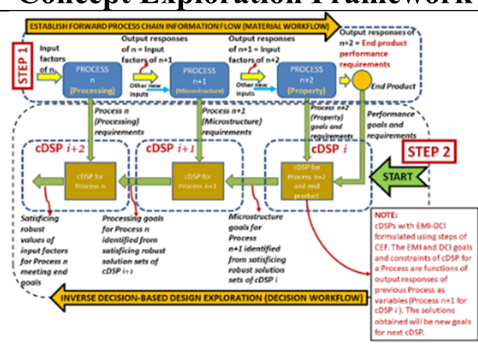
Requirements	Constructs of the Systems-based Design Architecture developed in this Dissertation	Research Hypotheses	Validation Examples
Systematic concept exploration	 **Concept Exploration Framework**	**RH2.1.** a concept exploration framework anchored in decision-based design construct – the cDSP can support the designer in formulating the design problem systematically and exploring the solution space to generate satisficing design specifications.	**1.** Integrated design of steel (material), manufacturing processes (rolling and cooling) and hot rolled rods (product) for automotive gears **AND** **2.** Horizontal Integration of a Multistage Hot Rod Rolling System  **AND** **3.** Explore the Solution Space for Microstructure After Cooling Stage to Realize the End Mechanical Properties of Hot Rolled Product
Inverse design exploration	 **Goal-oriented Inverse Design (GoID) Method**	**RH2.2.** a goal-oriented inverse design method that uses the concept exploration framework to facilitate the systems-based inverse design exploration	

Table 4.6: Secondary Research Question 2 and Hypotheses

Secondary Research Question 2	Research Hypothesis 2
RQ2. What are the computational foundations needed for performing the ***systematic*** and ***rapid concept exploration*** of complex engineered systems involving the material, product and manufacturing processes ***satisfying certain end performance requirements***, when simulation models are typically ***incomplete, inaccurate and not of equal fidelity***?	***H2.1.*** Developing a concept exploration framework anchored in decision-based design construct – the cDSP can support the designer in formulating the design problem systematically and exploring the solution space to generate satisficing design specifications (To address **G3**). ***H2.2.*** Developing a goal-oriented inverse design method that uses the concept exploration framework to facilitate the systems-based inverse design exploration of material microstructures and processing paths to meet multiple product level performance/property requirements (To address **G4**).

4.6 The Concept Exploration Framework (CEF)

The CEF is introduced in this dissertation as a general framework that includes systematic steps to identify design alternatives and generate *satisficing* design solutions. The CEF is inspired from the RCEM (Chen, Allen and coauthors 1997) with addition of features (processors) to consider different material and product models and options to explore the solution space for different design scenarios. Core to the CEF is the foundational mathematical construct – the compromise Decision Support Problem (cDSP) (Mistree, Hughes and coauthors 1993). The cDSP construct used here is anchored in the robust design paradigm first proposed by Taguchi. The fundamental assumption is that the models are not complete, accurate and of equal fidelity (Taguchi , Bras and Mistree 1993). The cDSP is a hybrid of mathematical programming and goal programming. Target values for each goal are defined in a cDSP and the emphasis of the designer is to satisfy these target goals as closely as possible. This is achieved by seeking multiple solutions through trade-offs among multiple conflicting goals. The solutions obtained are further evaluated by solution space exploration to identify solution regions that best satisfy the requirements identified. There are four keywords in the cDSP – *Given*, *Find*, *Satisfy* and *Minimize*. The overall goal of the designer using the cDSP is to minimize a deviation function – a function formulated using the deviations (captured using *deviation variables*) that exists from the goal targets.

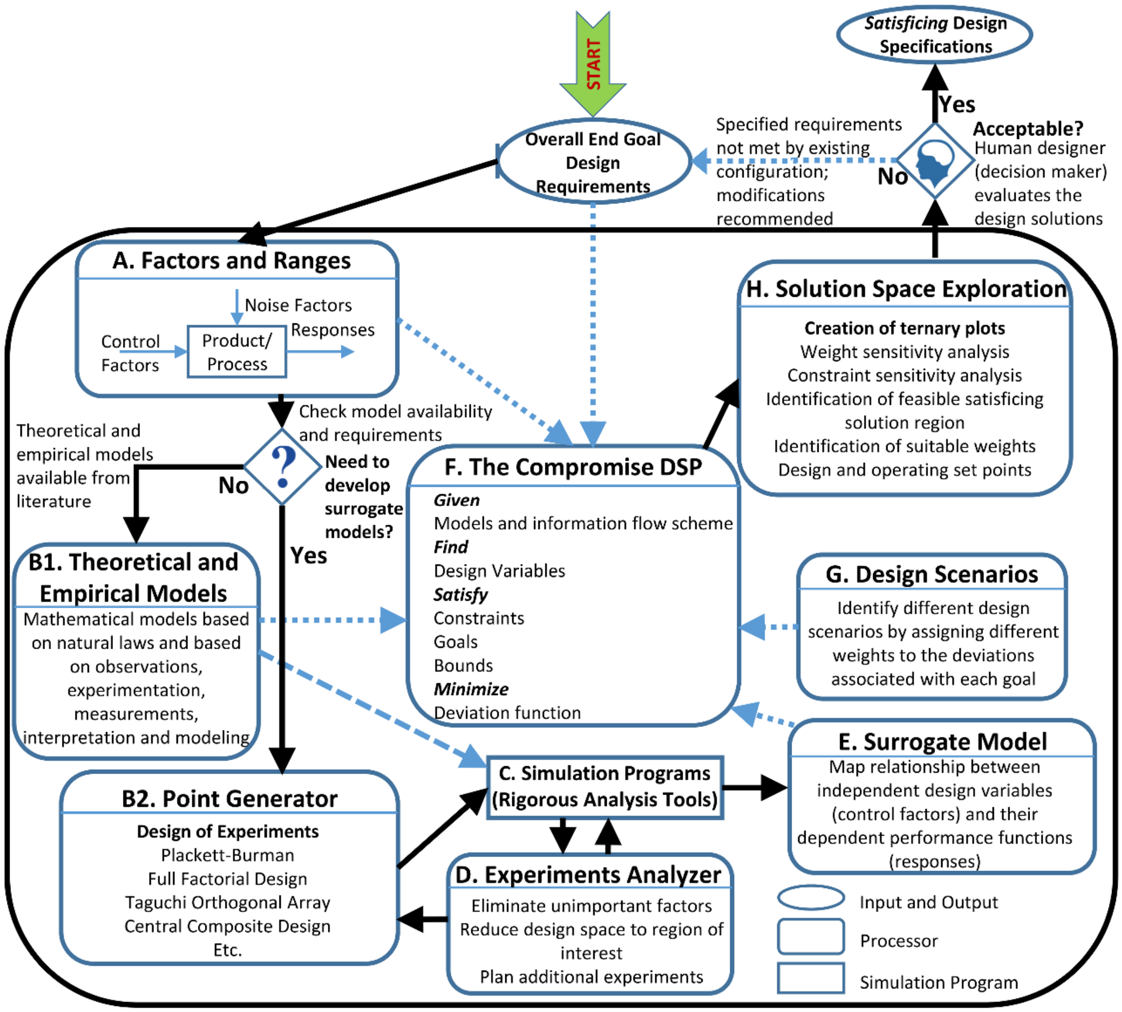


Figure 4.8: The computing infrastructure for Concept Exploration Framework (CEF)

The details regarding formulating and solving the cDSP are available (Bras and Mistree 1993, Mistree, Hughes and coauthors 1993) and explained in detail in Chapter 3 are not explained here.

Next, we explain the Concept Exploration Framework (CEF). In Figure 4.8, the computing infrastructure for the CEF is shown. The computing infrastructure for CEF includes 8 processors (A, B1, B2, D, E, F, G, H) and simulation programs (C). The application of the CEF begins with the designer identifying the overall end goal design requirements for the problem under study. The further steps in the CEF are below. The solid arrows in Figure 3 are used to highlight the steps of CEF in sequence. The dotted lines and dashed lines are used to represent information sharing within the framework.

***Step 1 using Processors A and B1*:** In this step, the initial concept exploration space is defined and the cDSP is formulated. For the requirements identified for the problem, the control factors (factors that the designer can control), noise factors (factors that the designer cannot control) and the responses (the performance goals identified) and their ranges are identified in processor A. This information is input to the foundational mathematical construct – the cDSP, processor F. In parallel with the identification of factors, ranges, and responses, a designer identifies the models available/required. For problems related to manufacturing processes such as hot rolling and cooling, several different models defining material/process behavior are available in the literature (Hodgson and Gibbs 1992, Majta, Kuziak and coauthors 1996, Kuziak, Cheng and coauthors 1997, Pietrzyk, Cser and coauthors 1999, Phadke, Pauskar and coauthors 2004). Such available theoretical and empirical models are identified in processor B1 and are communicated to the cDSP.

***Step 2 using Processors B2, D, E and Simulation Program C*:** In Step 2, the designer carries out low order screening experiments. If models for the problem are not available or if there is a need to develop reduced order or surrogate models so as to reduce the size of the problem, an experiment is designed to develop them. The point generator, processor B2 is used to design the experiments. The simulation program (C) is used to run the experiments. The simulation programs for manufacturing related problems may use some of the theoretical and empirical models from processor B1. This information flow is shown using the dotted arrow in Figure 4.8. An example of this is a finite element simulation (Simulation Program, C) for rolling that uses a constitutive model (empirical model, Processor B1) to define the flow behavior of the material. The experiments analyzer, processor D evaluates the simulation results and recommends additional experiments if needed. Regression analysis and ANOVA are used to evaluate the significance of the results. Processor E is used to create the surrogate models using the simulation program results that are acceptable to the designer.

***Step 3 using Processors F, G and H*:** All models are communicated to the cDSP, processor F. The cDSP is then exercised for different design scenarios as specified by processor G. These scenarios which are identified by assigning different weights to the deviations associated with the goals define a solution space. This solution space is then explored using processor H. Ternary plots are generated to visualize and explore the solution space to identify feasible solution regions that satisfy the requirements. A human designer evaluates the design solutions, checks feasibility and satisficing solution regions. If the overall end goal requirements are not satisfied or there are no feasible satisficing regions, the overall end goal requirements may be modified as in Figure 3. In such a situation, a designer can also make use of the ternary plots to carry out design trade-offs to identify regions that satisfy the modified end goal requirements instead of repeating the CEF.

Thus the generic functionalities offered by CEF in summary includes: i) identification of end goals and requirements for a problem, ii) systematic identification of control factors, noise factors that influence the responses of the goals and requirements, iii) systematic identification of mathematical models - theoretical, empirical models available from literature on the problem domain and systematic development of surrogate models using simulation programs and design of experiments, iv) systematic formulation of the design problem using the cDSP construct for the given information available for the problem, v) systematic planning of the design scenarios to be explored for the problem, vi) exercising the problem formulated for the design scenarios and vii) systematic analyzing of the solution space with the opportunity for the human designer to visualize the solution space and make design decisions. These functionalities can be used to formulate and execute any complex systems problem in a systematic fashion to provide decision support provided availability of required information. To facilitate the generic applicability of the CEF and extend the designer's abilities in making design decisions that are robust, flexible and modifiable particularly in the early stages of design, an ontology for design space exploration and a template-based ontological method that supports systematic design space exploration using CEF is proposed in Chapter 9 (Wang, Nellippallil and coauthors 2018).

The Concept Exploration Framework along with its features of multi-goal decision support can be readily incorporated into a design method that supports the design of the material and product (processing, composition and microstructure) as part of a larger overall systems design process. The framework can embody the hierarchy of process-structure-property-performance proposed by Olson (Olson 1997) by systematically accounting the information flow and mappings across these spaces and transforming overall design requirements into a set of satisficing design specifications for the material-product-and manufacturing process system of interest.

In Section 4.7, we describe the goal-oriented, inverse method in its generic form and the application of the method to explore the design space for the hot rod rolling process chain problem.

4.7 The Goal-Oriented, Inverse Method

4.7.1 Generic Form of the Goal-Oriented, Inverse Method

The basic idea of our method for finding satisficing solutions in a multi-level, multi-stage process chain that involves the Processing-Structure (PS), Structure-Property (SP) relations is passing down the satisficing solution ranges in an inverse manner, from given final performance range to the design space of the previous space (defined by model input and output) with designer having the flexibility to choose solution of preference. The method will be explained using the information flow diagram shown in Figure 4.9. It is a *goal-oriented* method because we start with the end goals that need to be realized for the product as well as process and then design the preceding stages to satisfy these end goals as closely as possible by exploring the design space. Then the design decisions that are made for the end requirements of the product/process after exploration are communicated to the stages that precede them to make logical decisions at those stages to satisfy the requirements identified thereby carrying out a design space exploration process in an inverse manner, as described by Steps 2.1 to 2.3, Figure 4.9. To demonstrate the generic nature of the method we call the different sequential processes as 'n' to 'n+2' and the decision support constructs as '*i*' to '*i+2*'.

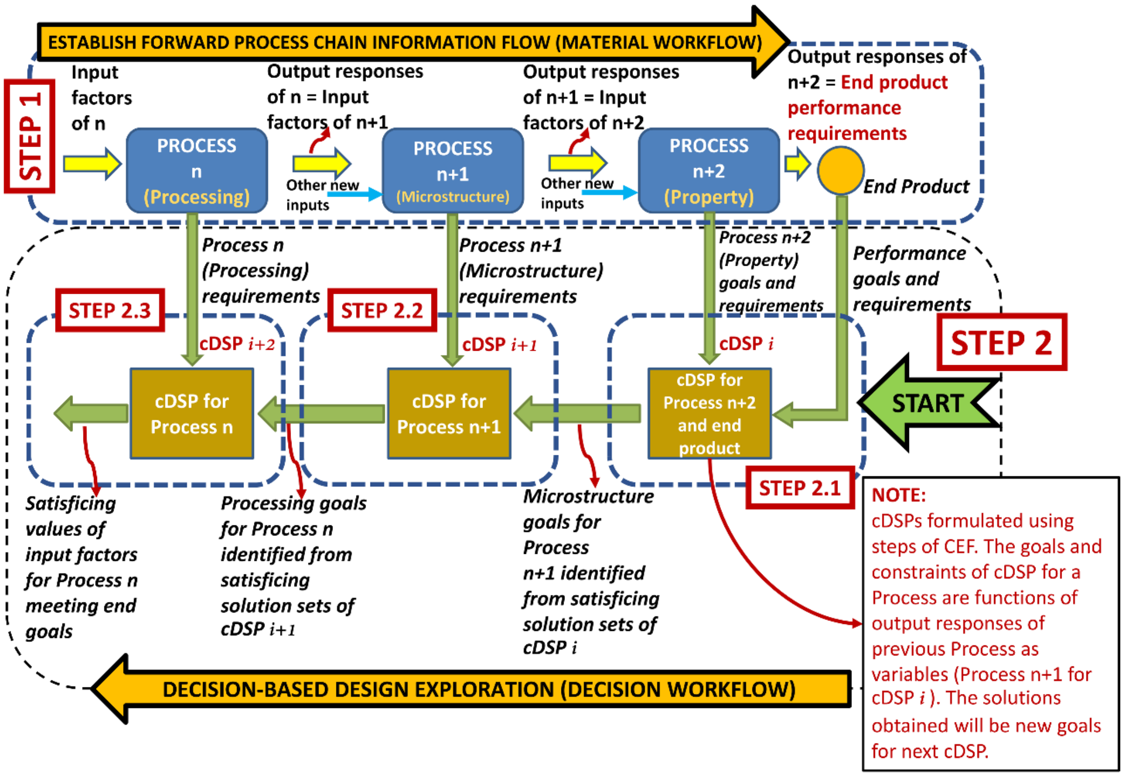


Figure 4.9: Generic form of the goal-oriented, inverse method illustrated using Steps 1 and 2

Step 1: Establish forward modeling and information flow across the process chain (forward material workflow)

Step 1 of the proposed method involves establishing the forward modeling and information flow across models. In Step 1, the designer makes sure that there is proper flow of information as models are connected across different 'Processes'. These processes could be different manufacturing processes that are sequentially connected to produce the product with information passing across processing-microstructure-property-performance spaces. Mathematical models are either identified or developed to establish the information flow. The Steps 1 and 2 of the Concept Exploration Framework are used to identify factors, ranges, responses, and models for the specific materials design problem under study. In Figure 4.9, Step 1 we see that the output of a Process serves as the input for the next Process along with other new inputs specific to the next Process with the final output being the end product. We can imagine these 'Processes n, n+1 and n+2' as Processing, Microstructure and Property Spaces respectively as shown in Figure 4 to understand the method clearly. Thus, Process n (Processing Space) generates output that serves as input for Process n+1 (the Microstructure Space). The output of Process n+1 (the microstructure identified) serves as the input for Process n+2. The output of Process n+2 defines the Property Space and this directly defines the final performance characteristics of the end product. From a design standpoint the input to a Process are design variables and the output response from the Process serves as input variables to next Process.

Step 2: Carry out decision-based design exploration starting from performance space and sequentially identifying satisficing regions of interest in previous spaces in an inverse manner

Step 2.1: Formulate cDSP *i* using CEF for achieving the desired end product properties and performances

In Step 2, we start the decision-based design exploration starting from the end goals and requirements and has Steps 2.1 to 2.3 to complete the process chain in Figure 4.9. cDSP *i* is formulated for Process n+2 in Step 2.1. The design variables of this cDSP will be the output responses from Process n+1 that serves as input to Process n+2. The property and performance goals that are desired are defined in this cDSP. On executing the cDSP for different design scenarios and exploring the solution space using CEF, the designer is able to identify the combination of output responses from Process n+1 (that serves as input for Process n+2) that best satisfy the conflicting property and performance goals defined. The identified values of output responses for Process n+1 that satisfies the goals defined for cDSP *i* are passed as goals for cDSP *i+1*. In Figure 4.9, Process n+1 represents the microstructure space, then the output of cDSP *i* will be the target values of microstructure factors that satisfies the properties and performances defined for the product. In Step 2.2, using cDSP *i+1* we analyze how these target microstructure values can be achieved in Process n+1 with the output responses from Process n as the input variables.

Step 2.2: Formulate cDSP *i+1* using CEF for achieving the goals identified for Process n+1 based on the exploration carried out in cDSP *i*

In Step 2.2, we formulate cDSP *i+1* for Process n+1. The target goals in this cDSP are the values of the design variables for cDSP *i* identified after solution space exploration in Step 2.1. The design variables for cDSP *i+1* are the output responses from Process n that serves as input to Process n+1. Executing this cDSP and exploring the solution space using CEF, the designer is able to identify the combination of input variables that best satisfies the target goals defined. From Figure 4.9, we see that the output will the combination of processing variables that best satisfy the microstructure targets defined in cDSP *i+1*. Again, we pass these identified values of design variables from cDSP *i+1* that satisfy requirements to next cDSP *i+2* as target goals.

Step 2.3: Formulate cDSP *i+2* using CEF for achieving the goals identified for Process n based on the exploration carried out in cDSP *i +1*

In Step 2.3, in a similar fashion to previous steps, the designer formulates cDSP *i+2* for Process n with target goals being the design variable values identified from cDSP *i+1*. On exploration of solution space, the designer is able to identify the combination of input factors of Process n that best satisfies the targets performance goals identified for cDSP *i+2*.

Thus, using this proposed method, the designer is able to carry out top-down driven, simulation-supported, decision-based design of processing paths and material microstructure to satisfy a ranged set of product-level performance requirements. The method is generic and can be applied to similar problems with information flow from one process to another as shown in Figure 4.9. The method supports coordination of information and human decision making and is suited for problems involving a network of forward, sequential information flow. Given any complex system that involve sequential flow of information across processes/levels, the proposed method has the potential to be applied to support information flow by making effective decisions across the processes/levels in order to realize an end goal.

4.8 Discussion on Concept Exploration Framework and Inverse Design Exploration Method

In this chapter, we present a goal-oriented, inverse method supported by the Concept Exploration Framework (CEF) to achieve the integrated design exploration of the material, product and manufacturing processes. The method is goal-oriented and inverse because we start with the end mechanical properties of the product and inversely maps the requirements to microstructure and processing spaces of the material to identify multiple solutions that satisfy the requirements. The utility of the proposed method is demonstrated by carrying out the integrated solution space exploration of the processing and microstructure spaces of the rolling and cooling processes to identify *satisficing solutions* that realize the end mechanical properties of the rod product. The method and its application are characterized by a confluence of different disciplines like engineering mechanics, materials science, manufacturing and systems engineering. The functionalities offered by the method supported by CEF includes:

- The method is based on requirements driven, “top-down” design of system and associated subsystems by taking a goal-oriented approach which is different to the standard practice of bottom-up modeling and design of material and product systems,
- There is the perception of obtaining a satisficing design space across process chains; augmenting the human ability to make design decisions - visualizing a solution space and making logical judgements through trade-offs to identify satisficing solution regions of interest,
- There is the capability to handling ‘n’ number of design variables – this is an advantage over other design exploration methods like IDEM where there is a limitation on the number of design variables,
- Propagation of end goal requirements (product performance or properties) across a process chain with the designer having the capability to check whether the end goals are actually achievable at previous spaces in their current configuration or not – designer can recommend adjustments in the design space if needed,

- Offers flexibility in design: The capability to define new goals and requirements at each level as the method uses individual cDSPs to facilitate information flow allowing to formulate a design space at each level - advantage over other design exploration methods like IDEM and pyDEM where the design space is defined by mapping from previous spaces (Choi, McDowell and coauthors 2008, Kern, Priddy and coauthors 2017),
- The capability to carry out rapid, integrated design exploration of material and products using simulation models that we accept are typically incomplete and inaccurate,
- The capability to coordinate information and human decision making,
- The CEF offers the capability to prioritize models, input factors, output responses and computational tools in terms of their value in design, and
- ensuring feasible design solutions that allows to invest on new complex material systems with confidence.

The proposed method and the concept exploration framework are generic and supports the integrated decision-based design of similar manufacturing processes involving the material and product. Given any complex systems problem that involve sequential flow of information across processes/levels, the proposed method has the potential to be applied to support information flow and human decision making across the processes/levels in order to realize an end goal. Through the proposed method an approach is proposed for *microstructure-mediated design* by *integrating the design of the material, product and associated manufacturing processes* involved.

4.9 On Verification and Validation – Theoretical Structural Validity (TSV)

4.9.1 TSV of Function-based Design

Theoretical structural validation refers to accepting the validity of individual constructs used in the systematic function-based approach and accepting the internal consistency of the way the constructs are put together. Theoretical structural validation involves systematically identifying the scope of the proposed approach's application, reviewing relevant literature and identifying the research gaps that is existing, identifying the strengths and limitations of the constructs uses based on literature review, determining the constructs and approaches that can be leveraged for the systematic function-based approach while reviewing literature on the advantages, disadvantages and accepted domains of application, and checking the internal consistency of the constructs both individually and when integrated.

In Chapter 4, we establish the generic nature of the systematic approach and why the approach is appropriate for concept generation during early stages of design for the integrated design materials, products and associated manufacturing processes. By carrying out literature search, it is shown that the systematic function-based approach and the associated constructs have been previously applied for problems in various domains in a successful manner and are verified and validated. The use of these generic systematic approach for the integrated design exploration of materials, products and associated manufacturing processes so as to establish systematic model integration and establishment of information workflow is not addressed in past literature.

Based on the critical review of literature in Chapter 4, it is inferred that the application of function-based systematic method is mostly on areas related to mechanical, control, software and process engineering and is mostly applied for selection of materials for different applications from existing classes of solutions. The focus is also more on product design by developing concepts at early stages of design. Our focus by using function-based design is in establishing model integration and information flow chain so as to facilitate systematic problem-oriented conceptual design via functional decomposition and representation of the problem in solution-neutral natural language taking into account the input and output flows. This allows to establish the integrated conceptual design of materials and products in a more systematic and domain-independent manner which helps in increasing the designer's flexibility and easy establishment of the information workflow for material/product system.

Once the phenomena and associated solution principles (models in our case) are identified, design catalogs are used to facilitate function-based systematic material and product design. Based on literature review in Chapter 4, it is established that design catalogs are previously used and validated for facilitating function-based systematic design in different domains successfully. However, the use of design catalogs for identifying and capturing material and product models to facilitate integrated materials and product design is not addressed in literature. The determination of phenomena and associated solution principles on multiple system levels is crucial and this allows for developing a wide range of principal solution alternatives and increase a designer's concept flexibility.

The use of design catalogs in past literature has been confined mechanical components like gearboxes, bearings, connections etc. The use of design catalogs for defining processing-structure-property-performance relationships via material models at multiple levels/scales using information generated through integration of such models is not addressed till now.

In this dissertation, the past efforts on function-based design and identification of phenomena and associated solution principles is leveraged to achieve the integrated design of materials, products and manufacturing processes. The focus in this dissertation is to establish processing-structure-property relations from a systems perspective by addressing phenomena and associate solution principles thereby integrating conceptual design of materials and products in a systematic and domain independent manner. To facilitate function-based systematic design at the level of phenomena and solution principles, the functionalities associated with design catalogs are leveraged to support a designer in designing material and product concepts in an integrated fashion.

The systematic approach followed is shown as a flow chart in Figure 1.7. The details are provided with description of each task in step by step manner in Chapter 4. The input needed, and the output generated is clarified, the internal information flow is checked to ensure sufficient information availability to execute next steps. Through critical evaluation of each step and the way individual constructs are put together, internal consistency of the systematic approach is verified and accepted.

The theoretical structural validity of the function-based systematic approach for conceptual materials and product design to achieve systematic model integration and information workflow is accepted by the logical procedure of literature review, gap analysis and development and evaluation individual and integrated constructs. Empirical studies need to be carried out to establish the usefulness and effectiveness of the approach and is addressed in Chapter 6.

4.9.2 TSV of Concept Exploration Framework and Goal-oriented Inverse Design Method

Theoretical structural validation refers to accepting the validity of individual constructs used in the concept exploration framework and the goal-oriented inverse design method and accepting the internal consistency of the way the constructs are put together. Theoretical structural validation involves systematically identifying the scope of the proposed framework's and design method's application, reviewing relevant literature and identifying the research gaps that is existing, identifying the strengths and limitations of the constructs used based on literature review, determining the constructs and approaches that can be leveraged for the concept exploration framework and inverse design method while reviewing literature on the advantages, disadvantages and accepted domains of application, and checking the internal consistency of the constructs both individually and when integrated.

In Chapter 1, the need for a concept exploration framework for the systematic concept exploration of materials and products is established. The CEF is inspired from the RCEM. The RCEM is critically reviewed in Chapter 3 and the functionalities and limitations associated with the method is established. The limitations of RCEM in terms of the following is discussed: i) RCEM does not take into account already available material and product models and relationships and focuses on establishing reduced order meta models/surrogate models, ii) RCEM has limitations in terms of exploration of solution space and does not have processors for establishing design scenarios for exercising the cDSP, iii) RCEM also lacks visualization tools and constructs for solutions space exploration and carry out design trade-offs, iv) RCEM cannot be individually used to support design exploration of process chains and thus needs support from a design method to achieve the same, v) RCEM in terms of EMI and DCI does not address robust design of a system having multiple conflicting goals that require different types of robust design across process chains. Based on these limitations, the requirements for an improved framework and a design method that facilitate the integrated design exploration of materials, products and associated manufacturing processes is established. To address the need for the inverse design method, the current research efforts focusing on inverse design exploration of material hierarchies are reviewed in detail in Chapter 1 and 2. The existing challenges and limitations are addressed and the need for a systems-based, top-down design exploration method is established in Chapters 1 and 2. In Chapter 4, the goal-oriented inverse design method is proposed. Several challenges associated with similar inverse design exploration methods like the IDEM is highlighted in Chapter 3 and some these challenges are addressed by the inverse design exploration method proposed in this dissertation. A detailed analysis of the functionalities offered compared to methods like IDEM is provided in Chapter 7. The basic idea of the method proposed in Chapter 4 for finding satisficing solutions in a multi-level, multi-stage process chain that involves the Processing-Structure (PS), Structure-Property (SP) relations is passing down the satisficing solution ranges in an inverse manner, from given final performance range to the design space of the previous space (defined by model input and output) with designer having the flexibility to choose solution of preference. The method is goal-oriented because the designer starts with the end goals that need to be realized for the product as well as process and then design the preceding stages to satisfy these end goals as closely as possible by exploring the design space. Then the design decisions that are made for the end requirements of the product/process after exploration are communicated to the stages that precede them to make logical decisions at those stages to satisfy the requirements identified thereby carrying out a design space exploration process in an inverse manner.

The proposed concept exploration framework is shown in Figure 4.8 and the goal-oriented inverse design method along with the associated steps is shown in Figure 4.9. The details of the framework and the design method with description of each steps to be performed to formulate, exercise and explore a complex systems design problem are provided in Chapter 4. The input needed, and the output generated is clarified, the internal information flow is checked to ensure sufficient information availability to execute next steps. Through critical evaluation of each step and the way individual constructs are put together, internal consistency of the concept exploration framework and the inverse design method is verified and accepted.

The theoretical structural validity of the concept exploration framework and the goal-oriented inverse design method to achieve inverse decision-based design exploration of process chains from a systems perspective is accepted by the logical procedure of literature review, gap analysis and development and evaluation individual and integrated constructs like the cDSP, surrogate modeling techniques, ternary analysis and plots, the inverse design method, etc. Empirical studies need to be carried out to establish the usefulness and effectiveness of the framework and the method. In Figure 4.10, a summary of validation of the systems-based design architecture developed in Chapter 4 is presented.

Theoretical Structural Validity (TSV) Validity of the constructs of the systems-based architecture • Chapter 4 – Based on literature reviews and gap analysis, it is remarked that, ✓ A function-based systematic method can be used to establish model integrations and information workflow for PSPP relationships ✓ A concept exploration framework integrated with an inverse design exploration method can facilitate integrated design exploration of materials, products and manufacturing processes	**Theoretical Performance Validity (ESV)** Usefulness of the architecture beyond examples • Generalizing Findings (Chapters 9, 10) • Arguing the validity of the systems-based design architecture developed beyond the example problems used in different domains (Chapter 10)
Empirical Structural Validity (ESV) Appropriateness of the examples chosen to verify the architecture • Horizontal Integration of Hot Rod Rolling Process Chain (Chapter 5) • Exploration of Microstructure Space for End Mechanical Properties of Rod (Chapter 5) • Vertical and Horizontal Integration of Hot Rod Rolling Process Chain (Chapters 6, 7, 8, 9)	**Empirical Performance Validity (EPV)** Usefulness of the architecture in examples • Systematic model integration (Chapter 6) • Inverse Design (Chapters 5, 6) • Robust Concept Exploration (Chapter 7) • Knowledge Capture, Reuse and Systematic Design Exploration (Chapters 8, 9)

Figure 4.10: Summary of validation of systems-based design architecture developed in Chapter 4.

4.10 Role of Chapter 4 and Connection with other Chapters in this Dissertation

In this chapter, the focus is on developing a systematic function-based approach for model integration and establishing information workflow. The function-based approach supports a designer in establishing the forward material workflow of the material/product system. Also, in this chapter, the focus is in developing a concept exploration framework that supports a designer in systematically formulating a design problem and exploring the solution space to identify satisficing design solutions. A goal-oriented inverse design method is proposed to support a designer in designing the system starting from the end goals and requirements. The method is proposed as a generic one with implications in several fields given there is models that establish the forward information workflow. The relationship of Chapter 4 with other chapters are shown in Figure 4.11. The utility of the systems-based design architecture developed in this chapter is tested using example problems in Chapter 5 and a comprehensive steel manufacturing example problem in Chapter 6. In Chapter 7, the concept exploration framework and inverse design exploration method proposed in this chapter are updated to include robustness. The interest in Chapter 7 for the designer is to identify satisficing robust solutions for multiple conflicting goals across a process chain.

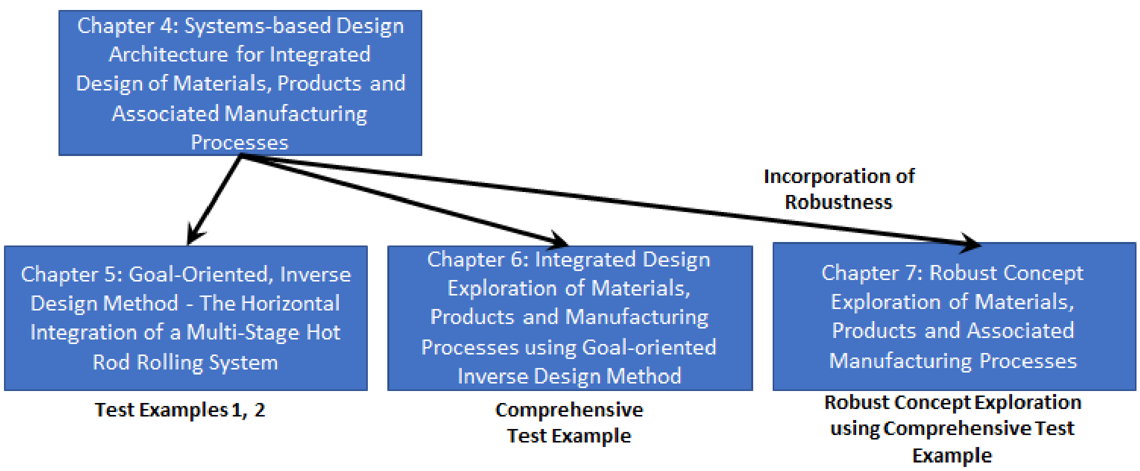


Figure 4.11: Relationship of Chapter 4 with other dissertation chapters.

Chapter 5: Goal-Oriented, Inverse Design Method - The Horizontal Integration of a Multi-Stage Hot Rod Rolling System

5.1 Test Example 1 – Model-based Horizontal Integration of Process Chains

Steel mills are involved in the production of semi-products such as sheets or rods with certain grades of steel. Process designers are very much aware of the operating constraints and process requirements for each of the operations as they are involved in the whole process day-in and day-out. Due to the advancements in material technology, new improved materials with enhanced properties are introduced to market posing a serious challenge to steel manufacturers. Suppose, that owing to the changing properties and performance requirements, manufacturers must produce a semi-product such as a rod with a newer grade of steel. This new steel grade has been used at laboratory scale to produce a rod, but the challenge posed to a steel manufacturer is to scale-up production. This requires the exploration of the ***design set points*** for each unit operation in the plant scale production of the rod (Tennyson, Shukla and coauthors 2015). Plant trials are one way of achieving this, which usually takes a lot of time and are expensive. Another option is to use computational models for exploring the design set points for these operations and thereby reduce the time and cost. However, these models are for specific phenomena that occur during an integrated process. Isolated models for individual processes will not give a true representation of the whole system and the desired solution. In this context, we define horizontal integration of processes as the facilitation of information flow from one process stage to another thereby establishing the integration of manufacturing stages to realize an end product. For exploring the design set points to achieve an end product, knowledge of the operation constraints and requirements are necessary for the newer grades of steel. However, this information is not available. Therefore, the first task is to identify operating constraints and design information for each unit operation. These operating constraints are imposed by the previous and subsequent unit operations as each process step is connected and information flows from one operation to another. Such process design problems are characterized by their complexity due to the large number of variables and their relationships at multiple stages. Two types of associations are possible for such problems – sequential and non-sequential. In the case of non-sequential association there is no definite order among the subsystems and most network problems falls under this category (Tiwari, Oduguwa and coauthors 2008).

In this chapter, we focus on demonstrating the inverse method for designing a multi stage hot rod rolling system for manufacturing a rod which is one of the semi-products in a steel manufacturing process chain. We view design as a decision-making process and believe that the fundamental role of a human designer is to make decisions. The hot rod rolling problem is sequential in which information flows from the first rolling stage/pass to the last rolling pass and the decisions made at the first pass influence the decisions that must be made at later passes (Tiwari, Oduguwa and coauthors 2008). We carry out the design process by means of a goal-oriented method that uses well established empirical models, response surface models along with the compromise decision support problem (cDSP) construct (Reddy, Smith and coauthors 1992, Mistree, Hughes and coauthors 1993, Allen, Seepersad and coauthors 2006) to support integrated information flow across different stages of rolling process. The method is goal-oriented because the decisions are first made based on the end requirements identified for the product and the process at the last rolling stage and these decisions are then passed to the preceding stages. Thus, the decisions at the first rolling stages are influenced by the decisions made at the last rolling stage thereby making this an inverse design scheme based on end goals. The cDSP is formulated using empirical models and the response surface models developed using simulation experiments and is then exercised for different design scenarios to explore the design space and to identify the best set of variables (design and operating set points) that meets the conflicting goals. Ternary plots are used to visualize these scenarios and to identify the appropriate feasible design space. The design of the multi-staged rolling process is carried out using the set points identified. The entire goal-oriented inverse design method is generic and has the potential to be applied to design any set of manufacturing processes where there is sequential flow of information (material) in order to realize an end product with specified target goals.

In Section 5.2, we describe the hot rod rolling process and the challenges associated with the modeling and design exploration of the process. In Section 5.3, we describe the problem in terms of the boundary defined and parameters considered in this study. The solution strategy in terms of process design scheme and the method adopted for this problem is also described in this section. In Section 5.4, we describe the empirical models and the response surface models developed. The mathematical formulation of the rod rolling problem using the cDSP construct is also presented in this section. The ternary analysis for visualizing and exploring the solution space is covered in Section 5.5. The key findings and closing remarks are presented in Section 5.6. We showcase the design calculations in Section 5.7.

5.2 The Hot Rod Rolling Process

Hot rod rolling is a complex, multi-stage manufacturing process that plays a critical role in producing specific grades of steel with specified target properties. The complexity in the process arises not only from the high working temperatures, but also because of the requirement to precisely control the process parameters to obtain the desired microstructure and properties. Due to increasing competition facing steel and aluminum manufacturers, there is an increasing need to make this process more flexible, agile and energy efficient**.** Process designers must determine cost effective solutions to assist in decision making and improve efficiency. Multi-pass rolling systems design (RSD) is the preparation of a set of rolls that are laid in series in the right sequence for different rolling passes to achieve a desired profile (Oduguwa and Roy 2006). RSD helps in producing workpieces with a desired work profile subject to the constraints of the mill with an acceptable quality, minimum cost and maximum output. This is equivalent to a search problem where the design space is explored to satisfy the requirements in order to determine the required number of passes to achieve a product of the required dimensions with minimum defects by controlling design variables. This requires considering different behaviors of the material during rolling including geometrical, mechanical, thermal, thermo-mechanical and metallurgical behaviors at multiple scales. Rolling is a multi-disciplinary process involving reheating, inter-stand operations, mill engineering, roll pass design, metallurgical transformations, etc. (Oduguwa and Roy 2006).

The challenges associated with the design of a rolling system arise from the complex nature of the process due to the large number of process parameters, constraints, bounds, etc., the multi-staged nature of process involving handshakes[1], the hierarchical nature in terms of process-structure-property-performance relationships, multi-disciplinary nature requiring knowledge and expertise from different fields, complex relationships between stress/strain-temperature and microstructure that requires model coupling at different scales (Roberts 1983, Lapovok and Thompson 1994, Michalewicz 1995, Shin 1995, Lapovok and Thomson 1997, Roy, Tiwari and coauthors 2000, Jupp 2001, Oduguwa and Roy 2001, Oduguwa and Roy 2002, Oduguwa, Tiwari and coauthors 2004, Oduguwa and Roy 2006). The challenges are addressed in detail below.

The challenges associated with the design of a rolling system are listed below in detail (Oduguwa and Roy 2006):

i) *Complex search space*: Rolling is a complex deformation process involving several process parameters, hard constraints and bounds so it is difficult to define the search space for rolling systems design (Michalewicz 1995, Roy, Tiwari and coauthors 2000). The functions involved in the process are non-linear, discontinuous and require coupling with models that are at different scales. Functions relating all the influencing parameters involved for carrying out design exploration are not directly available for this problem.

ii) *Multi-staged process*: Hot rolling is a multi-stage problem requiring multiple passes to produce the end product. Hence the sequential nature of linked unit operations that can be seen in a steel making process chain can be attributed to the hot rolling process. Each of these passes has essential requirements for achieving the desired property/performance of the end product. The output of one pass becomes the input of the next pass and there

[1] Handshake, the flow of information between passes as the output of one pass is the input to the next. Thus, the passes are linked by the relationships that exist when material flows between them.

is a handshake between each pass which must be designed (Oduguwa, Tiwari and coauthors 2004).

iii) *Hierarchical nature*: The hierarchical nature of the rolling process arises not only from process-structure-property-performance relationship in the material system but also from the way levels are defined in the system in terms of objectives to be met (Oduguwa and Roy 2002). For example, at the top level an engineer is interested in the productivity and quality of output from the system. At a lower level an engineer is interested in the number of passes required to achieve a target and the form of roll grooves for a particular operation, etc. (Lapovok and Thompson 1994, Shin 1995, Lapovok and Thomson 1997).

iv) *Multi-disciplinary problem*: The various aspects of the rolling process such as manufacturing, mill design, thermal aspects, material aspects, computational aspects, metallurgical phenomenon, modeling and simulation, process design, quality control, etc. requires knowledge, and expertise from a wide range of engineering fields making the entire process highly complex.

v) *Complex relationships:* Stress/strain, temperature and microstructure have such a complex relationship that is essential that they are analyzed for modeling the process (Jupp 2001). Accurate measures of each of them are required to fully describe the behavior of the material. For example, the temperature developed in the material while rolling involves the heat that is developed due to plastic deformation. This temperature developed influences the microstructure during rolling. Stress/strain that occurs in rolling affects the stored energy in the material and influences the recrystallization which changes the microstructure. Similarly, the deformation temperature, strain and strain rate affects the stress developed in the material while rolling (Jupp 2001). All these complex relationships need to be modeled precisely. This is a huge challenge from a design perspective.

vi) *Multi-dimensional:* Rolling involves various product and process parameters such as rolling speed, rolling temperature, reduction ratio, the geometry/work profile, spread of the workpiece in rolling, temperature distribution, friction conditions, heat transfer, cooling conditions, thermal conditions of roll, etc. (Roberts 1983). The challenge of bringing these varied parameters into a single formulation is a complex task.

vii) *Knowledge driven process:* Rolling system design is a knowledge driven process and is mostly qualitative in nature (Oduguwa and Roy 2001). The traditional way of rolling system design involved some expert personnel who has sound knowledge in the mixture of engineering fields that are involved, having many years of experience in practically handling the system. However, with the evolving trends in market and rise in competitions in the industry the requirement is to design the system as fast as possible in the best way with changing demands. This requires people with expertise in multidisciplinary areas to work together and share knowledge in order to effectively add value to the system design. Also, the rise in computational tools and techniques has to be exploited in the best possible way to bring in new design changes and modifications so as to improve the design process.

In this chapter, we address some of these challenges by developing a design method using simulation models along with the compromise decision support problem construct and solution space exploration techniques to design the multiple stages of a rolling system ensuring information flow to support horizontal integration of stages in order to realize an end product. The complex search space is managed by framing a proper boundary for the problem formulated and will be explained in Section 5.3. Well established empirical models along with a finite element model developed for rolling is used to define the complex relationships. The academic and industrial collaboration involved in this work between people from mechanical, design, material science and metallurgy domains helped to deal with the multi-disciplinary nature of the problem. The decision support problem constructs along with the solution space exploration techniques supports a designer to manage the uncertainty associated with models and addresses a way of handling such complex problems from a systems design perspective. In the next section, we describe the foundational construct for our work – the compromise decision support problem (cDSP) construct.

5.3 Foundational Constructs – The cDSP and Solution Space Exploration

In the model-based realization of complex systems, we have to deal with models that are typically incomplete, inaccurate and not of equal fidelity. This brings into the design process different types of uncertainties associated with the system, the parameters considered, the models considered and the uncertainties due to their interactions (McDowell, Panchal and coauthors 2009). From the decision-based design perspective, the fundamental role of a human designer is to make decisions given the uncertainties associated. In this regard, we define robust design as design that is relatively insensitive to changes. This involves achieving a desired performance for the system while the sensitivity of the performance objectives with respect to the system variables are minimized (Ebro and Howard 2016). Thus, the designer's objective here is to find '*satisficing'* solutions that showcase good performance given the presence of uncertainties and not optimum solutions that are valid for narrow range of conditions while performing poorly when the conditions are changed slightly. The cDSP is proposed by Mistree and coauthors for robust design with multiple goals (Bras and Mistree 1993, Mistree, Hughes and coauthors 1993). The fundamental assumption here is that the models are not complete and accurate; opposed to the fundamental assumption in optimization where the models are complete and accurate, and the objective function can be modeled accurately so that solution obtained is implementable. Hence the cDSP construct is anchored in the robust design paradigm first proposed by Taguchi (Taguchi). Using the cDSP construct several solutions are identified by carrying out trade-offs among multiple conflicting goals. The obtained solutions are then evaluated by carrying out solution space exploration in order to identify the best solutions that satisfy the specific requirements identified. The cDSP is a hybrid formulation based on mathematical programming and goal programming. In goal programming, the target values for each goal are defined and the emphasis is on achieving the target for each goal as close as possible. In cDSP, different weights are assigned to these goals and the compromised solutions obtained for different appropriate weights are explored.

The formulation and solving of the cDSP followed by exploration of solution space for any problem are carried out using the steps in Concept Exploration Framework (CEF). A generalized 4 step method is illustrated in Figure 5.1 that captures the overall steps of CEF in a simplified manner (Shukla, Goyal and coauthors 2014, Shukla, Goyal and coauthors 2015, Nellippallil, Song and coauthors 2016). After having defined the problem and requirements, Step 1 is to identify the theoretical and empirical models and relationships that exist for the process/problem of interest. Response surface models are developed to represent certain parameters as a function of the process variables. These response surface models are developed by carrying out simulation experiments, which could be finite element model-based experiments, or other similar experiments depending on the problem of interest. The response surface models developed through simulation experiments along with the theoretical and empirical models and relationships available are used to formulate the cDSP for the process/problem that is under study (Step 2).

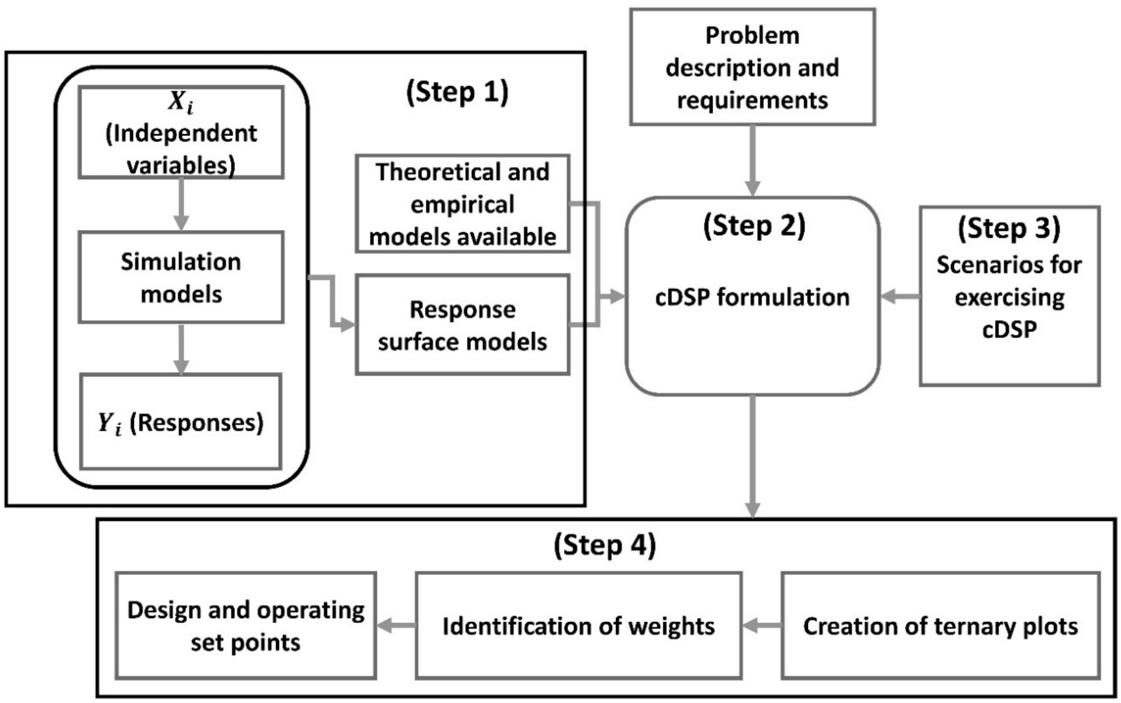


Figure 5.1: cDSP based steps to predict set points (Includes key steps of CEF – a simplified form)

In Step 3, we exercise the cDSP for different design scenarios and the results are recorded for each scenario. These scenarios are identified by assigning different weights to the goals of the cDSP formulated. The collective design results for different scenarios are visualized using ternary plots and the feasible design space that satisfies the design requirements in the best possible manner is identified (Step 4). Multiple solutions that satisfy the design requirements are identified from the feasible design space. The designer makes design decisions from the set of solutions depending upon the preferences set for the problem under study. For the manufacturing problem under consideration, these identified design solutions are the design and operating set points.

In the next section, we describe the goal-oriented method for carrying out sequential process design of manufacturing stages utilizing the cDSP construct and solution space exploration techniques to achieve the integrated design of the product and the processes. We use the hot rod rolling system design problem as an example to illustrate the efficacy of the method presented.

5.4 Problem Description and Application of Goal-Oriented Inverse Design Method

Rod *Quality* depends on many factors starting from the material microstructure to the macrostructure. Key factors influencing quality include steel composition, segregation of alloying elements, distribution of inclusions, microstructure and rod geometry. Ovality is one such geometrical property which is defined as the difference between the height of the rod section and the width from the center of the rod (Oduguwa and Roy 2002). Ovality is desirable in the initial roll passes as it helps to reduce the geometry of the square billet. However, is not desired in the end rod product as the output requirement is for a round/circular rod. Thus, there is a need to minimize/control the ovality induced at the last rolling stage. One way of minimizing ovality is to insure high contact between the workpiece and the roll. However, this requires in high rolling loads and thus minimization of ovality is possible at the expense of a high rolling load. Rolling load influences the overall functioning of the process and is representative of the overall process performance (Tiwari, Oduguwa and coauthors 2008). Rolling load ensures flow of material across passes. Higher rolling loads require increased rolling power requirements and can also yield deflections in the rolling system which is detrimental to the rolls themselves. This adds to the costs of the process. Hence maintaining the rolling load within a target value in an acceptable range is necessary but conflicts with the objective of minimizing ovality. Excessive rolling load resulting in roll breakage and wear are detrimental to production efficiency as it conflicts with rolling process *productivity* which is expressed in terms of throughput (Tiwari, Oduguwa and coauthors 2008). Therefore, this is a multi-objective design problem with three objectives: minimize ovality, maximize throughput and minimize rolling load subject to the rolling constraints.

In this process, the output of one stand is input for the next and there are successive reductions of the billet at each rolling stand. Therefore, modeling this process demands information exchange between these stands as the intermediate product developed in one stand will affect the form, properties and performance of the product developed at consecutive stands that follow which results in an impact on the end product. Therefore, a method to ensure the determination of the right combination of design variables to meet the constraints for each rolling pass and thereby meet the overall performance requirement is essential.

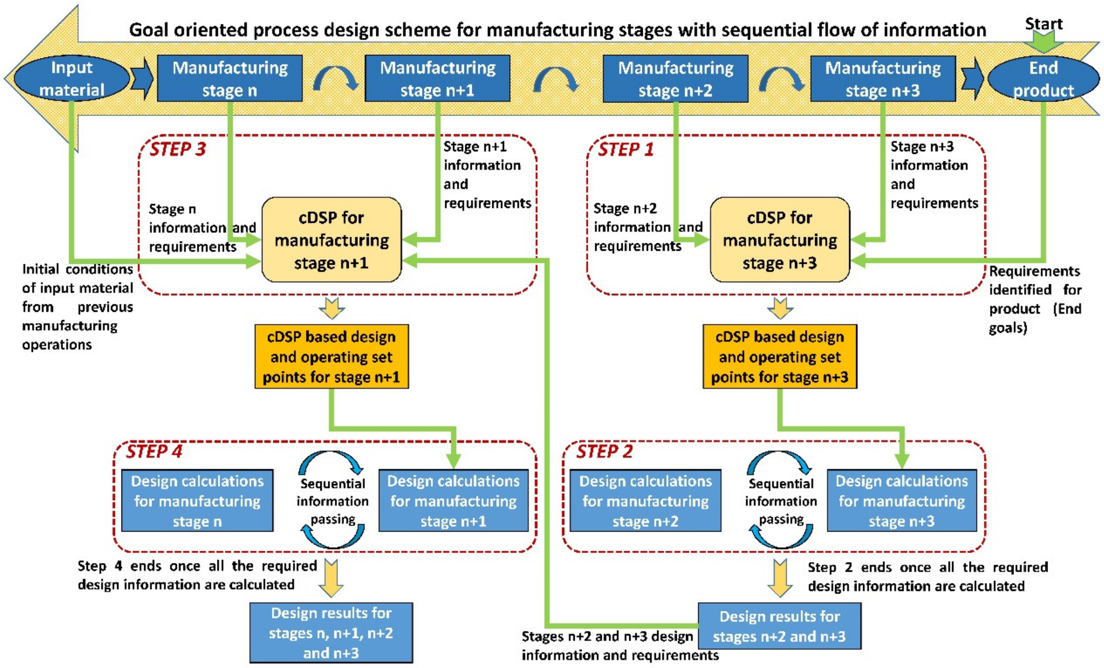


Figure 5.2: Goal oriented, Inverse Design method for manufacturing stages having sequential flow of information

We have developed a computational method for this sequential problem that has information exchange between rolling passes and is used to identify the set points of the various rolling passes involved. For this example, we assume that there are four passes that follow a square-oval, oval-round, round-oval and oval-round sequence moving from Pass 1 to Pass 4. The final requirement of the product of Pass 4 is to have minimum ovality, maximum throughput and a minimum rolling load value within an acceptable range. The different sequential relationships that exist among passes define the problem. The constraints for the process include the range for rolling load, range for throughput, maximum value of rolling wear, minimum and maximum values of elongation and spread for each pass. The cDSP for two passes – Pass 2 and Pass 4 are formulated. The cDSP for Pass 4 takes into account the end goals identified for the problem in terms of ovality, throughput and rolling load. The cDSP for Pass 2 is developed to support information flow across passes and perform the design of other passes. The goals for the cDSP for Pass 2 are maximization of throughput (maintaining target throughput values achieved for Passes 3 and 4) and achieving a target value of rolling load within a defined range. The ovality goal is an end goal for the rod produced after Pass 4 and is not required for Pass 2 as the material is again subjected to deformation to oval shape in Pass 3 to facilitate progressive breakdown of geometry.

This goal-oriented sequential inverse design method proposed to design the rolling system will be explained using the information flow diagram shown in Figure 5.2. In order to generalize the method, we are naming the four stages of rolling passes as "manufacturing stages" which are numbered from "n" to "n+3". We will be using the term "end product" for the rod developed after rolling and the term "input material" to refer the billet that comes from the continuous casting stage of the steel manufacturing process chain. The arrows that denote the flow of information needs to be followed to visualize the design process. There are four steps in the design method for designing these four manufacturing stages to realize the end product.

Step 1: *Formulation of cDSP for the last manufacturing stage (n+3) using the information from the end product to be realized and the sequential relationship existing between stages n+2 and n+3*

The whole design process starts with the identification of requirements for the end product to be produced after the manufacturing stage n+3 as shown in Figure 5.2. In Step 1, the cDSP for manufacturing stage n+3 is formulated. The cDSP is formulated using the information available on manufacturing stage n+3 and by incorporating the sequential relationship the stage n+3 has with manufacturing stage n+2. The requirements identified for both the end product and for the manufacturing stage n+3 are embodied in this cDSP as goals. The requirements from manufacturing stage n+2 along with the sequential relationships that exists are captured by the "Given" and "Satisfy" keywords of the cDSP formulated. The cDSP is exercised for different identified scenarios by assigning different weights for each goal and the scenarios that suits the design requirements the most are selected after carrying out solution space exploration using ternary plots. The system variables identified are basically the design and operating set points for manufacturing stage n+3.

Step 2: *Design of stages n+3 and n+2 using the design and operating set points identified and the information available from end product requirements*

In Step 2, the design and operating set points generated for manufacturing stage n+3 from Step 1 are used to design the stage by carrying out design calculations to determine information. Design calculations essentially involve analysis to check the achievement of goals and using the design and operating set points generated to calculate the values of parameters of both the manufacturing stages using the sequential relationships that exist between them that was incorporated in the cDSP formulated. First, the design and operating set points are used to generate information for stage n+3. The new design information generated for stage n+3 has a sequential relationship with manufacturing stage n+2 and hence they are passed to carry out the design of manufacturing stage n+2. Once new design information is generated for manufacturing stage n+2, they are again passed to manufacturing stage n+3 to come up with information which were unknown before. Thus, a cyclic process of information exchange is carried out at this step to generate new information for both the manufacturing stages using the design and operating set points identified in Step 1. Step 2 ends once all the required design information for the problem formulated is identified.

Step 3: *Formulation of cDSP for manufacturing stage n+1 using the design information generated for stages n+2 and n+3; and the sequential information existing between stages n and n+1; along with information on input material*

In Step 3, the cDSP for manufacturing stage n+1 is formulated. The design information generated for stages n+2 and n+3 are communicated to the cDSP for manufacturing stage n+1. The "Given" keyword of this cDSP captures the design information from stages n+2 and n+3. Along with that sequential information related to stages n and n+1, the initial conditions of input material are also captured during the formulation of this cDSP using the "Given" and "Satisfy" keywords. Specific requirements identified for manufacturing stage n+1 are formulated as system goals. The cDSP formulated is exercised for different scenarios to find design and operating set points for manufacturing stage n+1 that satisfies the requirements identified for the stage as well as the end requirements of product.

Step 4: *Design of manufacturing stages n+1 and n using the design and operating set points identified; the information available from input material and the information from stages n+2 and n+3*

In a similar fashion to Step 2, the design and operating set points identified for manufacturing stage n+1 are used to design the stage by carrying out design calculations. The design information generated for stage n+1 is passed to design manufacturing stage n using the sequential relationships that exists. The information available from the input material is also used at this stage to carry out the design of manufacturing stage n. The new design information generated for stage n is then communicated back to stage n+1 to determine stage n+1 information that was unknown before. The sequential information passing is carried out until the required design information for the problem formulated are identified. The design information generated for stages n and n+1 are also used to carry out design calculations for stages n+2 and n+3 as the information from those stages are available in the cDSP formulated for stage n+1. Hence the final result obtained using this goal-oriented, sequential method is the design information for all the four stages n, n+1, n+2 and n+3 in order to realize the requirements identified for the process as well as the end product.

The proposed four step method using the cDSP construct is generic and the method can be used for the design of other such unit operations where there is a sequential flow of information by identifying the design and operating set points that satisfy certain system goals and then design the entire system using these identified set points.

In Section 5.5, we describe the empirical models and theoretical models as well as the important relations that exist for the rod rolling problem under study. We also describe the response surface models that are developed as a part of the study here in this section. In Section 5.5.2, we explain the cDSP formulation for the Pass 4 (stage n+3) of the hot rod rolling problem. The cDSP for Pass 2 (stage n+1) which follows a similar pattern to that of Pass 4 will be explained in the Appendix A.1. In Section 5.6, we explain the scenarios identified for the cDSP for Pass 4 and visualization of the scenarios using ternary plots to identify the design and operating set points.

5.5 Designing a Multi-Pass Rolling System

The purpose of roll pass design is (Wusatowski 2013):

a) To ensure the production of a correct profile within permissible dimensional limits and with a good surface finish, free of surface defects, at the same time keeping the internal stress in the section being rolled to a minimum, b) to ensure the maximum output at minimum cost, c) to ease the working conditions of the rolling crew, d) to reduce roll wear to a minimum. For our hot rod rolling example problem, the design requirements are:

- Achieve a round profile by minimizing the ovality at the end of the fourth rolling pass.
- Maximize throughput while ensuring that product quality is not reduced.
- Maintain a minimum rolling load within a specified range and ensuring that it never exceeds the maximum.
- Control the elongation and spread during the rolling process within specified limits.
- Control the entry and exit speeds of the stock within specified limits.
- Ensure that the wear on the rolls is within an acceptable limit.
- Obey the sequential relationships between the different rolling passes (in terms of geometry and workpiece profile, etc.)

First a process model for rolling system is developed that ensures the flow of information through the sequential relationships between rolling passes as shown in Figure 5.2. In Figures 5.3a and 5.3b, we represent the geometry for the oval and round passes with key dimensions of interest for the rolling problem. The entire breakdown sequence consists of two more such passes in a cascaded fashion where the output of an oval pass is the input for a round pass. The rolls are laid horizontally and vertically for the oval and round passes respectively. Therefore, the horizontal major axis of the oval stock in Figure 5.3a coincides with the vertical axis of a round pass as in Figure 5.3b. A detailed description of the models along with the mathematical expressions related to the goals identified is provided in the following sections.

5.5.1 Major Relations and Calculations for the Rolling Pass Design Study

Condition of Constant Volume

This condition requires that the volume of the material rolled remains the same after each pass.

$$V = Fl = F_j l_j = V_j \qquad \textbf{Equation 5.1}$$

where V_j is the volume of the material after pass j, F_j is the cross-sectional area after pass j, l_j is the dimension of metal in the rolling direction. The cross-sectional area F_j is (Wusatowski 2013)

$$F_j = h_j b_j \qquad \textbf{Equation 5.2}$$

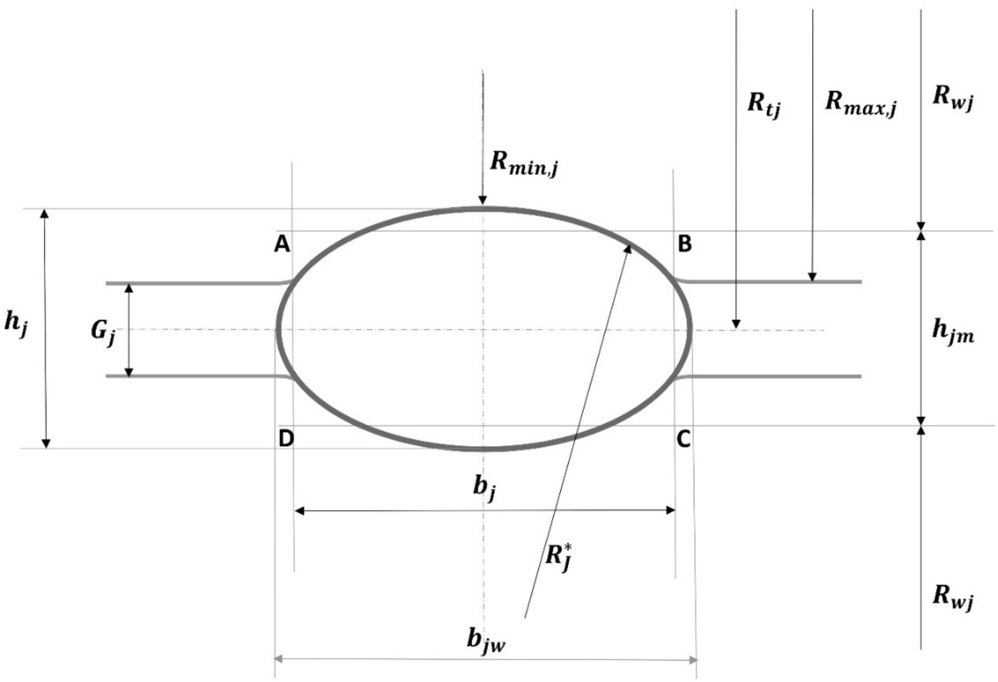
This expression is valid for the rolling of rectangular cross sections. For the rolling of non-rectangular cross sections such as bars, shapes, rails, etc., an additional term, the mean height of stock is introduced this is expressed as (Wusatowski 2013)

$$h_{jm} = \frac{F_j}{b_j} \qquad \textbf{Equation 5.3}$$

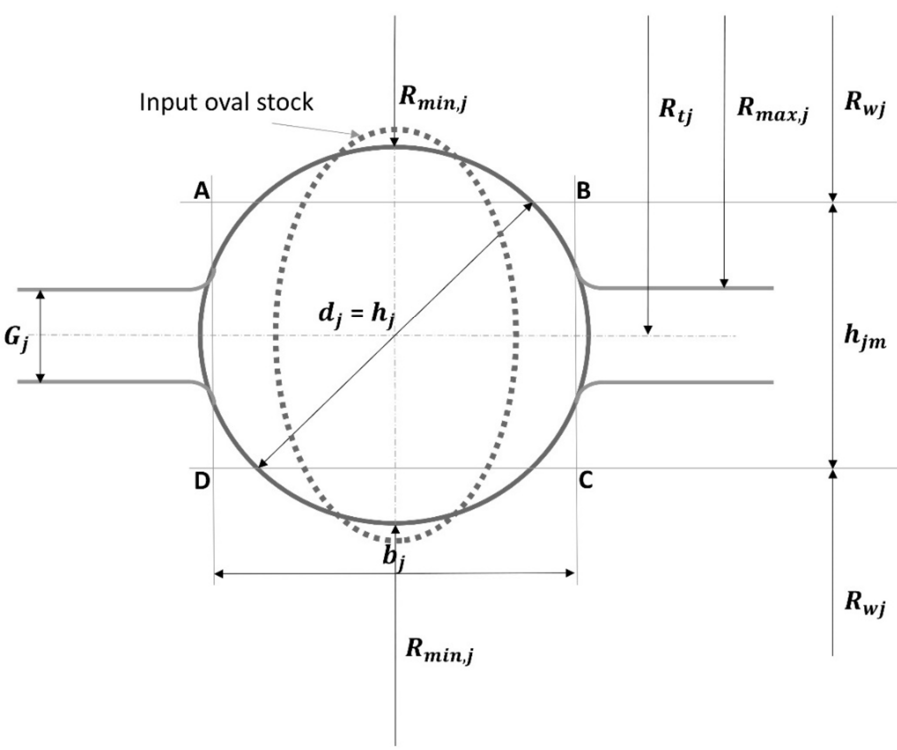
It is calculated by dividing the cross-sectional area F_j by the maximum breadth b_j of the filled section for a particular pass j.

Thus the condition of constant volume during rolling is (Wusatowski 2013)

$$\begin{aligned} V_0 = F_0 l_0 = h_{0m} b_0 l_0 = V_1 = F_1 l_1 = h_{1m} b_1 l_1 \\ = V_n = F_n l_n = h_{nm} b_n l_n \end{aligned} \qquad \textbf{Equation 5.4}$$



(a)



(b)

Figure 5.3 a and b: Oval and round passes respectively with key dimensions

On dividing these relations (Wusatowski 2013)

$$\frac{h_{2m}b_2l_2}{h_{1m}b_1l_1} = \gamma_m\beta\lambda = 1 \qquad \textbf{Equation 5.5}$$

where,

$$\gamma_m = \frac{h_{2m}}{h_{1m}} = mean\ coefficient\ of\ draught \qquad \textbf{Equation 5.6}$$

$$\beta = \frac{b_2}{b_1} = spread\ in\ rolling \qquad \textbf{Equation 5.7}$$

$$\lambda = \frac{F_1}{F_2} = \frac{h_{1m}b_1}{h_{2m}b_2} = \frac{l_2}{l_1} = \frac{w_2}{v_1} = coefficient\ of\ elongation \qquad \textbf{Equation 5.8}$$

where v_1, is the entry speed during a rolling pass, w_2 is the exit speed during the same pass. For round-oval rolling for rod production, an equivalent rectangle approximation (shown by ABCD in Figures 5.3a and 5.3b) is carried out and the geometrical parameters are identified during the design process.

Rod Ovality

The ovality of the final rod product is a serious concern for manufacturers. It is mainly due to: i) geometric factors such as the incoming width and height of the workpiece, radius of the roll, and the roll gap, ii) metallurgical parameters such as strain values, stress developed, temperature of material during rolling, iii) rolling process parameter such as rolling speed (Oduguwa and Roy 2002).

The geometric factors like incoming height (h_{j-1}) and width (b_{j-1w}) of the workpiece will define the amount of elongation and spread that occurs while rolling. This helps to determine the ovality of the rod produced. The roll radius (R_{max}) and roll gap (G_j) are critical parameters defining rolling contact and output size. Both of these parameters affect the ovality induced. The temperature (T_j) during rolling is also critical and determines the material flow. Higher temperature favors flow and thus plays a role in defining ovality. Also, the rolling speed (N_j, measured in rpm) affects the geometry formed.

Although these variables are known to influence the ovality during rolling, the exact relationships with respect to these variables are not available and therefore simulation experiments using finite element (FE) based rolling model are carried out to determine models to predict ovality as a function of the variables identified. Appropriate ranges for the variables of interest are identified and a two-level fractional factorial design of experiments (DoE) is carried out. The steps associated with the same are (Oduguwa and Roy 2002, Montgomery 2008):

Step 1: Fractional factorial design

The factors and factor levels for the simulations are depicted in Table 5.1.

Table 5.1: **Factors and factor levels for design simulation**

Level	h_{j-1} **mm**	b_{j-1w} **mm**	G_j **mm**	$R_{max,j}$ **mm**	T_j **K**	N_j **rpm**
1	22	55	5.5	200	1280	20
-1	18	52	3.5	155	1270	10

A two level six factor fractional factorial design is used for the DoE. FE simulations are carried out using the experimental design for the different runs of DoE. The coupled temperature-displacement finite element model developed for the fourth oval to round rolling pass in ABAQUS is shown in Figures 5.4 and 5.5.

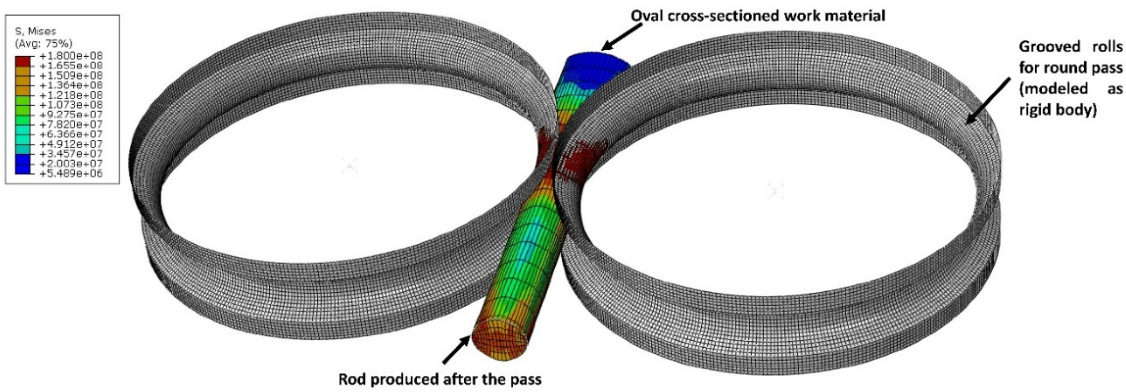


Figure 5.4 Geometry and mesh of the FE model developed for rod rolling

The material being rolled is modeled as a deformable body of oval shape and is meshed using C3D8RT, an 8-node thermally coupled brick element. The material properties, for example, conductivity as a function of temperature, elastic properties, etc. for steel is assigned to the billet. The plastic behavior of the material is described by assigning yield stress values for steel at different plastic strains. The rollers with round grooves are modeled as a discrete rigid body and are meshed using R3D4 elements. The surface profile of the rolls are modeled using the analytical models developed by Lee and co-authors (Lee, Choi and coauthors 2000). The oval shaped billet is constrained to move along the rolling direction. The rollers are constrained to only rotate along the axis of rotation. An initial temperature is input to the billet before rolling which serves as the temperature for rolling. A surface-to-surface contact is defined between the billet surface and the grooves of the rollers. The kinematic contact method is selected for mechanical constraint formulation. The heat transfer coefficient is defined between roll gap and to air and the reported values from literature are selected (Phaniraj, Behera and coauthors

2005). The coefficient of friction value is set to 0.3 for the rolling simulations to develop the response surfaces for ovality. In preliminary studies, the coefficient of friction was shown to have a negligible effect on ovality, however it does have an effect on roll wear as discussed later. The heat due to plastic deformation value of 0.9 is used (Galantucci and Tricarico 1999). The angular velocity of roll is applied based on average strain rate associated with the rolling pass schedule (Lee, Choi and coauthors 2002). The developed FE model is validated for temperature predictions at billet center and surface, stresses developed and geometry such as the final area of the rod produced following a similar pattern as in our previous works (Nellippallil, De and coauthors , Goh, Ahmed and coauthors 2014). The value of ovality in the rods is measured for each run and is recorded from the FE results as the absolute difference between the height and width of rod section from the center.

Step 2: Model fitting

In step 2, we develop response surface models for ovality by fitting the results obtained with a second order polynomial. We carry out ANOVA and find that the effect of roll radius is negligible by analyzing the *p*-values obtained and thus roll radius is eliminated from the list of factors. The parameters of the second order polynomial are determined using least squares regression analysis by fitting FE responses to input data. More detailed descriptions of RSM techniques and tools can be found in Myers and Montgomery (Montgomery and Myers 1995) and Simpson and co-authors (Simpson, Poplinski and coauthors 2001).

The response surface model thus developed for ovality with a R^2 value of 0.99 is

$$O_{vj} = 8.6153 \times G_j + 27.539 \times b_{j-1w} - 0.0009 \times N_j + 0.0001 \times h_{j-1} \times T_j - 0.0023 \times h_{j-1} \times N_j - 0.0041 \times G_j \times T_j - 0.0269 \times G_j \times N_j - 0.0216 \times b_{j-1w} \times T_j - 0.0026 \times b_{j-1w} \times N_j$$ **Equation 5.9**

The response surface of ovality model as a function of height and width of incoming workpiece with fixed values of other variables is shown in Figure 5.6a. In Figure 5.6b, we show the response of ovality model as a function of roll gap and roll rpm.

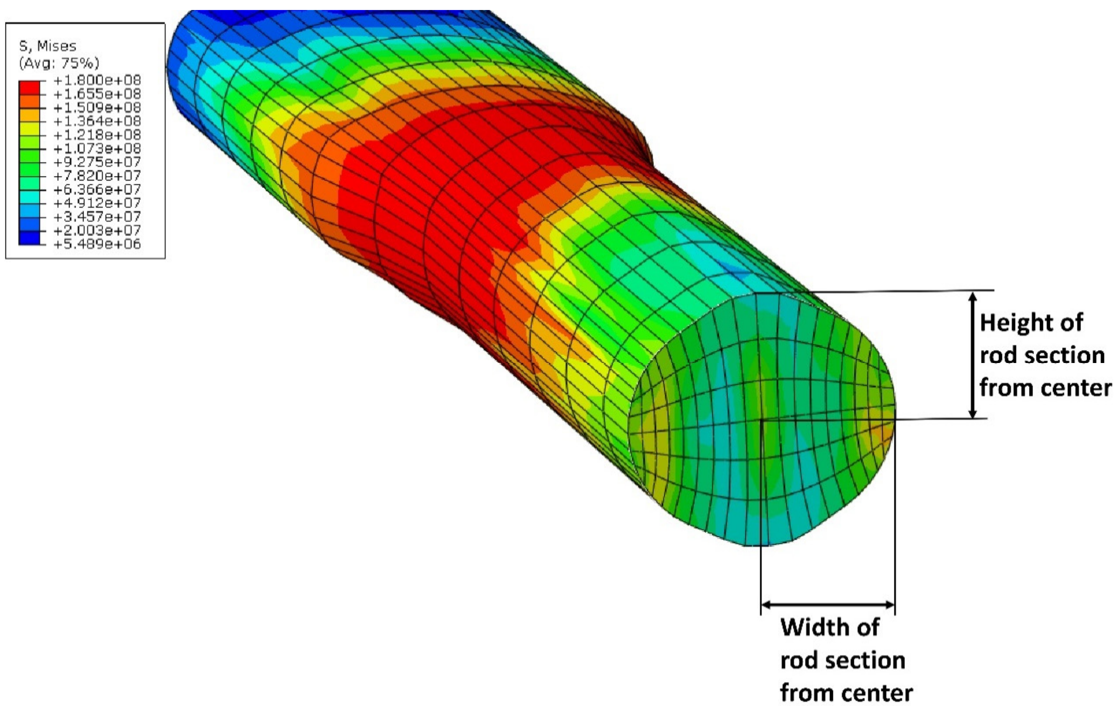


Figure 5.5: Cross section of rod produced using FE simulation showing the stress contours and the geometrical variables measured for calculating ovality

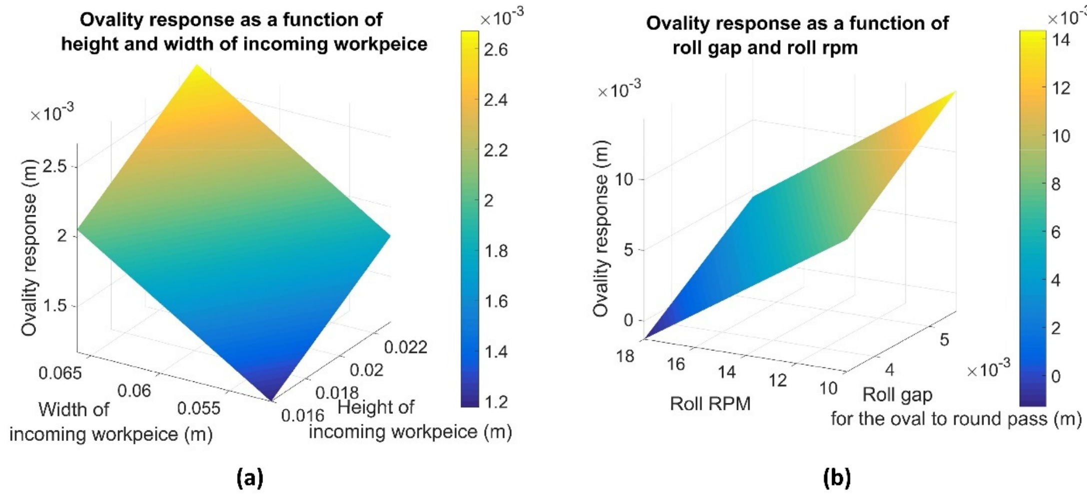


Figure 5.6 a and b: Ovality responses for different variables considered

Throughput

Throughput defines process productivity. Throughput is expressed as a function of exit speed during rolling (w_j) and the final stock cross sectional area (F_j) that leaves the roll (Wusatowski 2013). The subscript *j* refers to pass number.

$$T_{pj} = F_j w_j \qquad \textbf{Equation 5.10}$$

F_j , the area of cross section for the round pass is

$$F_j = \left(\frac{\pi h_j^2}{4}\right) \qquad \textbf{Equation 5.11}$$

where h_j = d_j = rod diameter of rod as shown in Figure 5.3b.

For an oval sectional with a defined (*b/h*) ratio, the cross-section area is (Wusatowski 2013)

$$F_j = \left(\frac{(\frac{b}{h})^2 h_j^2}{4.35} \right)$$ **Equation 5.12**

where b/h is a ratio defined for pass j. The equation is based on the values obtained from a nomogram for determining h_m/h_{max} for common ovals relative to s (roll clearance), h and b (Wusatowski 2013). The expression for b_{jw} is (Wusatowski 2013)

$$b_{jw} = (b/h)h_j$$ **Equation 5.13**

Hence from Equations 13 and 14

$$b_{jw} = \sqrt{4.35F_j}$$ **Equation 5.14**

Rolling load

Excessive rolling load in various passes can affect the productivity while minimum ovality is achieved through high contact and higher loads. Shinokira and Takai (Shinokura and Takai 1982) introduce a method for calculating the effective roll radius, the projected contact area, the non-dimensional roll force and the torque arm coefficient expressed as simple functions of the geometry of the deformation zone. The rolling load (P) is defined as a function of a multiplier (Q_s), projected contact area (F_p) and mean flow strength of material ($2k$).

$$P = Q_s F_p (2k)$$ **Equation 5.15**

The mean flow strength of material ($2k$) in the pass is approximated as the yield stress of material under plain compression as expressed in Sim's model (Sims 1954). The projected contact area is given by (Said, Lenard and coauthors 1999),

$$F_p = \frac{2}{\pi}\left(0.9b_j\right)L_d = 0.573b_jL_d \quad \textbf{Equation 5.16}$$

where b_j is the final width after a pass. The projected length of contact in the deformation zone is (Lee, Choi and coauthors 2002),

$$L_d = \sqrt{\left(R_{max} - \frac{h_o - G}{2}\right)(h_i - h_o)} \quad \textbf{Equation 5.17}$$

where R_{max} is the radius of the roll, G is the roll gap, h_i and h_o are the height of the incoming and outgoing workpiece, respectively. Since there is a 90° rotation from an oval to a round pass, the incoming height of the workpiece for a round pass will be the width from the oval pass that precedes it. For a typical round pass j, the formula becomes

$$L_d = \sqrt{\left(R_{max,j} - \frac{h_j - G_j}{2}\right)(b_{j-1w} - h_j)} \quad \textbf{Equation 5.18}$$

The multiplier Q_s is given by (Said, Lenard and coauthors 1999)

$$Q_s = -0.731 + 0.771M + \frac{1.61}{M} \quad \textbf{Equation 5.19}$$

where M depends on the projected contact area, F_p , and the initial and final cross sections, F_i and F_o respectively (Said, Lenard and coauthors 1999).

$$M = \frac{2F_p}{F_i + F_o} \quad \textbf{Equation 5.20}$$

For a typical pass j, $F_o = F_j$ and, $F_i = F_{j-1}$

Roll wear during rolling

Reducing the wear during rolling is important. To estimate it, we use an expression that estimates the change in the radius of a work roll due to wear during rolling (Roberts 1983). Roll wear is expressed as (Pietrzyk, Cser and coauthors 1999)

$$\frac{\Delta R}{l_j} = \frac{K\mu_j L_d^2 r\bar{\sigma} exp\left[\frac{\mu_j L_d}{h_i(2-r)}\right]}{D^2\sigma_{roll}}$$ **Equation 5.21**

where ΔR is the change in roll radius, l_j is the rolled length, K is the wear constant, μ_j is the coefficient of friction, L_d is the projected contact length, r is the reduction during rolling, $\bar{\sigma}$ is the flow strength of the material rolled, σ_{roll} is the flow strength of roll, D, the roll diameter. Here, we use a K = 8×10^{-5}, $\bar{\sigma}$ = 250 MPa for the material rolled and $\sigma_{roll} =$ 600 MPa (Roberts 1983, Pietrzyk, Cser and coauthors 1999). The rolled length l_j is

$$l_j = \lambda_j \times l_{j-1}$$ **Equation 5.22**

The value of l_{j-1} is assumed to be 3 m. The coefficient of friction, μ_j , is a system variable in this study and is between 0.3 to 0.45.

5.6 The cDSP For Roll Pass 4 (Step 1 of Method Proposed)

In this section we describe the mathematical formulation of the compromise decision support problem (cDSP) for Pass 4 of rod rolling. The cDSP for Pass 4 incorporates the end requirements identified for the rolling process. The cDSP is:

Given:

1) End requirements identified for the rod rolling process
   - Minimize ovality
   - Maximize throughput
   - Minimize rolling load
   - Minimum limit of rolling load, $P_{min} = 28\ t$ (metric)

- Maximum limit of rolling load, $P_{max} = 35\ t$ (metric)
- Minimum limit of throughput, $T_{pmin} = 0.0001\ m^3/sec$
- Maximum limit of throughput, $T_{pmax} = 0.0008\ m^3/sec$
- Target value for ovality, $O_{v,Target} = 0.001 \pm 0.001\ m$
- Target value for rolling load, $P_{Target} = 28\ t$
- Target value for throughput, $T_{p4,Target} = 0.0006\ m^3/sec$

2) Number of passes = 4
3) Initial billet size = 42 × 42 mm
4) Pass sequence = Square-oval-round-oval-round
5) Other parameter values for passes
6) The RSMs and well established empirical and theoretical correlations for the oval to round pass

   - Area of round section obtained after Pass 4

$$F_4 = \left(\frac{\pi h_4^2}{4}\right)$$ **Equation 5.23**

   - Coefficient of elongation for Pass 4

$$\lambda_4 = \frac{F_3}{F_4}$$ **Equation 5.24**

   - The theoretical width of oval Pass 3

$$b_{3w} = \sqrt{4.35F_3}$$ **Equation 5.25**

   - The height of oval Pass 3 for a defined (b/h) ratio

$$h_3 = \frac{b_{3w}}{(b/h)}$$ **Equation 5.26**

- The width of round Pass 4 for a defined spread β_4

$$b_4 = \beta_4 h_3$$ **Equation 5.27**

- Radius of curvature of oval pass

$$R_3^* = \frac{b_{3w}^2 + h_3^2}{4h_3}$$ **Equation 5.28**

- Mean height of the round rod produced after Pass 4

$$h_{4m} = \frac{F_4}{b_4}$$ **Equation 5.29**

- Theoretical diameter of roll for Pass 4

$$D_{t4} = 2\left(R_{max,4} + \frac{G_4}{2}\right)$$ **Equation 5.30**

- Effective diameter of roll for Pass 4

$$D_{w4} = D_{t4} - h_{4m}$$ **Equation 5.31**

- Entry speed of material for Pass 4

$$v_4 = \frac{w_4}{\lambda_4}$$ **Equation 5.32**

- Exit speed for material for Pass 3

$$w_3 = v_4$$ **Equation 5.33**

- Expression for ovality

$$O_{v4} = 8.6153G_4 + 27.539b_{3w} - 0.0009N_4 + 0.0001h_3T_4 - 0.0023h_3N_4 - 0.0041G_4T_4 - 0.0269G_4N_4 - 0.0216b_{3w}T_4 - 0.0026b_{3w}N_4$$ **Equation 5.34**

- Throughput for Pass 4

$$T_{p4} = F_4 \times w_4$$ **Equation 5.35**

- Rolling load in Pass 4

$$P_4 = Q_s F_p (2k)$$

Equation 5.36

7) Variability in system variables

The system variables and their ranges are provided in Table 5.2.

Table 5.2: System variables and ranges for cDSP

Sr. No	Variables	Ranges
1	X_1, diameter of rod after Pass 4 (h_4)	0.025-0.03 m
2	X_2, the coefficient of elongation for Pass 4 (λ_4)	1-3
3	X_3, the spread occurring in Pass 4 (β_4)	1-2
4	X_4, the exit velocity for Pass 4 (w_4)	0.5-3 m/sec
5	X_5, the maximum radius of roll in Pass 4 ($R_{max,4}$)	0.155-0.2 m
6	X_6, the roll rpm in Pass 4 (N_4)	10-20 rpm
7	X_7, the temperature during rolling (T_4)	1270-1280 K
8	X_8, the roll gap (G_4)	0.0035-0.0055 m
9	X_9, the coefficient of friction (μ_4)	0.3-0.45

Find:

System Variables

X_1, diameter of rod after Pass 4 (h_4)

X_2, the coefficient of elongation for Pass 4 (λ_4)

X_3, the spread occurring in Pass 4 (β_4)

X_4, the exit velocity for Pass 4 (w_4)

X_5, the maximum radius of roll in Pass 4 ($R_{max,4}$)

X_6, the roll rpm in Pass 4 (N_4)

X_7, the temperature during rolling (T_4)

X_8, the roll gap (G_4)

X_9, the coefficient of friction (μ_4)

Deviation Variables

d_i^-, d_i^+, *i =1,2,3*

Satisfy:

System Constraints

- Minimum coefficient of elongation constraint

$$\lambda_4(X_2) - 1.2 \geq 0 \quad \textbf{Equation 5.37}$$

- Maximum coefficient of elongation constraint

$$2 - \lambda_4(X_2) \geq 0 \quad \textbf{Equation 5.38}$$

- Minimum spread constraint

$$\beta_4(X_3) - 1.1 \geq 0 \quad \textbf{Equation 5.39}$$

- Maximum spread constraint

$$1.7 - \beta_4(X_3) \geq 0$$ **Equation 5.40**

- Exit speed constraint

$$w_4 - v_r(X_i) \geq 0$$ **Equation 5.41**

- Minimum load constraint

$$P(X_i) - P_{min} \geq 0$$ **Equation 5.42**

- Maximum load constraint

$$P_{max} - P(X_i) \geq 0$$ **Equation 5.43**

- Maximum wear constraint

$$0.0001 - \Delta R(X_i) \geq 0$$ **Equation 5.44**

System Goals

Goal 1:

- Minimize Ovality

$$\frac{O_{v,Target}}{O_v(X_i)} - d_1^- + d_1^+ = 1$$ **Equation 5.45**

Goal 2:

- Maximize Throughput

$$\frac{T_p(X_i)}{T_{p,Target}} + d_2^- - d_2^+ = 1$$ **Equation 5.46**

Goal 3:

- Minimize Rolling Load

$$\frac{P_{Target}}{P(X_i)} - d_3^- + d_3^+ = 1$$ **Equation 5.47**

Variable Bounds

Defined in Table 5.2

Bounds on deviation variables

$$d_i^-, d_i^+ \geq 0 \text{ and } d_i^- * d_i^+ = 0, \text{i} = 1,2,3$$ **Equation 5.48**

Minimize:

The aim for the designer using the cDSP is to minimize the over or under achievement of a goal from the target specified value. In the cDSP the objective function is represented as a weighted sum of the deviation variables and is known as the deviation function (Z). We minimize the deviation function

$$Z = \sum_{i=1}^{3} W_i(d_i^- + d_i^+); \sum_{i=1}^{3} W_i = 1$$ **Equation 5.49**

The objective for us through the cDSP formulation is to minimize these deviation variables and achieve the target values of the goals as close as possible.

In the next section, we exercise the cDSP formulated for different design scenarios by changing the weights associated with the deviation variables of each goals. The results for each of these scenarios are used to construct ternary plots to help a designer visualize and explore the solution space and identify design and operating set points for the rolling passes to meet the identified end requirements of the process. A similar cDSP for Pass 2 is formulated with only two goals, i.e., minimizing rolling load and achieving target throughput. The cDSP for Pass 2 is shown in Appendix A.1.

5.7 Exploration of Solution Space

We have exercised 19 different scenarios for Pass 4. Different weights are assigned to each goal in these scenarios. Details of the scenarios are provided in Table 5.3.

Table 5.3: Scenarios with weights for goals

Scenarios	W_1	W_2	W_3
1	1	0	0
2	0	1	0
3	0	0	1
4	0.5	0.5	0
5	0.5	0	0.5
6	0	0.5	0.5
7	0.25	0.75	0
8	0.25	0	0.75
9	0.75	0	0.25
10	0.75	0.25	0
11	0	0.75	0.25
12	0	0.25	0.75
13	0.33	0.34	0.33
14	0.2	0.2	0.6
15	0.4	0.2	0.4
16	0.2	0.4	0.4
17	0.6	0.2	0.2
18	0.4	0.4	0.2
19	0.2	0.6	0.2

Scenarios 1 to 3 are for a situation where the designer wants to achieve the target of one of the goals, minimizing ovality, maximizing throughput, or minimizing rolling load. For example, in scenario 1 the preference is only for achieving the ovality goal. Scenarios

4 to 6 are for a situation where equal preference is given to two of the goals while the third goal is not considered/relevant. Scenarios 7 to 12 are for situations where greater preference is given to one goal, a lower preference to the second goal while the third goal is assigned zero preference. Scenario 13 represents a situation where all the three goals are given equal preferences. Scenarios 14 to 19 are for situations where two goals have equal preference compared to the third goal with all being non-zero.

On exercising the cDSP for these different scenarios, we obtain the design and operating set points for the process and the achieved values of each of the goals. Ternary plots are constructed. A ternary plot is a diagram used to plot three (input or state) variables which sum to a constant, and to show a relationship between those variables (Sabeghi, Smith and coauthors 2015). In our context, the axes of the ternary plots represent the assigned weights (W_1,W_2, W_3) for each of the goals and the interior color contours represent the achieved value of the particular goal for which ternary plot is created. The achieved value is normalized to lie between 0 and 1 with 0 representing the minimum and 1 representing the maximum achieved value respectively. These values are indicated next to the color bar for the plots. These ternary plots are used to visualize and explore the solution space and identify a feasible solution space satisfying all requirements in the best possible manner. If the designer is unsure about the region of interest in terms of weights assigned, then the ternary plots are effective tools for identifying those regions that satisfy the requirements and thus choosing a good combination of goal weights. For further information about constructing ternary plots, see Sabeghi and co-authors (Sabeghi, Smith and coauthors 2015) . Next, we use these ternary plots to determine the weights for the goals and predict the required design set points.

For goal 1, a process designer is interested in identifying regions to minimize ovality to a value of nearly $0.001\ m$. This is an important goal and must be achieved as closely as possible since rods with ovality lead to a huge loss to the manufacturers. Here we assume that an ovality of a maximum to 0.002 m is acceptable. On analyzing Figure 5.7, in the region identified by the orange dashed line is an ovality value very close to the specified target value is achievable. Also, higher weights are assigned to the ovality goal, i.e. as the weight tends to 1, we approach the target value as closely as possible.

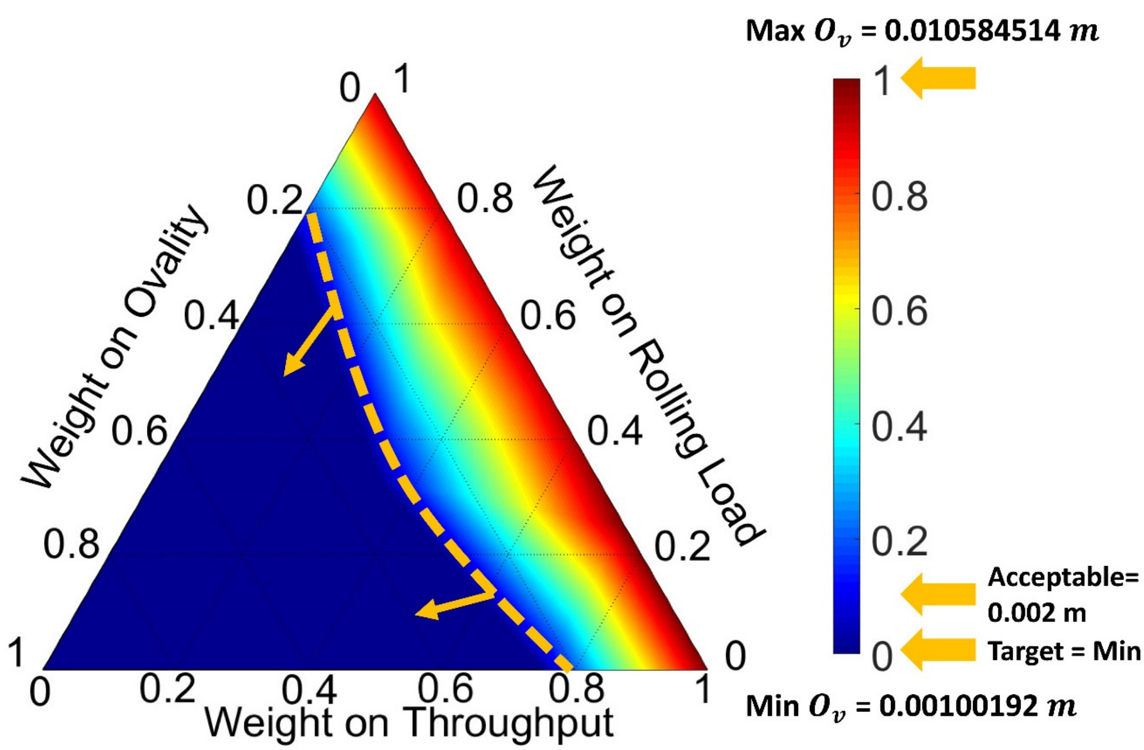


Figure 5.7: Ternary plot for Goal 1 – Ovality

For the goal 2, the process designer is interested in maximizing throughput and the target value identified is $0.0006\ m^3/sec$. In Figure 5.8, we see that the values in the region demarcated by the blue dashed line achieves the target.

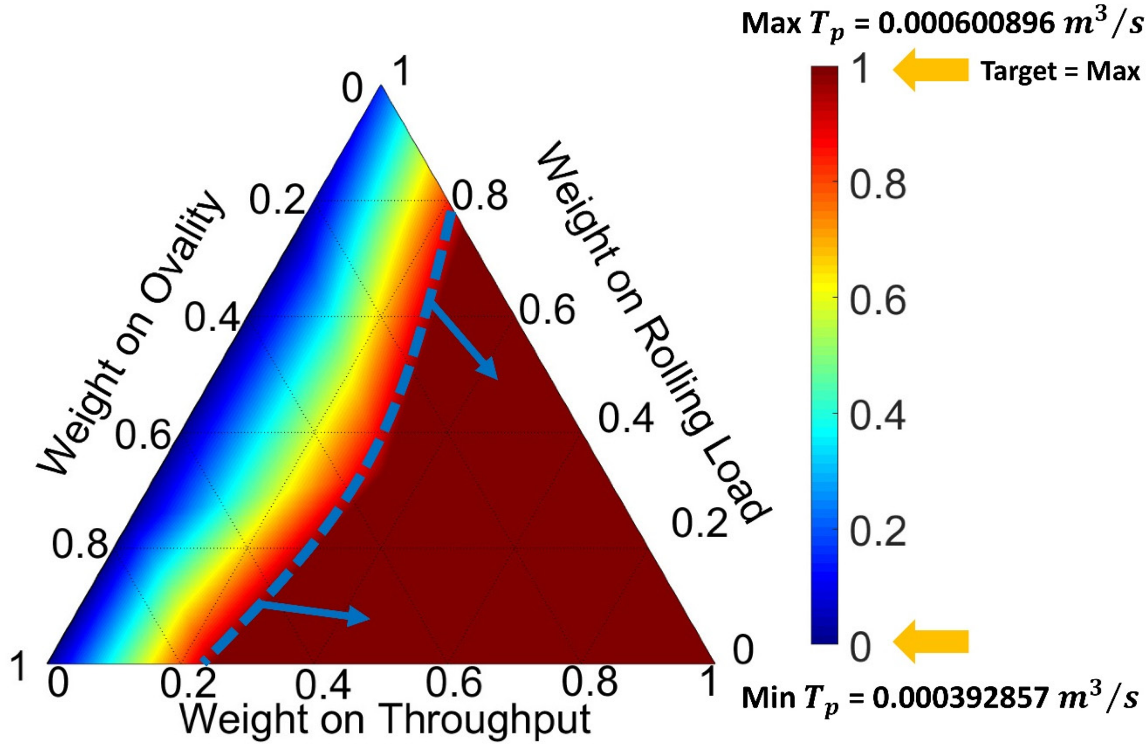


Figure 5.8: Ternary plot for Goal 2 –Throughput

For the goal 3, the interest of the process designer is to achieve the minimum rolling load within the defined limits. The target value for this goal is 28 t. On analyzing Figure 5.9, we see that the dark blue contour within the red dashed lines predicts the value of the goal close to the target.

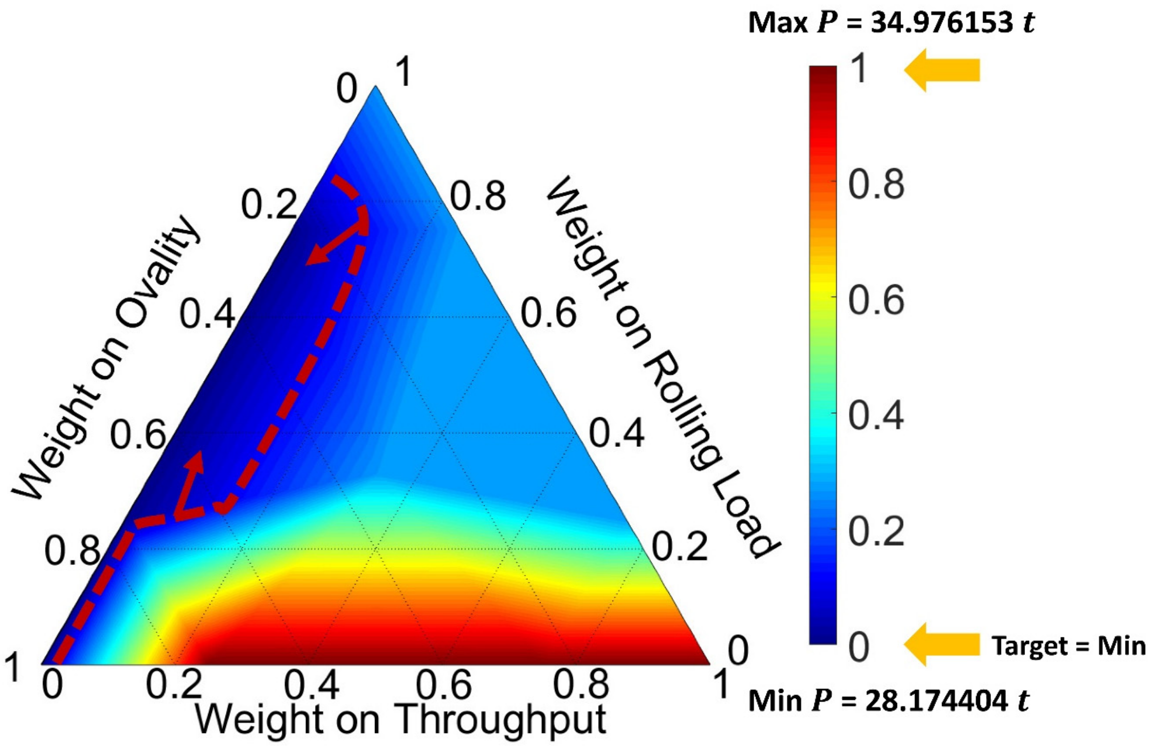


Figure 5.9: Ternary plot for Goal 3 – Rolling load

Now since the designer is interested in identifying regions that satisfy all the three goals mentioned above, there is a need to visualize these design spaces together in a single ternary plot. Therefore, we superimpose plots. The superimposed plot of the regions of interest in a ternary space is shown in Figure 5.10. In a superimposed plot, all the identified regions of interest for the three goals are merged in order to identify a single region that is common for the all the goals, if it exists. If not, the designer needs to make trade-offs among the goals. The region marked in light green satisfies the requirements for ovality and throughput, while the blue region satisfies the requirements of rolling load and ovality. There is no common region that satisfies all the three goals simultaneously. The designer can either choose solutions from the regions identified or reformulate the constraints/goals to identify feasible spaces.

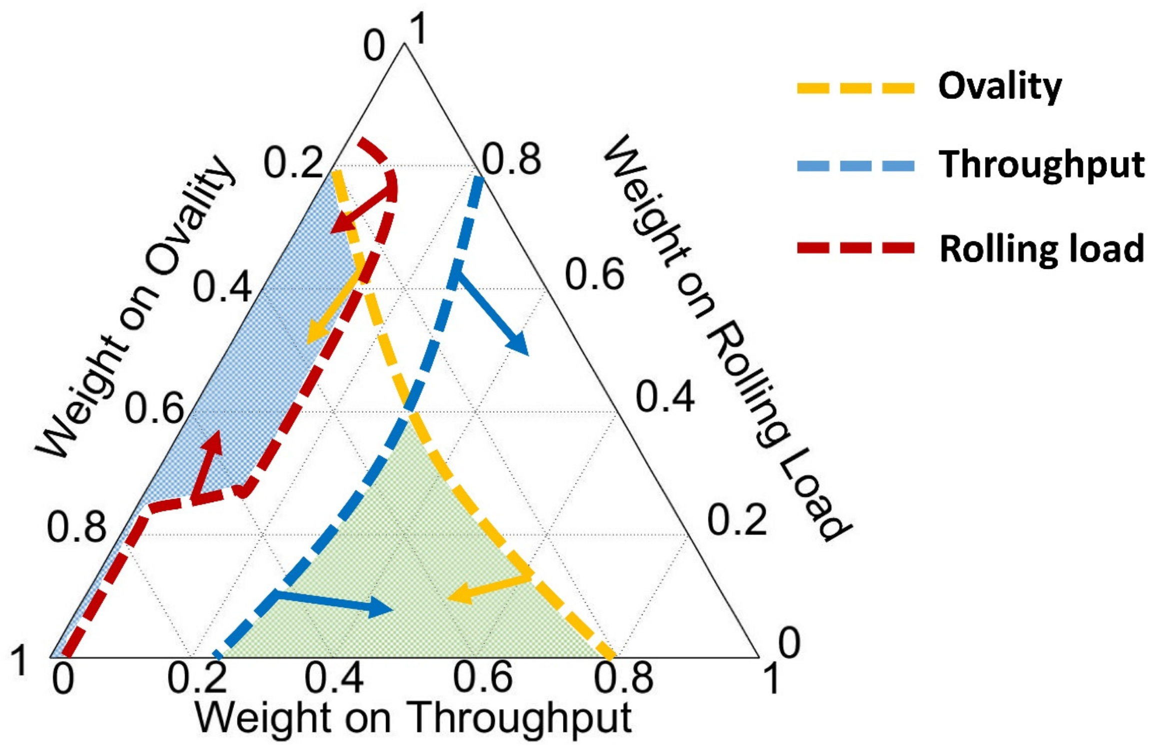


Figure 5.10: Superimposed ternary space for all goals

In this Section, we illustrate the utility of ternary plots to reformulate a problem according to new requirements and carry out solution space exploration to support decision making. For the problem under consideration, ovality goal is an important goal and cannot be relaxed at all. The goals on throughput and rolling load however can be relaxed. This is because of the fact that we view quality of the end product as a greater concern than productivity given that the performance criteria are met. Hence, we relax the goal on throughput even if its level drops to 0.0005 m^3/sec.

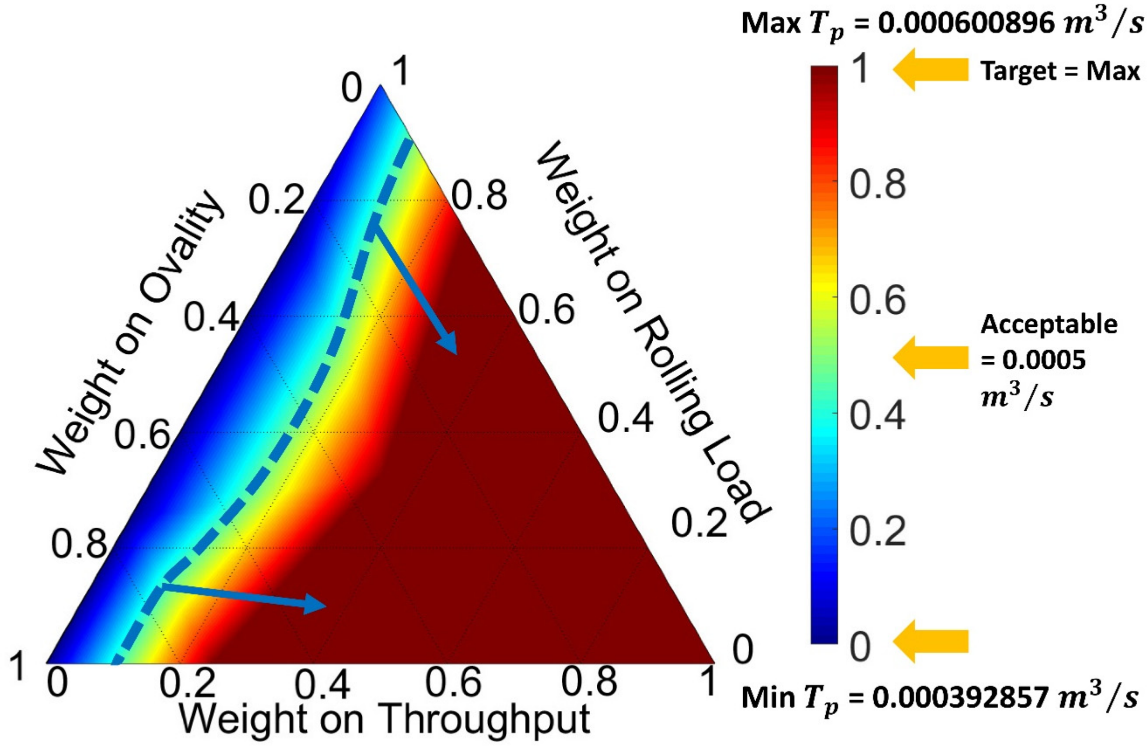


Figure 5.11: Ternary plot for Goal 2 – Throughput with relaxed requirements

This new region of interest is identified by the blue dashed line in Figure 5.11. Any combination of weights on goals in this identified region supports a throughput value greater than or equal to 0.0005 m^3/sec. We need to achieve minimum rolling load within the lower and upper bounds defined. Since the goal of achieving a minimum of 28 t is not possible unless compromises are made on other goals, we are relaxing the rolling load value to 32 t which is within the identified bounds. The acceptable new region in the ternary plot is identified by the dashed red line in Figure 5.12. Any combination of weights of goals in this identified region supports a rolling load value that is less than or equal to 32 t. We superimpose the new regions along with the region identified for minimizing ovality (Figure 6.7) to see if there is a common region that satisfies all three goals for the new design preferences, Figure 5.13.

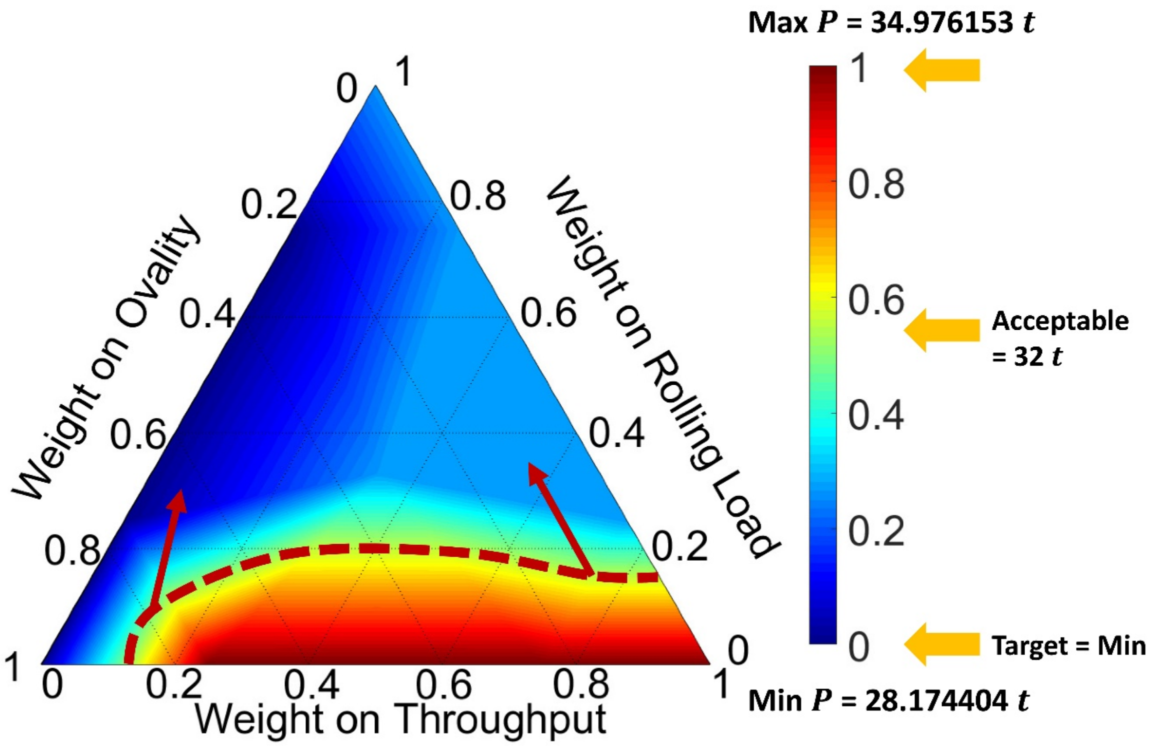


Figure 5.12: Ternary plot for Goal 3 – Rolling load with relaxed requirements

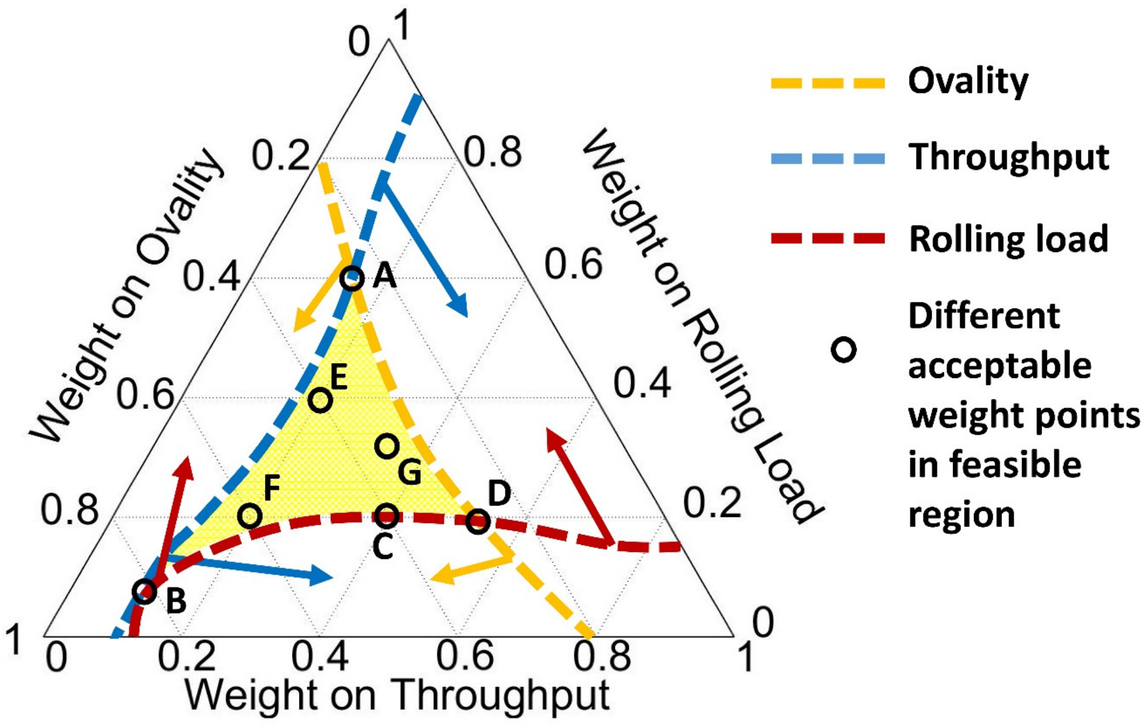


Figure 5.13: Superimposed ternary space for all goals after changes in design preferences

In the superimposed plot for the newly identified goals, the yellow region with multiple solutions within it denoted by the letters A to G satisfies all the newly identified goals. After exploring and analyzing each solution the designer can choose combinations from this region that meets requirements. Scenario 13 in Table 5.3 for which we have equal priority to the three goals ($W_1 = 0.33$, $W_2 = 0.34$, and $W_3 = 0.33$; point G in Figure 5.13) satisfies the three goals as closely as possible compared to the other solutions within the region; therefore, this scenario and the weights associated with it is the best combination. Thus, a designer is able to identify those weight combinations that when used in the cDSP formulation helps in predicting the design set points that satisfies the conflicting goals identified. The ternary plots thus are effective tools empowering the designer to make changes in design preferences according to the demands of the problem. The designer can then analyze and explore the new scenarios in order to make effective design decisions by identifying multiple possible solutions.

Next, we identify the system variable values for Scenario 13 obtained by solving the cDSP. These system variable values are presented in Table 5.4. We use these system variable values to design Pass 4 followed by Pass 3 by using the process design scheme described in Section 5.4 and illustrated in Figure 5.2. This is followed by formulating and solving the cDSP for Pass 2. The system variable values obtained by solving the cDSP and carrying out solution space exploration for Pass 2 are presented in Table 5.4. The design of Passes 1, 2 and 3 are carried out using the results from the Pass 2 cDSP. The calculation involved in the designing of passes is provided in Appendix A.2.

Table 5.4: cDSP results for Pass 4

System Variables for Pass 4 cDSP	Values obtained from running cDSP for Pass 4 (S13)
h_4	0.0260326 m
λ_4	1.3
β_4	1.15
w_4	1.12723 m/sec
$R_{max,4}$	0.155012 m
N_4	17.4642 rpm
T_4	1270 K
G_4	0.004 m
μ_4	0.3

Table 5.5: cDSP results for Pass 2

System Variables for Pass 2 cDSP	Values obtained from running cDSP for Pass 2
h_2	0.031 m
λ_2	1.3
β_2	1.2
w_2	0.79431 m/sec
$R_{max,2}$	0.155 m
G_2	0.004 m
μ_2	0.3

The design of all the passes by following the process design scheme is shown in Appendix A.2. The results of the roll pass design calculations are summarized in Table 5.6 and the pass dimensions are shown in Figures 5.14-5.17.

We discuss the design results summarized in Table 5.6 briefly here. We achieve a round rod of diameter 26 mm at the end of Pass 4 with ovality of $0.001004\,m$, throughput of almost $0.0006\,m^3/sec$ and a rolling load value of almost $30\,t$. This is achieved with a coefficient of elongation of 1.3 and spread of 1.15 occurring while the material is rolled in Pass 4. The entry speed of the material for Pass 4 is $0.866\,m/sec$ and exit speed is $1.127\,m/sec$. The effective roll diameter is obtained as $288.7\,mm$ for this pass.

The design of Pass 3 results in an oval stock of dimensions $18.3\ \times\ 55\,mm$. To design Pass 3 the spread value is assumed to be 1.5 and the coefficient of elongation is 1.0912. The entry speed of stock is $0.7943\,m/sec$ and the exit speed is the same as the entry speed of Pass 4. The maximum roll radius is assumed to be the same as Pass 4 and an effective roll diameter of $296.3\,mm$ for Pass 3 is based on this assumption. The design is able to achieve/maintain a throughput of almost $0.0006\,m^3/sec$ for Pass 3.

The design of Pass 2 results in a round stock with diameter of $31\,mm$. The coefficient of elongation and spread for this Pass are 1.3 and 1.2 respectively. The entry is 0.611 m/sec and the exit speed are the same as the entry speed of Pass 3. The effective diameter obtained for this pass is $285\,mm$. The target rolling load value of $40\,t$ for Pass 2 is achieved and the throughput is maintained at 0.0006 m^3/sec.

Table 5.6: Summary of key design results for all passes

Pass No.	Roll Stand No.	Dimensions mm	Cross-section F mm^2	Coefficient		Entry Speed v m/sec	Exit Speed w m/sec	Effective Diameter D_w mm	Goals Achieved		
				λ	β				Ovality O_v m	Throughput T_p m^3/sec	Rolling Load P t
0		Square 42×42	1764								
1	I	Oval 22×65.3	981.59	1.797	1.4	0.3401	0.611	333.3	NA	0.0006	NA
2	II	Round Ø31	755.07	1.3	1.2	0.611	0.79431	285.1	NA	0.0005997	40.82
3	III	Oval 18.3×55	691.93	1.0912	1.5	0.79431	0.86678	296.35	NA	0.0005999	NA
4	IV	Round Ø26	532.26	1.3	1.15	0.86678	1.1272	288.7	0.001004	0.0005999	30.002007

NA: Not applicable for the formulated problem under study

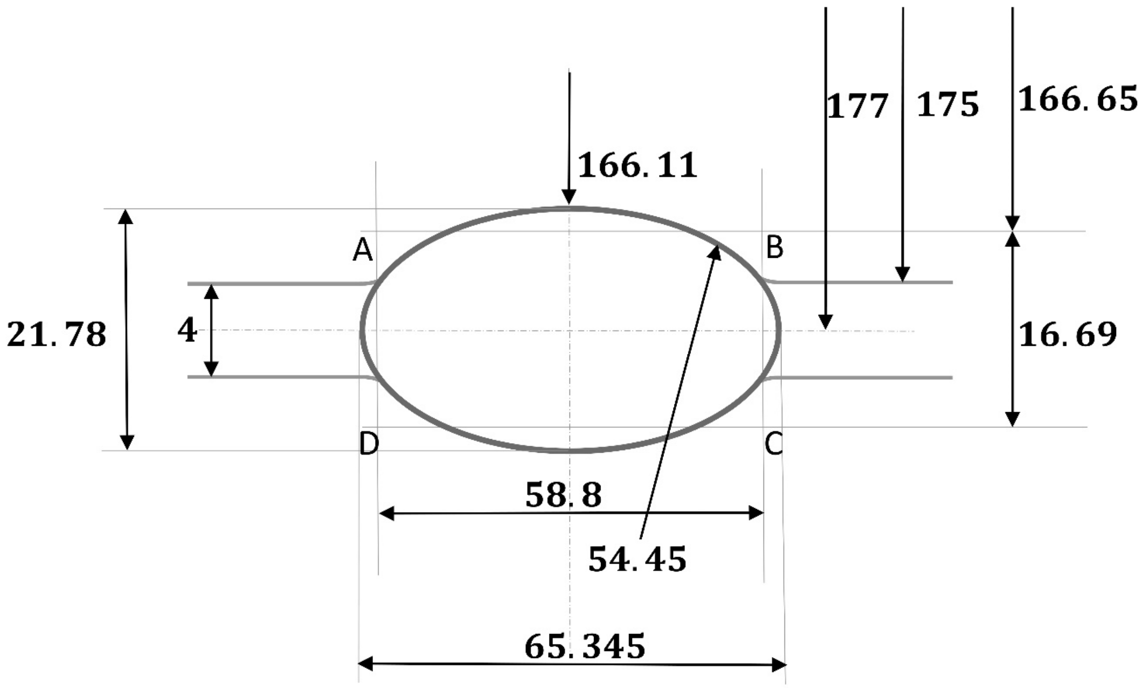


Figure 5.14: Pass 1 dimensions designed

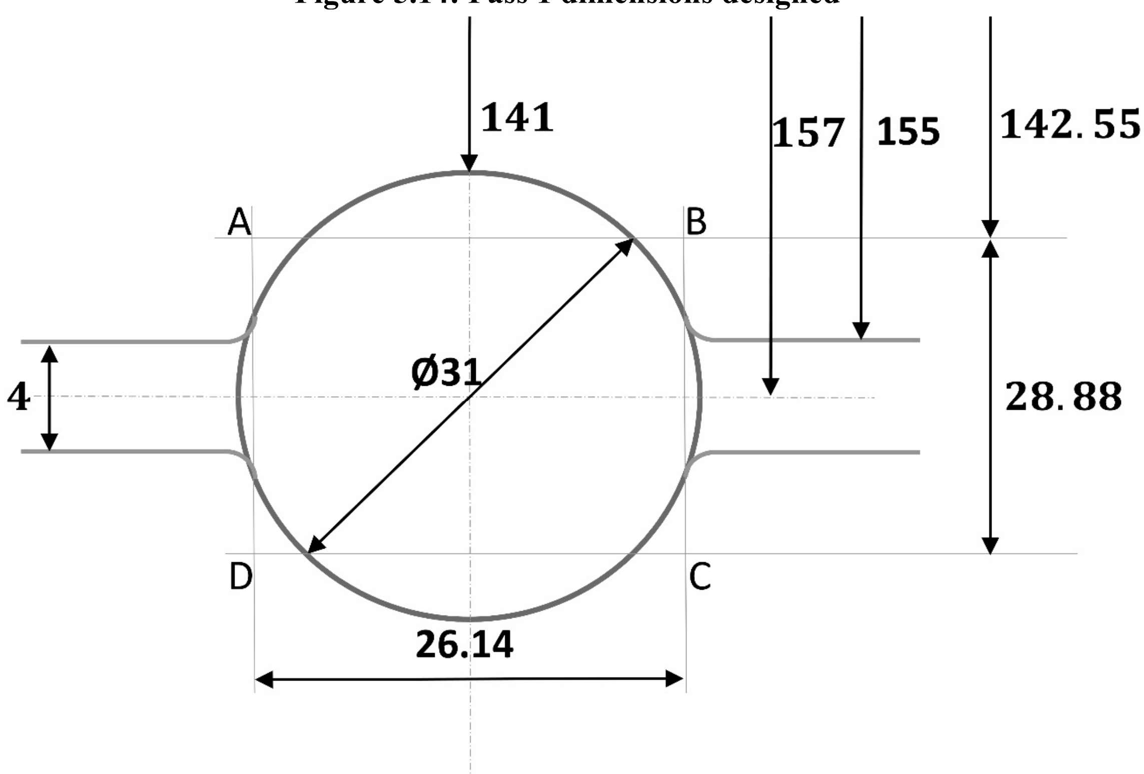


Figure 5.15: Pass 2 dimensions designed

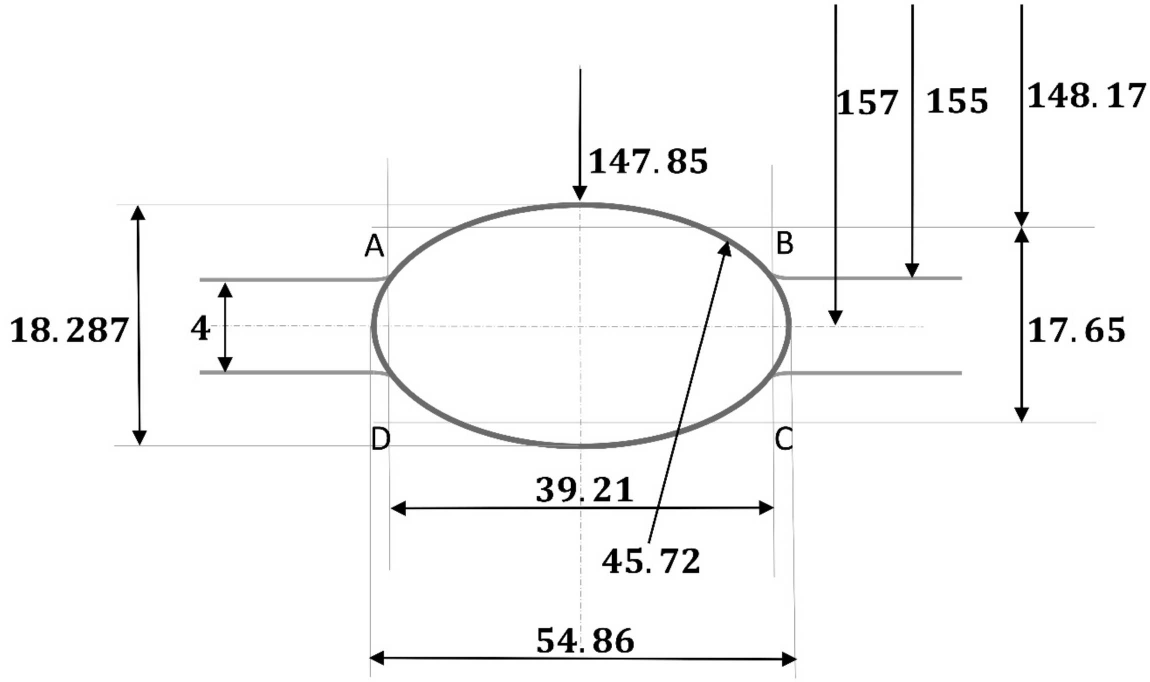


Figure 5.16: Pass 3 dimensions designed

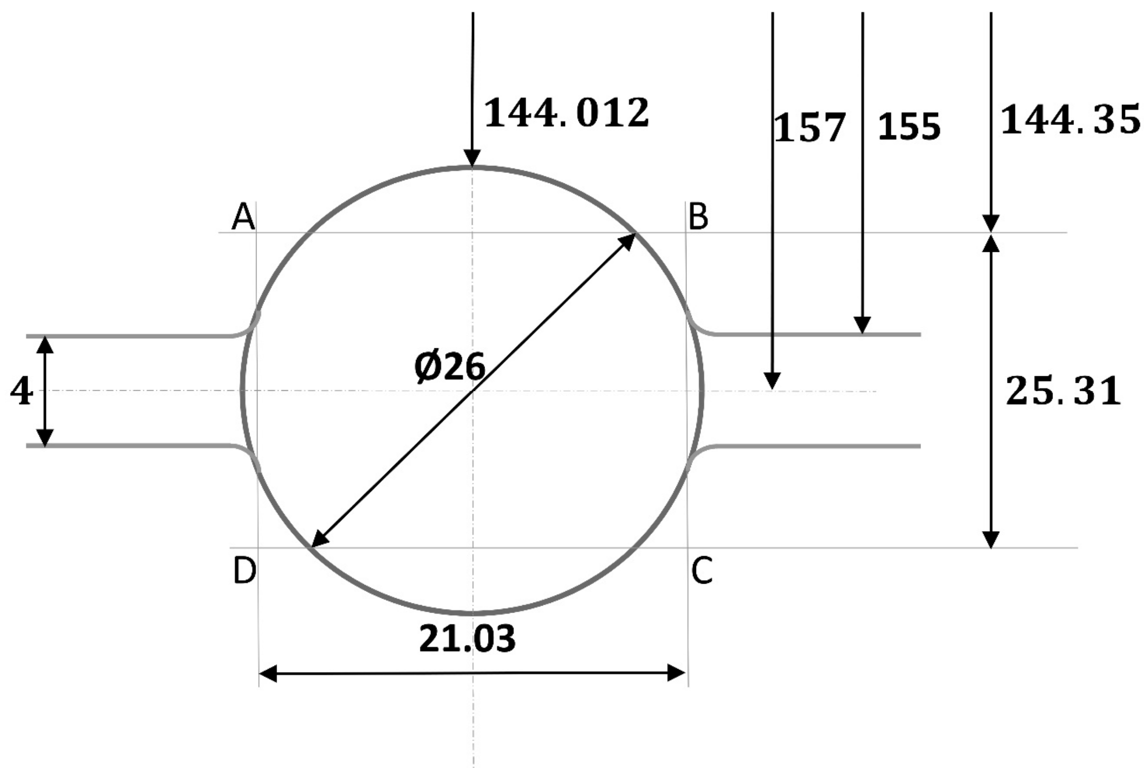


Figure 5.17: Pass 4 dimensions designed

The design of Pass 1 results in an oval stock of dimensions $22 \times 65.3\,mm$. The coefficient of elongation for this pass is 1.797. The spread value is assumed to be 1.4. The entry speed for this pass is $0.3401\,m/sec$. The exit speed is same as the entry speed of Pass 2. The maximum roll radius is assumed to be same as Pass 2 and Pass 4 and the effective roll diameter is $333\,mm$ based on this assumption. The throughput value of $0.0006\,m^3/sec$ is achieved with this configuration.

5.8 Test Example 2: Exploration of the Solution Space for Microstructure after Cooling Stage to Realize the End Mechanical Properties of Hot Rolled Product

Frame of Reference

Manufacturing a product involves a host of unit operations and the end properties of the manufactured product depends on the processing steps carried out in each of these unit operations. In order to couple the material processing-structure-property-performance spaces, both systems-based materials design and multiscale modeling of unit operations are required followed by integration of these models at different length scales (vertical integration). This facilitates the flow of information from one unit operation to another thereby establishing the integration of manufacturing processes to realize the end product (horizontal integration).

In this example, we use the goal-oriented inverse, design method to identify the design set points for hot rod rolling process chain that involves the cooling process to achieve certain specified mechanical properties. We illustrate the efficacy of the method by exploring the design space for the microstructure after cooling stage that satisfies the requirements identified for the end mechanical properties of a hot rolled product. Specific requirements like managing the banded microstructure to avoid distortion in forged gear blanks are considered for the problem.

The widespread popularity of steel as an engineering material in manufacturing industries is due to the fact that diverse range sets of mechanical properties and microstructures are possible by carefully managing the materials processing resulting in improved performances of products. The defining players for the properties of a steel product that is rolled are the chemical composition of material, the deformation history during the rolling process and the thermal history during subsequent cooling operation. Large number of plant trials are needed to produce a new grade of steel product mix having specific target properties and performances. In plant set-up, these trials are usually expensive and time consuming. The alternative is to exploit the advancements in computational modeling tools and frameworks to carry out simulation-based design exploration of different manufacturing processes involved in order to identify ranged set of solutions that satisfies the requirements identified for the process as well as the end product.

In the model-based realization of complex systems, we have to deal with models that are typically incomplete, inaccurate and not of equal fidelity. We believe that the fundamental role of a human designer is to make decisions given the uncertainties associated with the system (McDowell, Panchal and coauthors 2009). Thus, we try to find robust *satisficing* solutions that are relatively insensitive to change rather than optimum solutions that perform poorly when the conditions are changed. The compromise Decision Support Problem (cDSP) construct is proposed by Mistree and co-authors for robust design under multiple goals (Mistree, Hughes and coauthors 1993). Using the cDSP, several solutions are identified which are further explored to identify solutions that best satisfy specific requirements. We use the inverse design method and solution space exploration to determine the set points of the hot rod rolling and cooling stages to realize the microstructure and mechanical properties of the end product. Allen and co-authors describe the foundational problem that we are addressing in (Allen, Mistree and coauthors), and addressed in detail in Chapter 1 of dissertation. Nellippallil and co-authors describe the goal-oriented inverse design method, the cDSP construct and illustrate the utility of the same for roll pass design in (Nellippallil, Song and coauthors , Nellippallil, Song and coauthors 2016); addressed in detail in Chapters 4 and 5 of dissertation. Information on the mathematical models we use to achieve integration of different processes in hot rod rolling process chain and the framework that we use to formulate the cDSPs is presented by Nellippallil and co-authors in (Nellippallil, Allen and coauthors 2017); addressed in detail in Chapter 6 for the comprehensive example problem.

Using this example, we explore the solution space for the microstructure after cooling stage that satisfies the goals identified for the mechanical properties of end product. We identify the influence of different fractions of ferritic and pearlitic microstructures on end mechanical properties like yield strength, tensile strength, toughness (impact transition temperature) and hardness. We demonstrate the efficacy of the method and solution space exploration by designing the microstructure after cooling to realize the end product mechanical properties. In Section 5.9, we describe the problem and the proposed goal-oriented inverse decision-based design method. In Section 5.10, we highlight the results obtained. We close the test example with our remarks in Section 5.11.

5.9 Problem Description and Application of GoID Method

There has been an increasing trend in developing algorithms for predicting the behavior of materials during complex manufacturing processes like the hot rod rolling, as the final properties of end steel product produced depends on its processing route (Nellippallil, De and coauthors , Hodgson and Gibbs 1992, Majta, Kuziak and coauthors 1996, Kuziak, Cheng and coauthors 1997, Phadke, Pauskar and coauthors 2004). One of the major issue during the hot rod rolling process is the segregation of alloying elements such as manganese (Mn) during the progress of solidification in casting and affects the entire downstream processing as well as the mechanical properties of the end product (Jägle 2007). These segregates, known as microsegregates, are typically of the size of grains and are formed due to limited solid solubility of these solutes. and During the hot rolling process, the concentration profile changes due to the deformation of these structures. During the subsequent cooling process, austenite to ferrite phase transformation occurs. Supposing the steel is of hypo eutectoid composition the ferrite phase will form in regions with low content of austenite stabilizing solute content and the rest of the phase will be pearlite. Thus due to the alternate layers of low and high solute regions induced during hot rolling, we will see a banded microstructure formation having both ferrite and pearlite (Jägle 2007). These banded microstructures are a major factor for distortions in gear blanks after forging process. Thus, managing the factors associated with banding will indirectly affect the final mechanical properties of the product. To predict the final mechanical properties of the product as a function of the composition variables, rolling and cooling parameters, there is a need for series of modeling integrations, both vertical and horizontal. We define the integration of multiple length scale models within a process as vertical integration and the integration of the different stages or processes ensuring information flow as horizontal integration. More information on the specific problem addressed and the vertical and horizontal integration of models are provided in reference (Nellippallil, Allen and coauthors 2017) and is addressed in detail in Chapter 6 for the comprehensive example problem.

Application of Goal-Oriented Inverse Design Method

The goal-oriented, inverse design method applied in this example is explained using the information flow diagram shown in Figure 5.18. The method is goal-oriented because we start with the end goals that needs to be realized for the product as well as process. The decisions that are taken for the end requirements of the product/process are then communicated to the stages that precedes to make logical decisions at those stages that satisfies the requirements identified thereby making it an inverse design process. Brief descriptions of the steps are provided below.

Step1: Establish forward modeling and information flow across models for the problem formulated. In Step 1, the designer makes sure that there is proper flow of information as models are connected across different stages (from rolling to cooling to end product mechanical properties). Mathematical models are either identified or developed in this step.

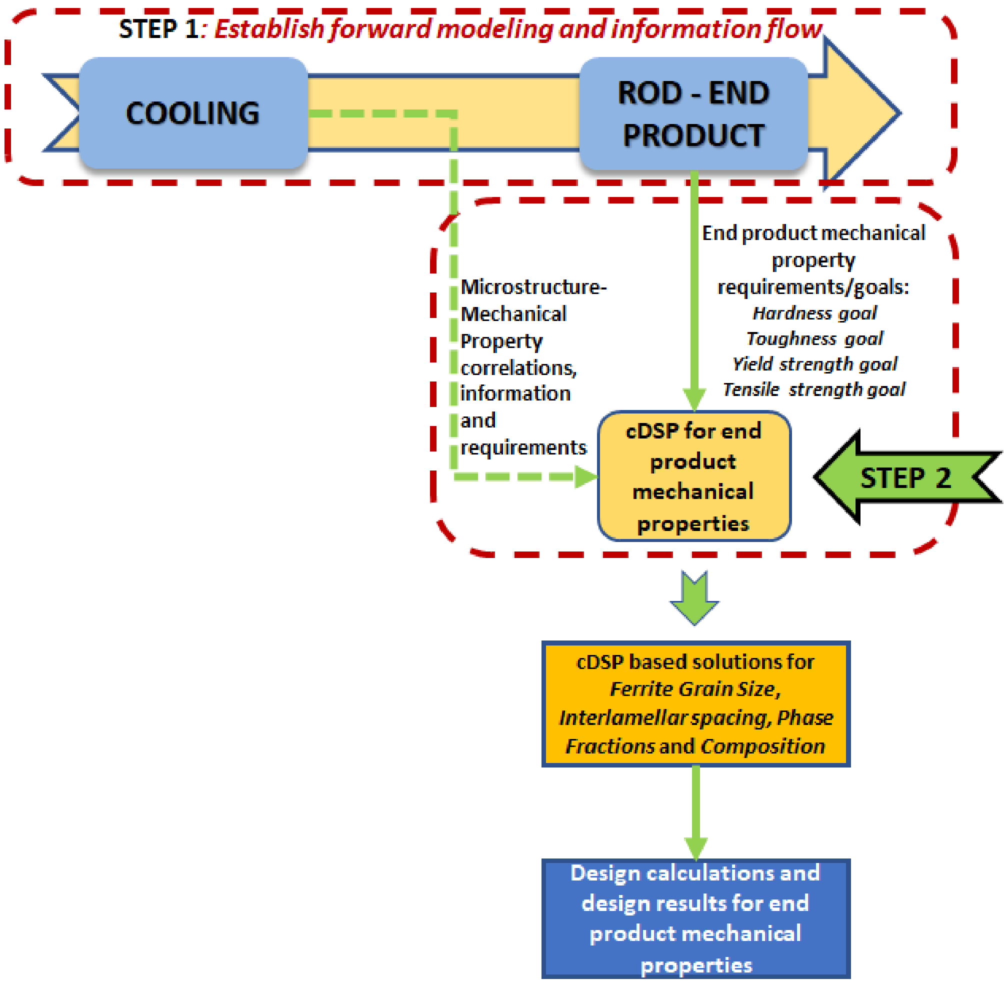


Figure 5.18: Goal-oriented inverse design method applied to test example 2 problem

Step2: In Step 2, a cDSP for the mechanical properties of the final end product is formulated using the models identified in Step 1. Information, requirements (manage banding) and the correlations of mechanical properties with microstructure after cooling stage (ferrite grain size, interlamellar spacing, phase fractions and composition) are communicated to this cDSP formulated. For the hot rod rolling problem formulated, the end mechanical property goals and requirements for yield strength, tensile strength, hardness and toughness (impact transition temperature) are identified. On exercising the cDSP, the best combinations for ferrite grain size, phase fractions, interlamellar spacing and compositions that satisfy the requirements for properties are identified.

5.10 Exploration of Solution Space for Microstructure after Cooling Stage to Realize the End Mechanical Properties of Hot Rolled Product

In this test example, we address the following inverse problem: Given the end mechanical properties of a new steel product mix, what should be the microstructure after cooling that satisfies the requirements identified? We address this problem by carrying out exploration of microstructure solution space. In Table 5.7, we list the requirements identified for the end product as well as the requirements after the cooling stage. The end product mechanical properties like yield strength, tensile strength, impact transition temperature and hardness and their target values/ranges are defined. The requirements from the cooling stage are to have a high ferrite fraction (≥0.8) and to achieve a minimum ferrite grain size after cooling. The ferrite fraction is defined as a goal in the cDSP to manage banded microstructure. A very high ferrite fraction denotes a less banded structure as there is less amount of the pearlite phase. This is true in case of a very high pearlite fraction too as there will be less ferrite leading to less banded structure.

Table 5.7: Target values and design preferences for the requirements identified

Requirements/Goals	***Target Ranges/Values***	***Design Preferences***
Yield Strength Goal (YS)	220-400 MPa	Maximum Possible
Tensile Strength Goal (TS)	500-780 MPa	Maximum Possible
Ferrite Fraction Goal (X_f)	≥0.8 (Min Banded Microstructure)	Close to Target

Impact Transition Temperature (ITT) Requirement	-90 to -30 ℃	Minimum Possible
Hardness Requirement (HV)	150-250	Maximum Possible
Ferrite Grain Size Requirement	5-10 μm	Minimum Possible

In Table 5.8, we list the system variables and their corresponding ranges. More information on the dependence of the system variables on the final mechanical properties are available in (Nellippallil, Allen and coauthors 2017) and in Chapter 6 for the comprehensive example problem.

Table 5.8: System variables and their ranges

System Variables	***Ranges Defined***
Ferrite Grain Size (FGS) (μm)	5-25
Ferrite Fraction (X_f)	0.1-1.0
Pearlite Interlamellar Spacing (S_0) (μm)	0.15-0.25
Chemical Composition of Silicon (%)	0.18-0.3
Chemical Composition of Nitrogen (%)	0.007-0.009

The cDSP is exercised for different scenarios by assigning different weights to the goals associated. Ternary plots are created using the design and operating set points generated after exercising the cDSPs. We use these ternary plots to determine the appropriate weights for the goals and predict the required design set points. We showcase these ternary plots in Figures 5.19-5.22.

For Goal 1, the process designer is interested in maximizing the yield strength of the end product to a target value of 400 MPa. On analyzing Figure 5.19, we see that the values in the dark red contour region demarcated by the blue dashed line achieves the maximum yield strength of around 329 MPa. For Goal 2, the process designer is interested in maximizing the tensile strength of the of the end product to a target value of 780 MPa. On analyzing Figure 5.20, we see that the values in the dark red contour region identified by the green dashed lines achieves the maximum tensile strength of 759 MPa. For Goal 3, the process designer is interested to manage the banded microstructure by identifying high ferrite fraction regions. On analyzing Figure 5.21, we see that region in the red contour identified by the violet dashed line has ferrite fraction from 0.7 to 0.99609 with maximum being at the same region where yield strength is seen to have the highest value. Similarly, we see in Figure 5.21 that the blue region identified with the violet dashed lines have the lowest ferrite fraction (0.3 to 0.100049) leading to high pearlite fraction. This region corresponds with the region where tensile strength is seen to have the maximum value. The region in between these two dashed violet lines has the highest banded microstructure of ferrite and pearlite. Thus, it is clear from the ternary analysis that the ferrite fraction plays a major role in defining the yield strength and tensile strength of the end product. A high ferrite fraction improves the yield strength of the product while compromising the tensile strength and a high pearlite fraction improves the tensile strength of the product while compromising the yield strength of the product. Another requirement identified is to have a minimum impact transition temperature (ITT) for the product. We plot the solution space for ITT in Figure 5.22. We see from Figure 5.22 that the ITT drops in those regions with high ferrite fraction. The target regions for ITT of -30℃ and -90℃ are identified by the red dashed lines in Figure 5.22.

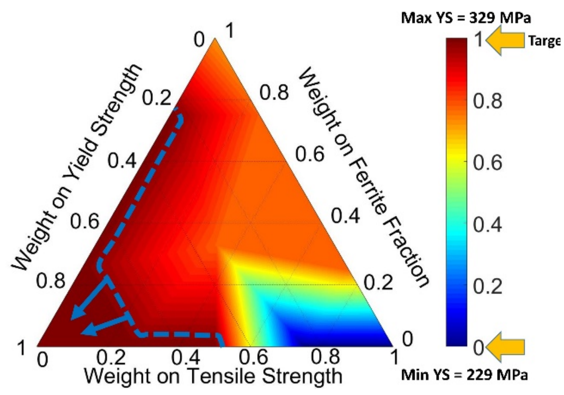


Figure 5.19: Ternary plot – Yield Strength

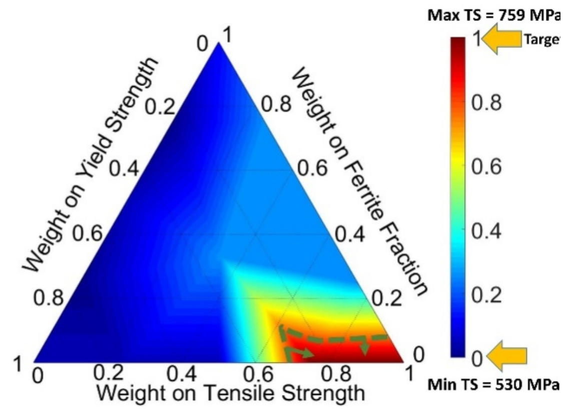


Figure 5.20: Ternary plot – Tensile Strength

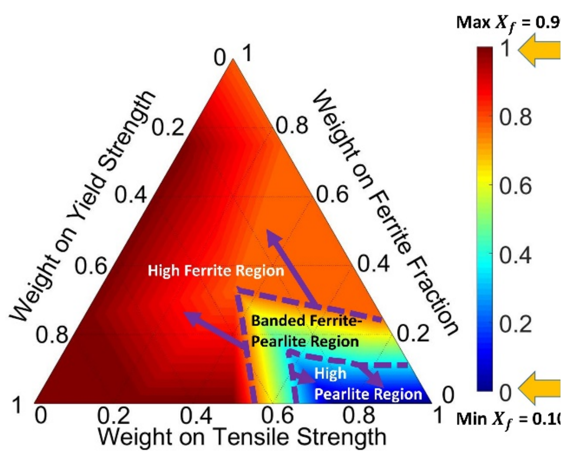


Figure 5.21: Ternary plot – Ferrite Fraction

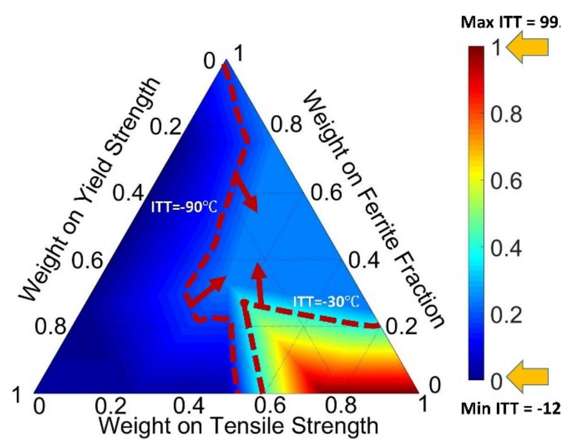


Figure 5.22: Ternary plot – ITT Solution Space

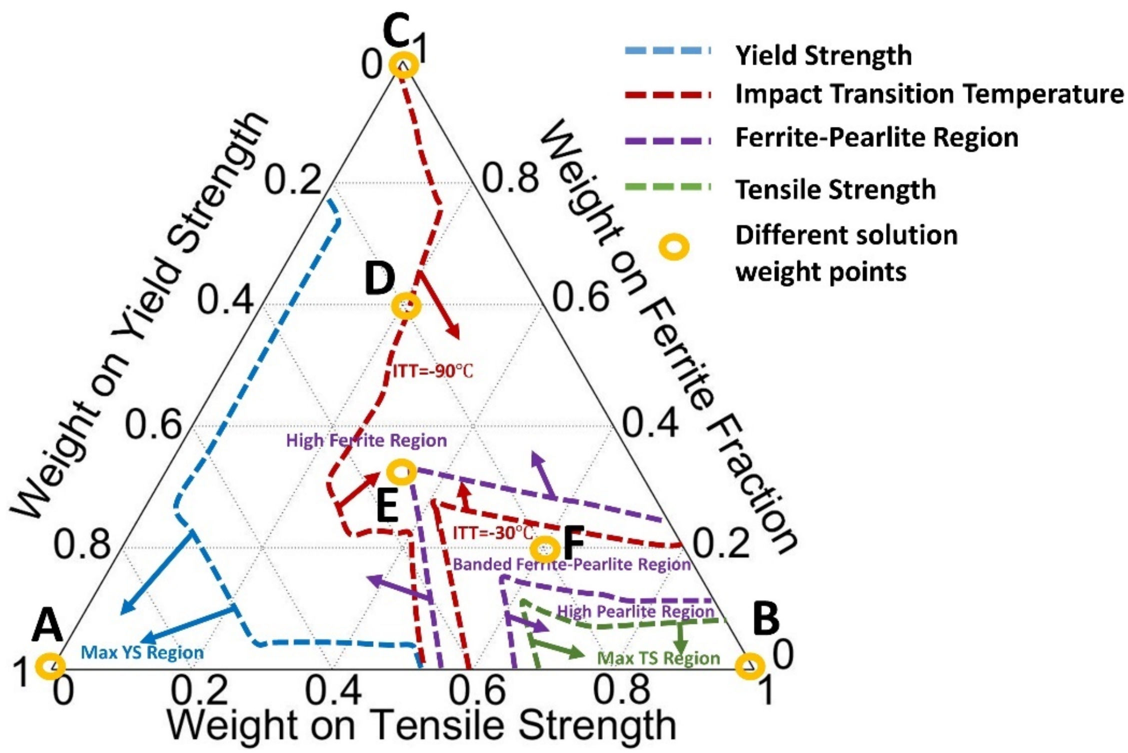


Figure 5.23:Ternary plot – Superimposed Ternary Plot

Now, since the designer's interest is in identifying regions that satisfy all the conflicting requirements, there is a need to visualize all the design spaces in one ternary plot. Therefore, we plot the superimposed ternary plot shown in Figure 5.23. If there is a common region that satisfies all the requirements identified, then we select solutions from that region. If not, we identify compromised solutions that satisfy our requirements to the best possible. From the superimposed ternary plot, we are analyzing 6 solution points A, B, C, D, E and F in Table 5.9.

Table 5.9: Solution points for microstructure after cooling and end mechanical properties

Sol. Pts	FGS (μm)	X_f	S_0 (μm)	%Si	%N	YS MPa	TS MPa	ITT ℃	HV
A	5	0.996	0.15	0.3	0.009	328.7	541.8	-120.7	166.1
B	5	0.1	0.15	0.299	0.0089	229	759.35	99.81	242.65
C	5	0.8	0.15	0.18	0.007	306.9	589.05	-72.5	182.7
D	5	0.87	0.15	0.299	0.0089	314.76	572.17	-90	176.76
E	5	0.7997	0.15	0.299	0.0089	306.9	589.05	-72.5	182.7
F	5	0.55	0.15	0.299	0.0089	279.13	649.46	-10.95	203.97

On analyzing the solution points in Table 5.9, we see that ferrite grain size (FGS) and pearlite interlamellar spacing (S_0) is low for all the solution points. Thus, a smaller ferrite grain size and smaller interlamellar spacing is preferred to enhance the end mechanical properties of the product. This is an important information that is generated which has to be communicated as the goal for the preceding rolling and cooling stages that produces the end product. Solution point A with highest ferrite fraction has the highest YS and lowest ITT while achieving a TS and HV that is acceptable. Solution point B with highest pearlite fraction has the highest TS and HV while falling short in YS and ITT leading to rejection of the point. Solution points C, D, E with ferrite fraction around 0.8 and above achieves acceptable targets for YS, TS, ITT and HV. Solution point F with a ferrite fraction of 0.55 achieves better TS and HV than points C, D and E but the values drops for YS and ITT respectively. This point is also rejected due to the highly banded microstructure generated. Based on the analysis carried out, we pick solution point D that generates the best combination of values of the system variables that satisfies the requirements of YS, TS, ITT and HV.

5.11 On Verification and Validation – Empirical Structural and Performance Validation

Empirical structural validation involves accepting the appropriateness of the example problems used to verify the performance of the framework and the method. The CEF and the inverse design method is first tested using two example problems in Chapter 5. In the first example problem, the horizontal integration of rod rolling is considered. Using the framework and method, the integrated design of rolling passes and the final rod product is carried out in an inverse manner starting from the end goals. The example thus is appropriate to demonstrate the utility of the framework and method as it involves complex information flow across manufacturing stages that needs systematic problem formulation and exploration across stages to design the entire system. In this example, only macrostructural effects associated with hot rod rolling is considered. Using the second example, our goal is to illustrate the utility of the method and framework in supporting the design of the material microstructure for given end mechanical properties of the product. To illustrate the same, a rather simple problem is formulated to design the microstructure after cooling process to satisfy certain end mechanical properties like yield strength, tensile strength, hardness and toughness of the rod produced. The example is appropriate as the example supports in demonstrating the utility of method and framework in carrying out microstructure-mediated design. The example is further improved and expanded to the comprehensive problem on vertical and horizontal integration of hot rolling process chain in Chapter 6. Using the comprehensive example problem in Chapter 6, the utility of the framework and the method is tested for the integrated design exploration of materials, products and manufacturing processes.

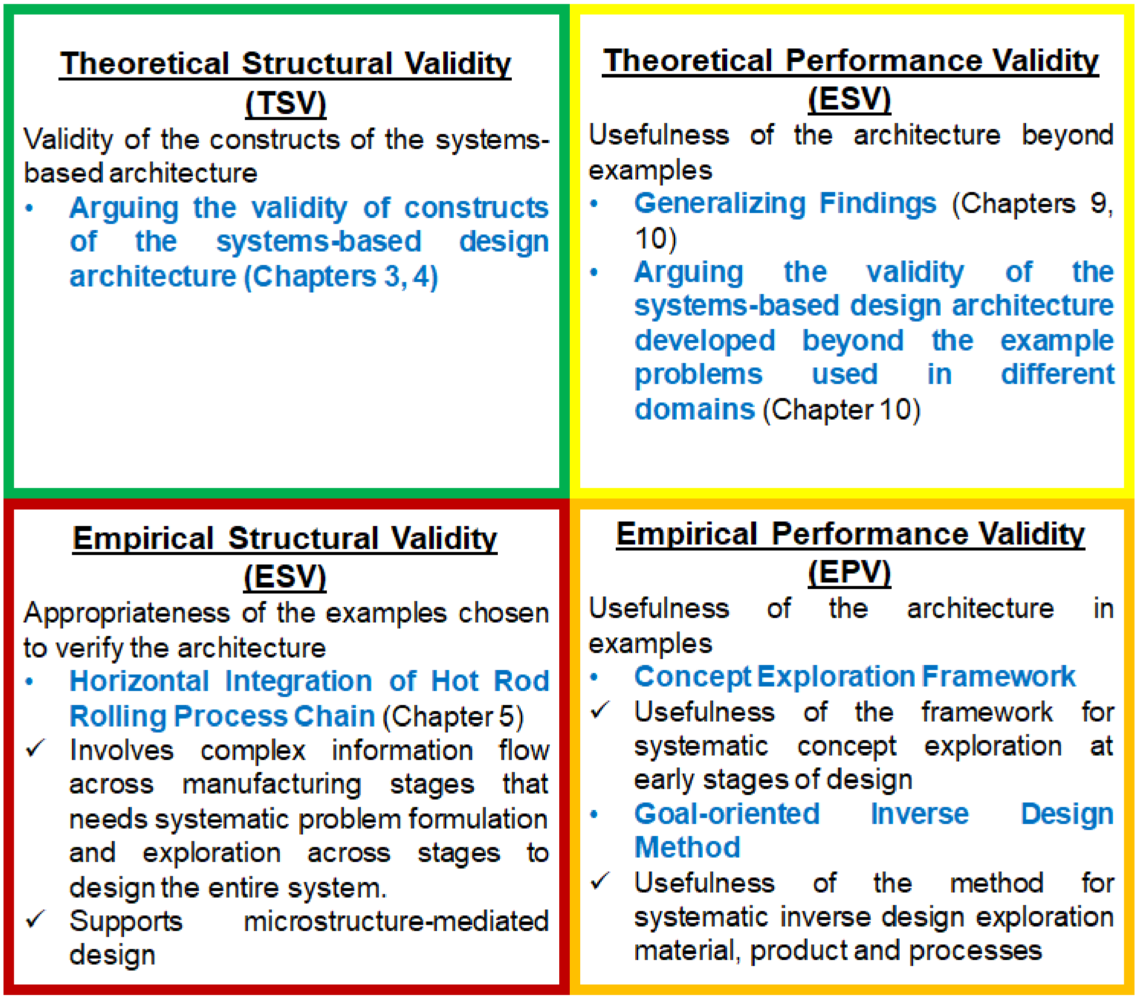


Figure 5.24: Verification and validation aspects addressed in Chapter 5

5.12 Role of Chapter 5 in this Dissertation

In this Chapter, a method is proposed based on well-established empirical models and response surface models developed through simulation experiments along with the compromise Decision Support Problem (cDSP) construct to support integrated information flow through different stages of a multi-stage hot rod rolling system (horizontal integration). The method is specific form of the generic goal-oriented inverse design method proposed in Chapter 4. We illustrate the efficacy of the proposed goal-oriented, sequential inverse design method using hot rod rolling as an example. Here the design decisions are first made at the last rolling pass based on the end requirements of the process. We allow these design decisions to be passed to the preceding rolling passes by following the sequential relationships existing between the passes in an inverse manner. We carry out the design of individual passes by allowing design information to be passed back and forth between passes using the sequential relationships. The formulation of individual cDSPs for passes helps to organize the sequential information flow and provides the ability to the designer to consider specific goals associated with each rolling pass and integrating them with the end goals. The ternary analysis feature incorporated in the method provides the designer with the capability of exploring the solution space and identifying feasible regions that satisfies the different goals identified for a particular stage of the manufacturing process chain. The proposed method has the potential to be used for identifying design set points for a chain of unit operations that are connected in sequence. Once the information flow between operations and the empirical and the simulation/response surface models necessary to establish relationships are available, a designer will be able to use this method to achieve the integrated decision-based design of the product and the processes.

Using Test Example 2

In this chapter, we demonstrate the utility of the proposed goal-oriented inverse decision-based design method by exploring the solution space for the microstructure after cooling stage that satisfies the requirements for the end mechanical properties of the product. Through this method and the problem formulated, we study the effect of ferrite fraction, ferrite grain size, pearlite interlamellar spacing and composition in defining the mechanical properties like yield strength, tensile strength, toughness and hardness. We illustrate the efficacy of ternary plots to explore microstructure space solutions that satisfies the conflicting mechanical property goals in the best possible manner by carrying out design trade-offs. The results for microstructure space obtained will be studied further to design (identify design and operating set points) preceding manufacturing stages like rolling and cooling by following the proposed design method in order to realize the end product (Chapter 6). The proposed inverse decision-based design method is generic and supports the integrated decision-based design exploration of manufacturing stages that are connected. The primary advantage of the proposed method is in enabling a process designer to rapidly explore the design space for manufacturing processes using simulation models there by reducing the need for expensive plant trials resulting in reduced time and cost involved in the production of a new grade of product mix.

Chapter 6: Integrated Design Exploration of Materials, Products and Manufacturing Processes using Goal-oriented Inverse Design Method

6.1 Frame of Reference – Establishing context from Chapter 1 and need for this research

Steel manufacturers focus on developing new grades of steels with improved properties and performance. Careful managing of material processing during steel manufacturing will lead to the development of steels with a range of mechanical properties resulting in the improved performance of products. A round rod is produced after passing the raw steel through several manufacturing processes such as casting, reheating, rolling and cooling. This round rod forms the input material for gear production. The chemical composition of the steel including the segregation of alloying elements, the deformation history during rolling, the cooling after rolling and the microstructure generated define the end properties of the rolled product. The presence of large numbers of design variables, constraints and bounds, conflicting goals and sequential information/material flow during material processing makes the steel rod making process chain highly complex. Many plant trials are therefore required to produce a new steel grade with desired properties and performance. These trials are usually expensive and time-consuming. An alternative is to carry out simulation-based, integrated design exploration of the different manufacturing processes involved in exploiting the advances in computational modeling and identifying a ranged set of solutions that satisfy the requirements both of the steel manufacturing process and the end rod product.

In practice design is involved with the selection of a suitable material for a given application. The classical material selection approaches are being replaced by a materials design revolution that is underway in the recent past where the focus is to design the material microstructure or mesostructure to achieve certain performance requirements such as density, strength, ductility, toughness, hardness and so on. The demands on the microstructure placed by these multiple performance requirements are often in conflict.

Our interest lies in formulating and solving the inverse problem: given the required end properties/performance, what should be the input parameters in terms of material microstructure and processing paths for the model-based realization of the material, product, and the manufacturing processes?

From a systems design perspective, we view design as a *top-down, simulation-supported, integrated, decision-based process to satisfy a ranged set of product-level performance requirements* (McDowell, Panchal and coauthors 2009, Allen, Panchal and coauthors 2015). Keeping with this and the discussions by Olson on Materials-by-Design (Olson 1997), we view the integrated design of materials, products and processes as *fundamentally an inverse, goal-oriented synthesis activity in which the designer (decision-maker) aims at identifying material structures and processing paths that achieve/satisfy certain required product and process-level properties and performances*. From the standpoint of design community, design process is always the inverse process of identifying design variables to realize desired properties or performances. However, the word "inverse" is used here from the perspective of materials design community and will be explained in the sections that follow.

The philosophical underpinning of the goal-oriented approach to materials design has been provided by Olson (Olson 1997) and reiterated by many others (McDowell, Panchal and coauthors 2009, Horstemeyer 2012, Horstemeyer 2018, McDowell 2018). The conventional way of modeling hierarchical processes and systems is a “bottom-up”, cause and effect (deductive) approach of modeling the material’s processing paths, microstructures, resulting properties, and then mapping the property relations to performance functions, as shown in Figure 6.1. Over the years the focus in materials design has turned to provide high-throughput decision support and develop inverse methods for materials design exploration as discussed by McDowell and Kalidindi (McDowell and Kalidindi 2016). There are several works in this vein. Adams and coauthors (Adams, Kalidindi and coauthors 2013) present a framework that utilizes highly efficient spectral representations to arrive at invertible linkages between material structure, its properties, and the processing paths used to alter the material structure. The Materials Knowledge Systems approach by Kalidindi and coauthors (Kalidindi, Niezgoda and coauthors 2010, Kalidindi, Niezgoda and coauthors 2011) showcase advances in rapid inverse design to estimate local responses. However, all these approaches including the strategy proposed by Olson (McDowell and Olson 2008) fall to specific classes of materials design problems and demands considerable knowledge and insight in mechanisms, material hierarchy and information flow. Thus, these classes of inverse design approaches are mostly suited for detailed design and not for “design exploration” (McDowell 2018).

In our work, we seek “top-down”, goals/means, inductive or inverse methods especially at early stages of design to explore the design space of processing paths and resulting microstructures of a material *satisfying* a set of specified performance requirements, see Figure 6.1. Approaches to pursue top-down design exploration by employing multiscale modeling and systems-based design especially at early stages of design are addressed in limited literatures. Choi and coauthors (Choi, Mcdowell and coauthors 2008, Choi, McDowell and coauthors 2008) propose the Inductive Design Exploration Method (IDEM); a multi-level, robust design method that makes it possible to consider propagation of all three types of uncertainty (Nellippallil, Mohan and coauthors 2018), such as that arising in hierarchical materials design problems that incorporates process-structure-property relations. The two major design objectives using the IDEM for material and product design are (McDowell and Olson 2008): i) to guide bottom-up modeling so as to conduct top-down, goal-oriented design exploration, ii) to manage the uncertainty in chains of process-structure-property relations. Kern and coauthors (Kern, Priddy and coauthors 2017) propose pyDEM a generalized implementation of the IDEM as an open-source tool in the Python environment. The top-down, goal-oriented approach of materials design comes with several challenges as highlighted by McDowell and co-authors (McDowell, Choi and coauthors 2007). In this chapter, we address the challenge of incorporating the design of the material as part of a larger overall systems design process embodying the hierarchy of process-structure-property-performance set forth by Olson (Olson 1997) with consideration on supporting coordination of information and human decision making.

To carry out design space exploration across the material processing-structure-property-performance spaces there should be flow of information via simulation models integrated across multiple scales and across multiple manufacturing processes – defined as the vertical and horizontal integration of models. We define *vertical integration* as the integration of models and simulations of different phenomenon that occur at multiple length scales for a specific manufacturing process so as to generate information that can be passed to other manufacturing processes that follow. We define *horizontal integration* as the integration of different such manufacturing processes using simulation models ensuring proper flow of the information generated through vertical integration at each manufacturing process thereby establishing the processing-structure-property-performance route to realize an end product (Nellippallil, Song and coauthors , Tennyson, Shukla and coauthors 2015), see Figure 6.1.

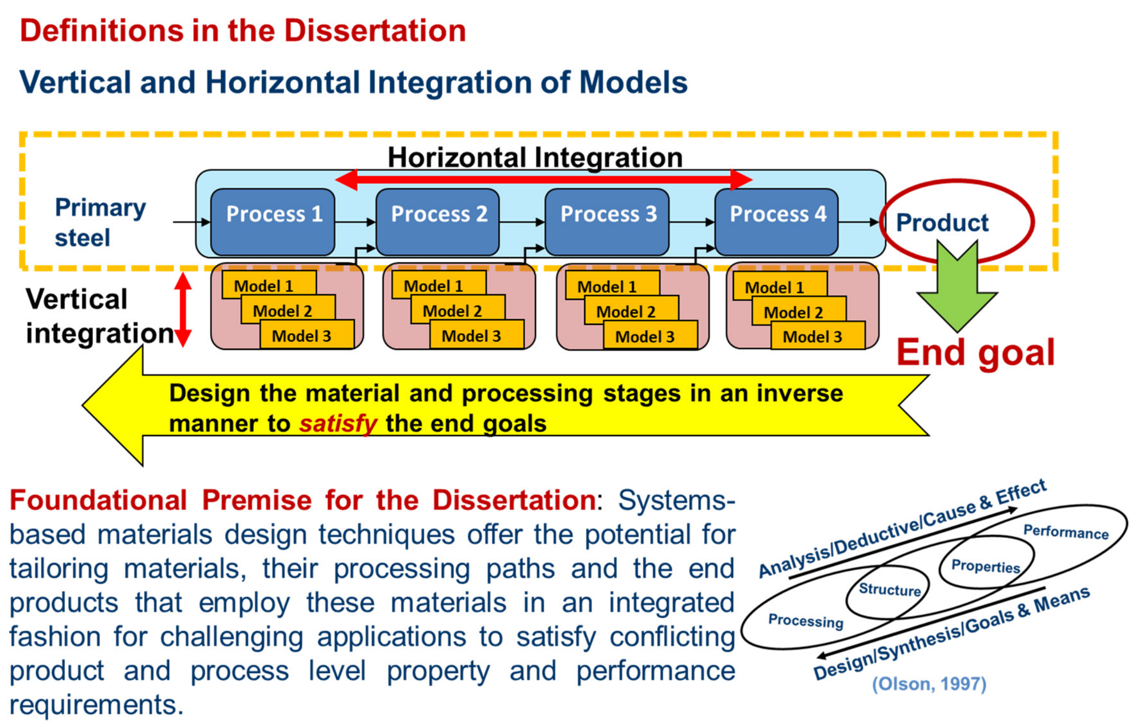


Figure 6.1: Vertical and Horizontal Integration and Systems-based Materials and Product Design

To achieve vertical and horizontal integration of models, there must be analysis models linking different manufacturing processes and phenomenon which predict the material properties associated with these processes and ensure the proper forward flow of information. Once we achieve forward modeling, we carry out top-down (goal-oriented), decision-based design exploration of the material microstructure and processing paths to achieve the required product properties. The primary mathematical construct used in the method is the compromise Decision Support Problem (cDSP) supported by the Concept Exploration Framework (CEF) to generate *satisficing* design solutions (Mistree, Hughes and coauthors 1993). Our intention in solving the compromise DSP is to *satisfice* a set of goals and thus we approach the problem from the school of thought of a *satisficer*; more information available in (Mistree, Patel and coauthors 1994). The Concept Exploration Framework is inspired from the Robust Concept Exploration Method (RCEM) proposed by Chen and co-authors (Chen, Allen and coauthors 1997) to systematically generate satisficing, top-level specifications.

In Section 6.2, we describe the vertical and horizontal integration of models from the perspective of the steel manufacturing process chain problem focused on hot rod rolling (HRR) process that we are addressing. In Section 6.3, we apply the proposed goal-oriented, inverse method for the problem described. The empirical models and the response surface models for computational analysis of the problem are presented in Section 6.4. The mathematical formulation of the hot rod rolling process chain is provided in Section 6.5 and the ternary analysis for visualizing and exploring the solution space is covered in Section 6.6 with closing remarks in Section 6.7.

6.2 Integrated Design of Materials, Products and Processes – The Steel Manufacturing Process Chain Problem (Comprehensive Example)

Many algorithms for establishing forward relationships have been developed. These models are used to predict the behavior of materials during complex manufacturing processes as the final properties of the end steel product depend on its processing route (Nellippallil, De and coauthors , Hodgson and Gibbs 1992, Majta, Kuziak and coauthors 1996, Kuziak, Cheng and coauthors 1997, Phadke, Pauskar and coauthors 2004, Jägle 2007). It is beneficial for steel manufactures to develop computer algorithms/tools that provide the capability to establish inverse relationships; i.e., relate the end properties of the steel product as a function of process variables. These computer algorithms/tools need to be developed using mathematical models that predict the microstructure and mechanical properties of the material as a function of the manufacturing process conditions. The challenge here is in considering all the different phenomenon that happens during the processing of the material and establishing the processing-structure-property-performance relationship in an inverse manner using models. In this problem, we are interested in developing an integrated method that is generic and has the ability to relate the end mechanical properties of the material with good accuracy to the different processing and microstructure routes available for the material. The efficacy of the method is illustrated for the specific steel manufacturing process chain problem addressed below. The industry inspired problem is contributed by Tata Consultancy Services Research and Tata Steel in India; the focus being to integrate the design of steel (material), manufacturing processes and automotive gears (end product) (Shukla, Goyal and coauthors 2015).

A difficulty during steel making is the distortion that happens in gear blanks during forging and heat treatment requiring more machining in the later stages of the manufacturing process. This distortion is mainly due to the banded microstructure that forms due to the presence of segregates. The segregation of alloying elements like manganese (Mn) occurs during casting solidification and this impacts the entire downstream processing affecting the end product mechanical properties. These segregates form due to the limited solubility of alloying elements in the melt during casting. These micro segregation patterns usually remain in the material at the later stages as complete removal of these patterns through processes like reheating is not feasible from a manufacturing stand point as it demands large reheating time leading to increased manufacturing costs. In the hot rolling process, deformation of these structures takes place resulting in a change in the concentration profile. The regions are flattened with alternate layers of high solute and low solute develop during rolling. During the following cooling process, phase transformation occurs and austenite to ferrite phase transformation occurs.

If the steel has hypo eutectoid composition the ferrite phase forms in regions with low austenite stabilizing solute and the remainder transforms to pearlite. Due to the alternate layers of low and high solute regions induced during hot rolling, a banded microstructure having ferrite and pearlite forms with that finally leading to distortion in gear blanks. To manage the effects of distortion at the end of forging, these segregates must be tracked in the previous manufacturing stages and the factors must be managed effectively. These factors could be the operating set points needed for rolling and cooling to produce a specific microstructure. Managing these factors will affects the final mechanical properties of the product. Thus, to predict the mechanical properties of the product as a function of the composition, rolling and cooling factors, there must be an integration of models.

6.2.1 Systematic Approach of Modeling the Hot Rolling Process Chain

The first step is the multilevel function structure creation through functional analysis, abstraction and synthesis, Figure 6.1. This is carried out based on the clarified problem defined in Section 6.2.

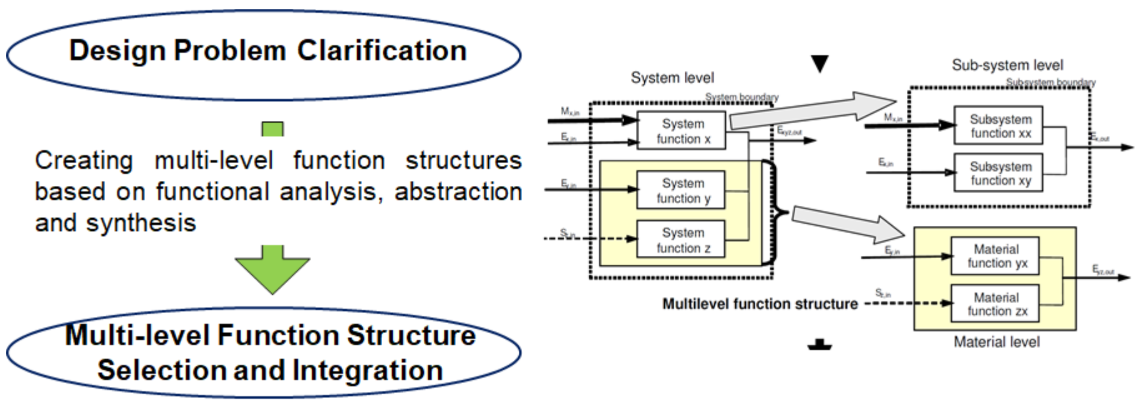


Figure 6.2: Step 1 of systematic model integration – creation of multilevel function structure

In terms of the steel manufacturing process chain problem clarified in Section 6.2, the system level functionalities that material-product-manufacturing process system should fulfill are to ***transform*** a square billet into a rod; ***transform*** austenite phase of steel to different phases of steel like ferrite and pearlite; ***transform*** by breaking down the initial austenite grain size to smaller equiaxed grains of austenite and further to ferrite; ***manage*** banded microstructure of ferrite and pearlite; ***manage/control*** micro segregation effects caused by banded microstructure by controlling the manganese content; ***improve*** yield strength; ***improve*** tensile strength; ***improve*** hardness; ***improve*** toughness.

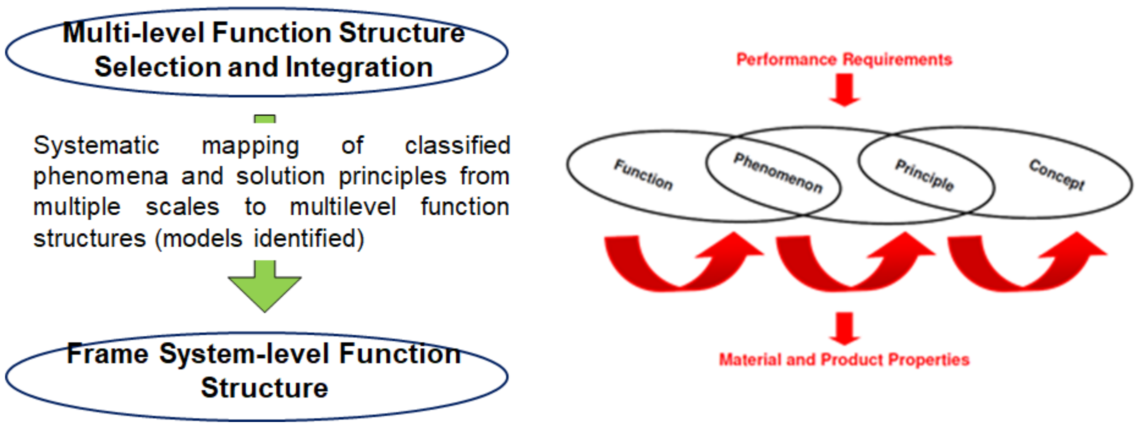


Figure 6.3: Mapping phenomena to core functions

The focus in this section is on the systematic mapping of phenomena to the core functions identified. The phenomena, input and output for the phenomena to establish the information flow chain across the system is identified. The forward material workflow starts with the hot rolling process which includes a hot deformation module, recrystallization module, flow stress module and a grain growth module. The input is the chemical composition, initial austenite grain size after reheating, and the rolling schedule (strain, strain rate, interpass time, number of passes). These are used to predict the temperature evolution, flow stress, and to estimate the austenite grain size after rolling. The output after the vertical integration of these modules is passed to cooling process models. In the vertical integration of cooling process, time-temperature transformations and simultaneous transformations must be considered for the transformations from austenite to different steel phases. This will provide a way to model the banding that occurs during cooling. Here, we consider austenite transformations to ferrite and pearlite phases only. The input to this module is the chemical composition, final austenite grain size after rolling, and the cooling conditions (cooling rate). After the vertical integration of these modules, the output is the phase fractions (final microstructure after cooling), pearlite interlamellar spacing and the ferrite grain size. This output and the chemical composition serves as the input for the property module to predict the mechanical properties, the yield strength, tensile strength, hardness, and toughness. Through these model and simulation integrations specific problem dependent information is passed from one manufacturing process to the other thereby developing a link between the manufacturing processes. This is the horizontal integration of the manufacturing processes to realize the end product (rod produced after rolling and cooling for this problem) by establishing the process-structure-property-performance relationships.

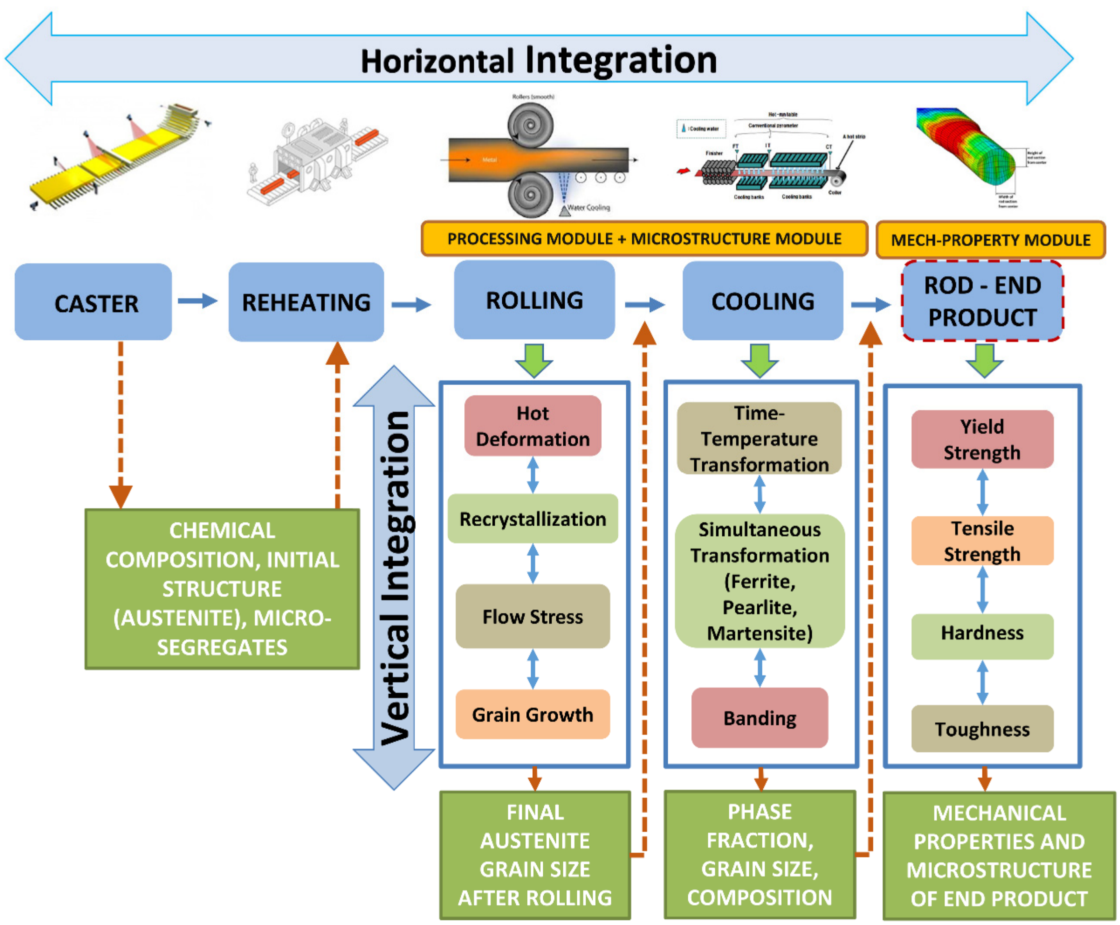


Figure 6.4: The vertical and horizontal integration of models with information flow for the hot rod rolling process chain

The vertical integration of models at multiple length scales and horizontal integration of different processes ensures proper flow of information across processing-microstructure-final mechanical property/performance spaces, see Figure 6.4.

Design catalogs classifying solution principles (models for our case) associated with the phenomenon identified is developed next. The most promising and suiting solution principles for addressing the characteristics of the problem are selected and evaluated further. The design catalogs in our case includes models identified to establish the relationships associated with the problem. Extensive literature search is carried out to identify the possible models for the problem addressed in this dissertation. Some examples of design catalogs in terms of the models identified are shown below. The design catalog for ultimate tensile strength, yield strength and ferrite grain in terms of different models identified is shown in Table 6.1, 6.2 and 6.3 respectively.

Table 6.1: Design catalog for tensile strength models

Model Source	Equation
(Gladman, McIvor and coauthors 1972)	$\sigma_u = X_f^{1/3}(246 + 1143[N]^{0.5} + 18.1(0.001D_\alpha)^{-0.5}) + 97[Si] + (1 - X_f^{1/3})(719 + 3.5S_0^{-0.5})$
(Choquet, Fabregue and coauthors 1990)	$\sigma_u = 237 + 29[Mn] + 79[Si] + 5369[N] + 700[P] + 7.24X_f(0.001D_\alpha)^{-0.5} + 500(1 - X_f)$
(Hodgson and Gibbs 1992)	$\sigma_u = 164.9 + 634.7[C] + 53.6[Mn] + 99.7[Si] + 651.9[P] + 472.6[Ni] + 3339[N] + 11(0.001D_\alpha)^{-0.5}$
(Kuziak, Cheng and coauthors 1997)	$\sigma_u = X_f(20 + 2440[N]^{0.5} + 18.5(0.001D_\alpha)^{-0.5}) + 750(1 - X_f) + 3(1 - X_f^{0.5})S_0^{-0.5} + 92.5[Si]$

Table 6.2: Design catalog for yield strength models

Model Source	Equation
(Gladman, McIvor and coauthors 1972)	$\sigma_y = 63[Si] + 425[N]^{0.5} + X_f^{1/3}(35 + 58[Mn] + 17(0.001D_\alpha)^{-0.5}) + (1 - X_f^{1/3})(179 + 3.9S_0^{-0.5})$
(Gladman, Dulieu and coauthors 1977)	$\sigma_y = 88 + 37[Mn] + 83[Si] + 2900[N]^{0.5} + 17(0.001D_\alpha)^{-0.5}$
(LeBon and deSaint-Martin 1977)	$\sigma_y = 190 + 15.9(0.001D_\alpha)^{-0.5}$
(Kejian and Baker 1993)	$\sigma_y = \sqrt{\{70 + 37[Mn] + 83[Si] + 1500[N] + 18.6(0.001D_\alpha)^{-0.5}\}^2 + \sigma_d^2}$
(Choquet, Fabregue and coauthors 1990)	$\sigma_y = 63 + 23[Mn] + 53[Si] + 5000[N] + 700[P] + X_f\left(15.4 - 30[C] + \frac{6.094}{0.8 + [Mn]}\right)(0.001D_\alpha)^{-0.5} + (1 - X_f)(360 + 2600[C]^2)$
(Hodgson and Gibbs 1992)	$\sigma_y = 62.6 + 26.1[Mn] + 60.2[Si] + 759[P] + 212.9[Cu] + 3286[N] + 19.7(0.001D_\alpha)^{-0.5}$
(Majta, Kuziak and coauthors 1996)	$\sigma_y = 75.4[Si] + 478[N] + 1200[P] + X_f(77.7 + 59.5[Mn] + 9.1(0.001D_\alpha)^{-0.5}) + (1 - X_f)(145.5 + 2.5S_0^{-0.5})$
(Kuziak, Cheng and coauthors 1997)	$\sigma_y = X_f(77.7 + 59.5[Mn] + 9.1(0.001D_\alpha)^{-0.5}) + 478[N]^{0.5} + 1200[P] + (1 - X_f)[145.5 + 3.5S_0^{-0.5}]$

Table 6.3: Design catalog for ferrite grain size

Steel	Model Source	Equation
C-Mn	(Sellars and Beynon 1984)	$D_\alpha = (1 - 0.45\varepsilon_r^{1/2}) \times \{1.4 + 5C_r^{-1/2} + 22[1 - exp(-1.5 \times 10^{-2}D)]\}$
C-Mn $C_{eq} <$ 0.35	(Hodgson and Gibbs 1992)	$D_\alpha = \left(1 - 0.45\varepsilon_r^{1/2}\right) \times \{\left(-0.4 + 6.37C_{eq}\right) + \left(24.2 - 59C_{eq}\right)C_r^{-0.5} + 22[1 - exp(-0.015D)]\}$
C-Mn $C_{eq} >$ 0.25	(Hodgson and Gibbs 1992)	$D_\alpha = \left(1 - 0.45\varepsilon_r^{1/2}\right) \times \{\left(22.6 - 57C_{eq}\right) + 3C_r^{-0.5} + 22[1 - exp(-0.015D)]\}$
C-Mn	(Senuma, Suehiro and coauthors 1992)	$D_\alpha = \left[5.51 \times 10^{10} D^{1.76} \exp\left(\frac{-21430}{T_{.05f}}\right) X_f\right]^{1/3}$
C-Mn	(Donnay, Herman and coauthors 1996)	$D_\alpha = \{13 - 0.73[1000([C] + 0.1[Mn])^{0.45}]\}D^{0.3}C_r^{-0.15}$
Nb	(Sellars and Beynon 1984)	$D_\alpha = (1 - 0.45\varepsilon_r^{1/2}) \times \{2.5 + 3C_r^{-1/2} + 20[1 - exp(-1.5 \times 10^{-2}D)]\}$
V-Ti	(Roberts, Sandberg and coauthors 1983)	$D_\alpha = 3.75 + 0.18D + 1.4C_r^{-0.5}$

V-Ti	(Sellars and Beynon 1984)	$D_\alpha = (1 - 0.45\varepsilon_r^{1/2}) \times \{3 + 1.4C_r^{-1/2} + 17[1 - exp(-1.5 \times 10^{-2}D)]\}$
V-T	(Kuziak, Cheng and coauthors 1997)	$D_\alpha = \frac{D}{1 + (0.036 + 0.0233C_r^{.5})D}$

Similar design catalogs are developed for other functions and the system level function structure based on the phenomena and solution principles is developed. The system level function structure after the selection and integration of models showing the information flow across the processing-structure-property-performance spaces of material, product and manufacturing processes is shown in Figure 6.5.

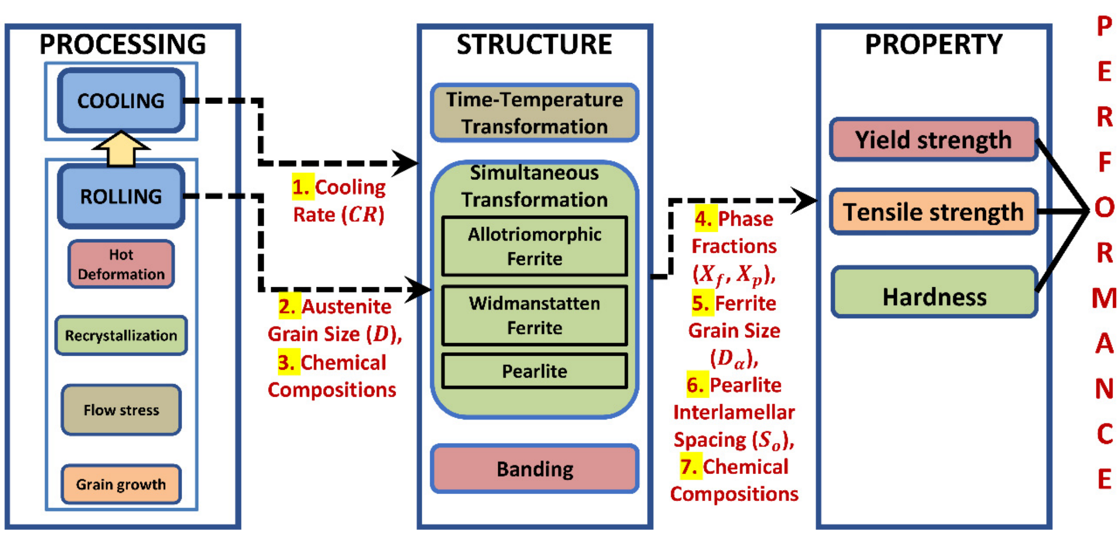


Figure 6.5: System-level function structure and information flow chain for the problem addressed

The selection/identification of the solution principles from the design catalogs for the problem discussed in this dissertation is provided in Section 6.5 of this chapter and are not detailed here.

To illustrate the goal-oriented inverse method, we define a boundary within the problem. Here, we focus on using the proposed method to establish processing-microstructure-property relations between the rolling, cooling module (processing and microstructure) and the property module of the product that defines the end performance. In Section 6.3, the Concept Exploration Framework that is used to systematically formulate the problem and identify ranged set of satisficing solutions is discussed.

6.3 The Concept Exploration Framework – From the standpoint of Processing-Structure-Property-Performance Relationship

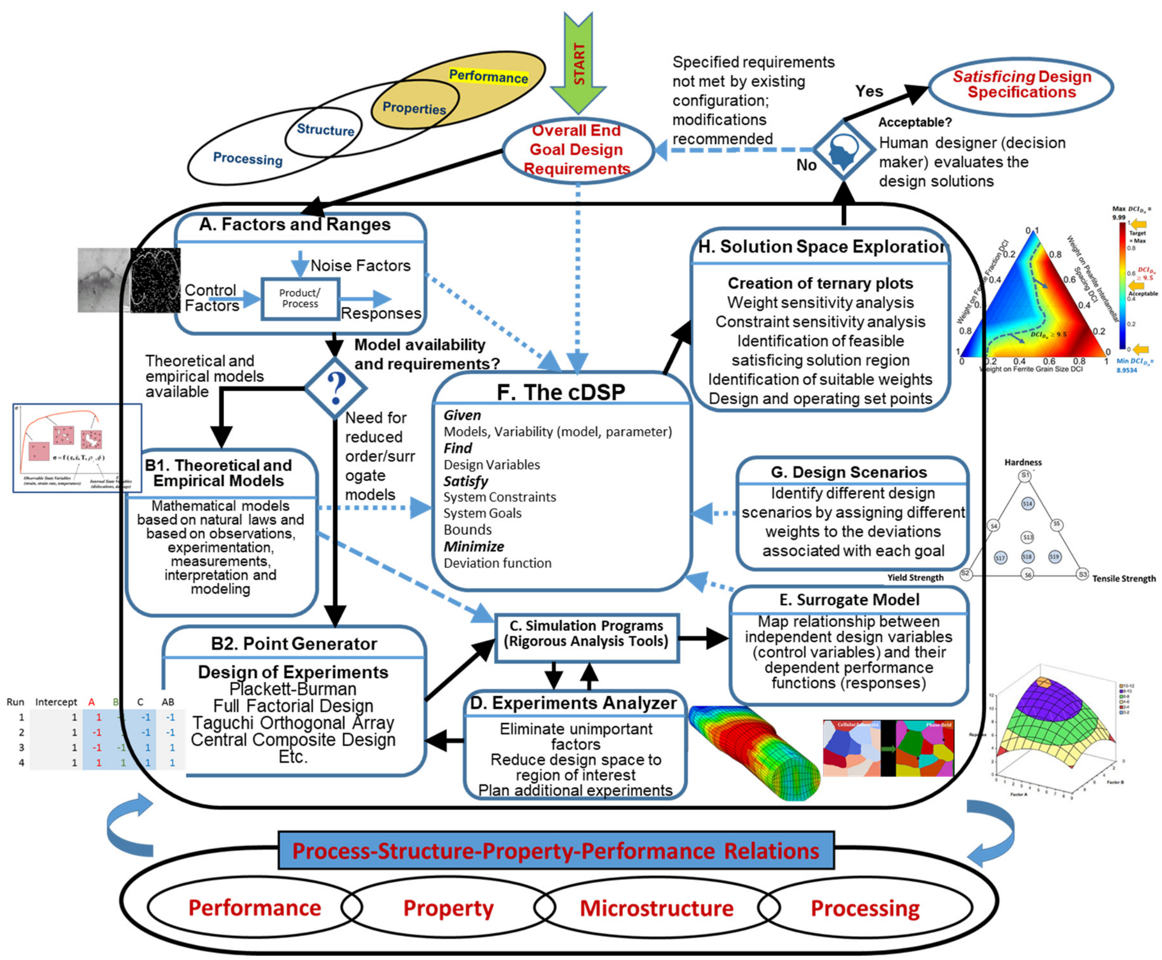


Figure 6.6: The CEF for PSPP Exploration

The CEF is introduced in this chapter as a general framework that includes systematic steps to identify design alternatives and generate *satisficing* design solutions across the processing-microstructure-property-performance spaces. The CEF is inspired from the RCEM (Chen, Allen and coauthors 1997) with addition of features (processors) to consider different material and product models and options to explore the solution space for different design scenarios. The foundational mathematical construct of the CEF is the compromise Decision Support Problem (cDSP) (Mistree, Hughes and coauthors 1993). The cDSP construct used here is anchored in the robust design paradigm first proposed by Taguchi. The fundamental assumption is that the models are not complete, accurate and of equal fidelity (Taguchi , Bras and Mistree 1993). The cDSP is a hybrid of mathematical programming and goal programming and the emphasis of the designer using the cDSP is to satisfy specified target goals as closely as possible. This is achieved by seeking multiple solutions through trade-offs among multiple conflicting goals. The solutions obtained are further evaluated by solution space exploration to identify solution regions that best satisfy the requirements identified. The four keywords in the cDSP – *Given*, *Find*, *Satisfy* and *Minimize* support a designer in formulating the problem systematically and the overall goal of the designer using the cDSP is to minimize a deviation function.

The Concept Exploration Framework along with its features of multi-goal decision support can be readily incorporated into a design method that supports the design of the material and product (processing, composition and microstructure) as part of a larger overall systems design process. The framework can embody the hierarchy of process-structure-property-performance proposed by Olson (Olson 1997) by systematically accounting the information flow and mappings across these spaces and transforming overall design requirements into a set of satisficing design specifications for the material-product-and manufacturing process system of interest. The designer can start with the performances/properties that he or she wants and use the CEF to identify satisficing solutions for microstructure, see Figure 6.6. This can be further repeated to identify satisficing solutions for the processing space that meets microstructure requirements.

6.4 Application of Goal-oriented Inverse Design Method and CEF for the Hot Rod Rolling Process Chain Problem

In Figure 6.7, we show the schematic application of proposed goal-oriented, inverse method to carry out the integrated design exploration of the hot rod rolling process chain problem of interest.

Step 1: Establish forward modeling and information flow across the process chain

For the hot rod rolling process chain problem addressed in this chapter, the mechanical property goals and requirements for yield strength (YS), tensile strength (TS), hardness (HV) and toughness measured by impact transition temperature (ITT). These mechanical properties are dependent on the final microstructure after cooling like the ferrite grain size after cooling (FGS, D_α), the phase fractions of ferrite (X_f) and pearlite ($1 - X_f$), the pearlite interlamellar spacing (S_0) and the composition variables like silicon $[Si]$, nitrogen $[N]$, phosphorous $[P]$ and manganese $[Mn]$. These microstructure factors are defined by the rate (CR) at which cooling is carried out and the final austenite grain size after rolling (AGS, D) and composition variables like carbon $[C]$ and manganese $[Mn]$. The AGS is determined by the processing carried out at rolling stage which requires the modeling of hot deformation, recrystallization, grain growth, etc. The input to the cooling stage is D, CR, $[C]$ and $[Mn]$ from the rolling process. The outputs are D_α, X_f and S_0 which along with the composition variables define the YS, TS, ITT and HV of end rod produced. The models used to establish these relationships are presented in Section 6.5.

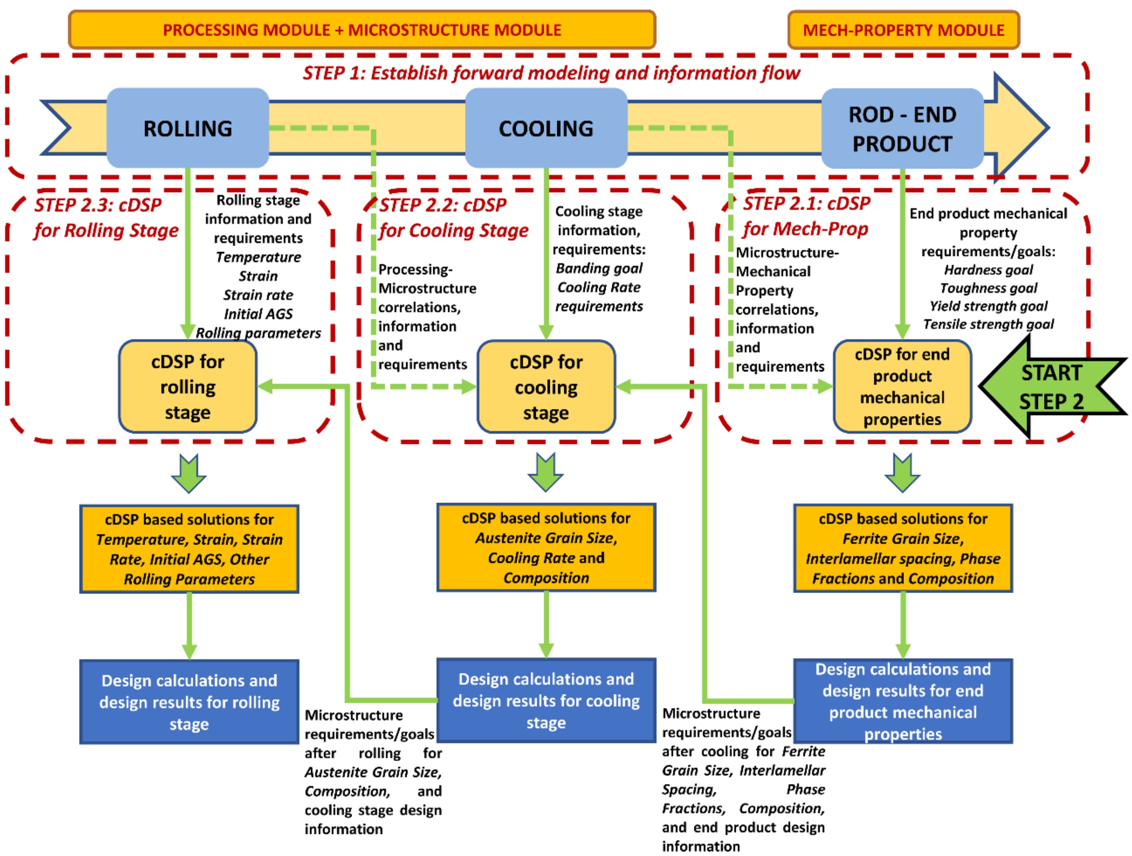


Figure 6.7: Schematic of the proposed goal-oriented, inverse method for the hot rod rolling process chain problem

Step 2.1: Formulate cDSP for end mechanical properties of rod to explore the processing and microstructure space for cooling stage

In Step 2.1, the cDSP for the mechanical properties of the final end product is formulated. Information, requirements and the correlations between mechanical properties and microstructure after cooling (ferrite grain size, pearlite interlamellar spacing, phase fractions, and composition) are communicated to this cDSP. The end mechanical property goals are requirements for yield strength, tensile strength, hardness and toughness (impact transition temperature). On exercising the cDSP and carrying out solution space exploration of the microstructure space after cooling, the combinations for ferrite grain size (D_α), phase fractions X_f, pearlite interlamellar spacing S_0 and compositions that best satisfy the requirements for end properties are identified and are communicated to the next step. The formulation of the cDSP is provided in Section 6.6 and the solution space exploration is carried out in Section 6.7.

Step 2.2: Formulate cDSP for cooling stage to explore the processing and microstructure space of rolling

In Step 2.2, a similar process to that in Step 2.1 is carried out to formulate the cDSP for cooling. This cDSP has target goals and requirements for ferrite grain size D_α, phase fraction X_f, and composition that are based on the solutions obtained from the first cDSP. Also, information from cooling stage such as banding requirements, cooling rate requirements are included into this cDSP. The information, requirements, and correlations of variables at the end of rolling (austenite grain size, composition) and the cooling stage parameters are communicated to the cDSP. The goals for this cDSP are target ferrite grain size and target phase fractions subject to constraints. On exercising the cDSP, the combinations for austenite grain size D, cooling rate CR, and composition elements like carbon (C) and manganese (Mn) that best satisfy the requirements are identified. The formulation of this cDSP is in Section 6.6 and the solution space exploration is carried out in Section 6.7.

Step 2.3: Formulate cDSP for rolling to carry out design exploration of rolling process variables

In Step 2.3, we follow a similar procedure to Steps 2.1 and 2.2 to formulate the cDSP for rolling considering the information generated from cooling and the rolling information and requirements identified. This cDSP has a grain growth module, static, dynamic and meta dynamic recrystallization modules and a hot deformation module.

Due to the complexity and size of the problem we are demonstrating the efficacy of method by carrying out the design space exploration of the hot rolling process chain problem by addressing the cDSPs in Steps 2.1 and 2.2. The cDSPs in Steps 2.1 and 2.2 spans the processing, microstructure and property spaces and is thus sufficient for framing a well-defined problem boundary for the method demonstration.

6.5 Mathematical Models for Hot Rod Rolling Process Chain Design (Establishing Step 1 Of Method)

The mathematical models used to formulate the hot rod rolling (HRR) process chain problem are introduced and brief descriptions are provided here. These models, the control variables, noise factors, parameters, responses and allowable ranges are identified by carrying out Steps 1 and 2 of the CEF as described in Section 4.6 in Chapter 4 and briefly addressed in Section 6.3. From the problem perspective, we accomplish Step 1 of the goal-oriented, inverse decision-based design method by identifying these forward models to establish the relationships described in Section 6.4. In Section 6.5.1 we describe the microstructure-mechanical property correlation models that establish relationships between the mechanical properties of the rod product and the microstructure generated after cooling stage. In Section 6.5.2 and 6.5.3, we describe the models for phase transformation on cooling after hot rolling.

6.5.1 Mechanical Property-Microstructure Correlation Models

The required mechanical properties for the rod are yield strength (YS), tensile strength (TS), toughness measured by impact transition temperature (ITT) and hardness (HV). Gladman and co-authors (Gladman, McIvor and coauthors 1972, Gladman, Dulieu and coauthors 1977) predict the mechanical properties of plain carbon steel products as a function of the ferrite-pearlite microstructure. Models with improved predictive power were later developed by Hodgson and Gibbs (Hodgson and Gibbs 1992), Majta and co-authors (Majta, Kuziak and coauthors 1996), Kuziak and co-authors (Kuziak, Cheng and coauthors 1997) and Yada (Yada 1987), Table 6.4. Details on these models and the reason for their selection are presented by Nellippallil and coauthors (Nellippallil, Allen and coauthors 2017) and described next. The models identified are summarized in Table 6.4.

Model for Yield Strength (YS)

Yield strength (lower yield stress) is an important mechanical property that defines the stress at which the material begins to deform plastically. We have selected a semi-empirical model (Equation 6.1) by Kuziak and co-authors that describes the lower yield stress YS, of carbon-manganese steels as a function of ferrite grain size after cooling D_{α}, cooling rate CR, ferrite fraction X_f, the pearlite interlamellar spacing S_o, and the composition elements in the steel (Kuziak, Cheng and coauthors 1997). The model is developed following the concept of Hall-Petch relationship. The reason for the selection of this model is because of the fact that it takes into account the influence of pearlite through the factors X_f and S_o compared to other models available.

$$YS = X_f(77.7 + 59.9 \times [Mn] + 9.1 \times (0.001D_\alpha)^{-0.5}) + 478[N]^{0.5} + 1200[P] + (1 - X_f)[145.5 + 3.5S_0^{-0.5}] \quad \textbf{Equation 6.1}$$

where YS is in MPa, S_o in μm, D_α in μm.

Model for Tensile Strength (TS)

Tensile strength represents the resistance of the material to breaking when subjected to tensile loads. We have selected the model (Equation 6.2) by Kuziak and co-authors that describes the tensile strength TS, of carbon-manganese steels as a function of ferrite grain size after cooling D_α, cooling rate CR, ferrite fraction X_f, the pearlite interlamellar spacing S_o, and the composition elements in the steel (Kuziak, Cheng and coauthors 1997). Again, we have opted for the model as it takes into account the influence of pearl-ite.

$$TS = X_f(20 + 2440 \times [N]^{0.5} + 18.5 \times (0.001D_\alpha)^{-0.5}) + 750(1 - X_f) + 3(1 - X_f^{0.5})S_0^{-0.5} + 92.5 \times [Si] \quad \textbf{Equation 6.2}$$

where TS is in MPa, S_o in μm, D_α in μm.

Model for Hardness (HV)

Hardness represents the resistance to plastic deformation usually by indentation. Hardness (HV) is represented as a function of ferrite and pearlite fractions, average austenite to ferrite transformation temperature (T_{mf}) and the weight percentage of silicon (Si) as depicted in Equation 6.3 based on the investigation by Yada (Yada 1987).

$$HV = X_f\left(361 - 0.357T_{mf} + 50[Si]\right) + 175(1 - X_f) \qquad \textbf{Equation 6.3}$$

We have assumed the value of T_{mf} as 700 ℃ in this work.

Model for Impact Transition Temperature (ITT)

The impact transition temperature denotes the boundary between brittle and ductile failure when subjected to impact loads and is a measure of the material's impact toughness. This temperature is extremely important during material selection. We have selected the model (Equation 6.4) developed by Gladman and co-authors (Gladman, McIvor and coauthors 1972) for impact transition temperature of high-carbon steels as a function of ferrite grain size D_α, ferrite fraction X_f, pearlite interlamellar spacing S_o, pearlite colony size p, carbide thickness t and composition elements.

$$\begin{aligned} ITT = {} & X_f(-46 - 11.5D_\alpha^{-0.5}) \\ & + \left(1 - X_f\right)(-335 + 5.6S_0^{-0.5} - 13.3p^{-0.5} \\ & + (3.48 \times 10^6)t) + 49[Si] + 762[N]^{0.5} \end{aligned} \qquad \textbf{Equation 6.4}$$

where D_α, S_o, p and t are in mm in Equation 6.4.

We assume the value of pearlite colony size p as 6 μm and carbide thickness t as 0.025 μm.

Table 6.4: Mechanical property models

Mechanical Property	Model	Reference
Yield Strength	$YS = X_f(77.7 + 59.9 \times [Mn] + 9.1 \times (0.001D_\alpha)^{-0.5}) + 478[N]^{0.5} + 1200[P] + (1 - X_f)[145.5 + 3.5S_0^{-0.5}]$ where YS is in MPa, S_o in µm, D_α in µm	Kuziak and co-authors (Kuziak, Cheng and coauthors 1997)
Tensile Strength	$TS = X_f(20 + 2440 \times [N]^{0.5} + 18.5 \times (0.001D_\alpha)^{-0.5}) + 750(1 - X_f) + 3(1 - X_f^{0.5})S_0^{-0.5} + 92.5 \times [Si]$ where TS is in MPa, S_o in µm, D_α in µm	Kuziak and co-authors (Kuziak, Cheng and coauthors 1997)
Hardness	$HV = X_f(361 - 0.357T_{mf} + 50[Si]) + 175(1 - X_f)$ Average austenite to ferrite transformation temperature (T_{mf}) is assumed as 700 ℃	Yada (Yada 1987)

Impact Transition Temperature	$ITT = X_f(-46 - 11.5D_{\alpha}^{-0.5}) + (1 - X_f)(-335 + 5.6S_0^{-0.5} - 13.3p^{-0.5} + (3.48 \times 10^6)t) + 49[Si] + 762[N]^{0.5}$ where D_{α}, S_o, p and t are in mm. We have assumed the value of pearlite colony size p as 6 μm and carbide thickness t as 0.025 μm	Gladman and co-authors (Gladman, McIvor and coauthors 1972)

6.5.2 Models for Phase Transformation on Cooling after Hot Working

Classical nucleation and grain growth theory quantitatively describe the kinetics of decomposition of austenite. Using classical Johnson-Mehl-Avrami theory, we describe the transformation of a single phase to a product phase (Jägle 2007). The transformations that occur in steel are often simultaneous resulting in the formation of multiple phases such as allotriomorphic ferrite, Widmanstätten ferrite, bainite, pearlite, and martensite. Therefore, one requirement for a kinetic model for the phase transformation of steel is that it must allow for simultaneous phase transformations resulting in different steel phases. Robson and Badeshia (Robson and Bhadeshia 1997) and Jones and Badeshia (Jones and Bhadeshia 1997) address this requirement by numerically solving all impingement equations and choosing the appropriate nucleation and grain growth equations. The simultaneous transformation of austenite into allotriomorphic ferrite, Widmanstätten ferrite, and pearlite are considered by Jones and Badeshia (Jones and Bhadeshia 1997); details can be found in (Jones and Bhadeshia 1997, Jones and Bhadeshia 1997, Jägle 2007). We have used the program STRUCTURE developed by

Jones and Badeshia to predict the simultaneous transformation of austenite (and, H. K. D. H and coauthors Last accessed 4, February 2017.).

Response surface models (RSMs) are used to calculate the microstructure (allotriomorphic ferrite, Widmanstätten ferrite, and pearlite) of steel as a function of percentages of carbon $[C]$ manganese $[Mn]$, cooling rate CR and austenite grain size $[D]$ using the STRUCTURE program. These predictors are selected because of their substantial contribution to austenite transformation and the formation of banded microstructure (Jägle 2007). Values for the other required input are based on the work of Jones and Badeshia (Jones and Bhadeshia 1997). A fractional factorial design of experiments is carried out to develop response surface models for the transformation of austenite to ferrite and pearlite [23, 25], Table 6.5. The response surface models are shown in Table 6.6. The RSMs are verified by comparing the predictions with experimental (measured) data reported by Bodnar and Hensen (Bodnar and Hansen 1994), see (Nellippallil, Allen and coauthors 2017).

Table 6.5: Factors and factor levels for DoE

Level	$\boldsymbol{CR}$ **K/min**	$\boldsymbol{AGS}$ $\boldsymbol{\mu m}$	$[\boldsymbol{C}]$ **%**	$[\boldsymbol{Mn}]$ **%**
1	11	30	0.18	0.7
2	55	55	0.24	1.1
3	100	100	0.3	1.5

Response Surface Model Verification

The developed RSMs are verified by comparing the predictions with experimental (measured) data reported by Bodnar and Hensen (Bodnar and Hansen 1994). We observe from the comparison showcased in Figure 6.8 that the predictions using RSM lies more or less in the vicinity of the straight line depicting the measured values. However, as we can observe from Figure 6.8, the model is not fully accurate and the uncertainties associated with the model have to be dealt with in future analysis.

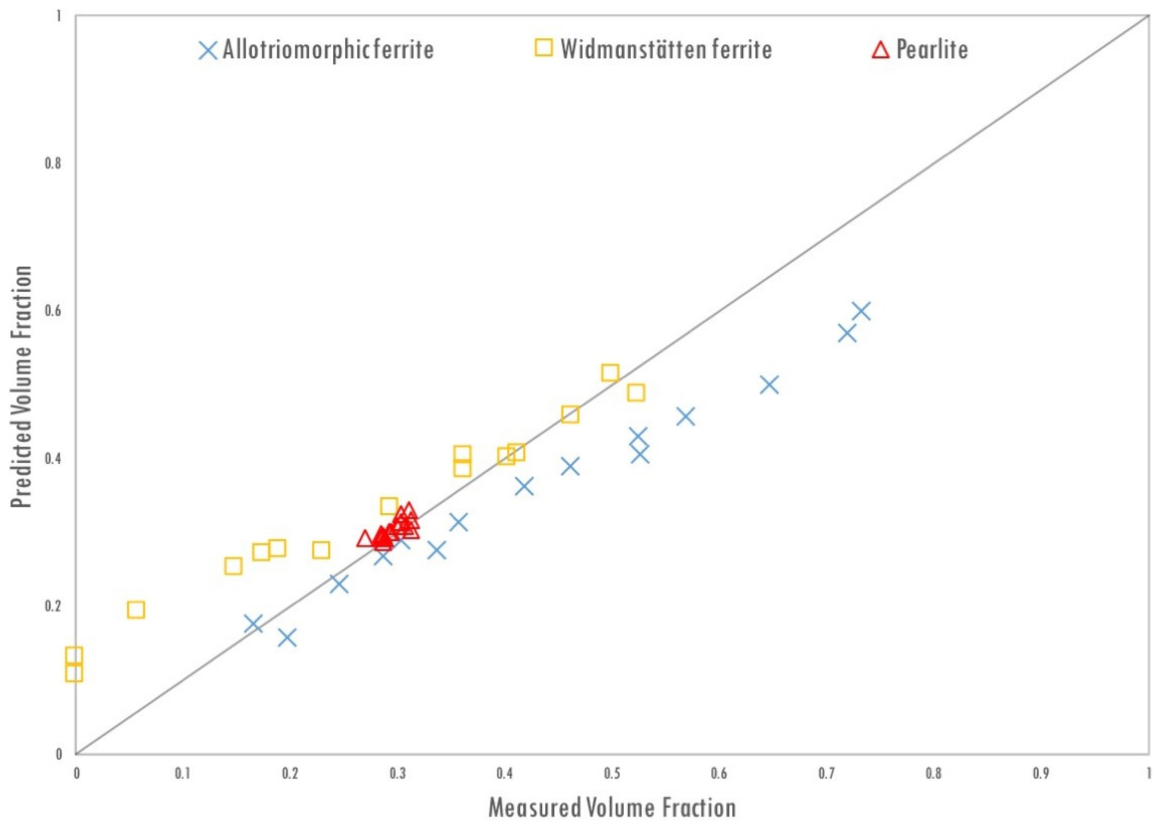


Figure 6.8: Comparison of RSM predictions with measured volume fractions from literature (Bodnar and Hansen 1994)

The response surface model developed by carrying out the experimental runs using the STRUCTURE program is listed in Equations 6.5-6.8 and summarized in Table 6.6. The response surface model developed for fraction of allotriomorphic ferrite X_{fa} with R^2 value of 0.98 is

$$X_{fa} = 1.59 - 0.26[C] - 0.00856CR - 0.0105D - 3.08[C] + 0.000826[Mn]CR + 0.0009[Mn]D + 0.7647[Mn][C] + 0.000011CR * D + 0.002CR[C] + 0.0032D[C] - 0.05058[Mn]^2 + 0.00004CR^2 + 0.000036D^2 + 2.483[C]^2 \quad \textbf{Equation 6.5}$$

The response surface model developed for fraction pearlite X_p with R^2 value of 0.99 is

$$X_p = 0.206 - 0.117[Mn] - 0.0005CR - 0.00113D + 0.248[C] + 0.00032[Mn]CR + 0.000086[Mn]D + 0.9539[Mn][C] - 4.259 \times 10^{-6}CR * D + 0.00726CR[C] + 0.0023D[C] - 0.0305[Mn]^2 - 0.0000056CR^2 + 4.859 \times 10^{-6}D^2 + 0.79[C]^2 \quad \textbf{Equation 6.6}$$

Widmanstätten ferrite X_{fw} is represented as the fraction that is left after transformations of austenite to allotriomorphic ferrite and pearlite.

$$X_{fw} = 1 - (X_{fa} + X_p) \quad \textbf{Equation 6.7}$$

The total ferrite is calculated as the sum of allotriomorphic ferrite and Widmanstätten ferrite.

$$X_f = (X_{fa} + X_{fw}) \quad \textbf{Equation 6.8}$$

Table 6.6: Design catalog - RSM for phase fractions

Phase Fraction	**Response Surface Model Developed**	**R^2 value**
Allotriomorphic Ferrite	$X_{fa} = 1.59 - 0.26[C] - 0.00856CR - 0.0105D - 3.08[C] + 0.000826[Mn]CR + 0.0009[Mn]D + 0.7647[Mn][C] + 0.000011CR * D + 0.002CR[C] + 0.0032D[C] - 0.05058[Mn]^2 + 0.00004CR^2 + 0.000036D^2 + 2.483[C]^2$	0.98
Pearlite	$X_p = 0.206 - 0.117[Mn] - 0.0005CR - 0.00113D + 0.248[C] + 0.00032[Mn]CR + 0.000086[Mn]D + 0.9539[Mn][C] - 4.259 \times 10^{-6}CR * D + 0.00726CR[C] + 0.0023D[C] - 0.0305[Mn]^2 - 0.0000056CR^2 + 4.859 \times 10^{-6}D^2 + 0.79[C]^2$	0.99
Widmanstätten Ferrite	$X_{fw} = 1 - (X_{fa} + X_p)$	–
Total Ferrite	$X_f = (X_{fa} + X_{fw})$	–

6.5.3 Models for Ferrite Grain Size (D_α) and Pearlite Interlamellar Spacing (S_o)

As the hot worked steel cools, austenite is transformed into various phases. The most important parameters are the ferrite grain size and pearlite interlamellar spacing because they contribute to the steel's mechanical properties. The models for these parameters are summarized in Table 6.7.

Ferrite Grain Size

As the hot worked steel cools down to a lower temperature, austenite transforms to different phases. Out of the newly formed phases, the ferrite grain size is one important parameter that contributes to the strength of the compositions. The factors affecting ferrite grain size D_α are final austenite grain size after rolling D and retained strain ε_r, both related to the deformation history of the material from rolling side, the composition and cooling rate which are external influences (Pietrzyk, Cser and coauthors 1999). We are adopting the models by Hodgson and Gibbs (Hodgson and Gibbs 1992) (Equations 6.9 and 6.10) for defining ferrite grain size.

$$D_\alpha = (1 - 0.45\varepsilon_r^{0.5}) \times \{(-0.4 + 6.37C_{eq}) + (24.2 - 59C_{eq})CR^{-0.5} + 22[1 - \exp(-0.015D)]\} \quad \text{for } C_{eq} < 0.35 \qquad \textbf{Equation 6.9}$$

$$D_\alpha = (1 - 0.45\varepsilon_r^{0.5}) \times \{(22.6 - 57C_{eq}) + 3CR^{-0.5} + 22[1 - \exp(-0.015D)] \quad \text{for } C_{eq} > 0.35$$ **Equation 6.10**

where C_{eq} is the carbon equivalent given by Equation 7.11.

$$C_{eq} = (C + Mn)/6$$ **Equation 6.11**

Pearlite Interlamellar Spacing

Pearlite interlamellar spacing is a very important microstructural factor that influences the mechanical properties of steel as the steel turns more into a fully pearlitic microstructure (Vander Voort 2015). We are adopting the model (Equation 6.12) by Kuziak and co-authors (Kuziak, Cheng and coauthors 1997) where pearlite interlamellar spacing S_o is defined as a function of carbon C, manganese Mn and cooling rate CR.

$$S_o = 0.1307 + 1.027[C] - 1.993[C]^2 - 0.1108[Mn] + 0.0305CR^{-0.52}$$ **Equation 6.12**

In Section 6.6, we showcase the cDSP formulations for end product mechanical properties and cDSP for cooling stage using the models identified in Section 6.5.

Table 6.7: Design catalog - Models for D_α and S_o

Parameter	Model	Reference
Ferrite Grain Size	$D_\alpha = (1 - 0.45\varepsilon_r^{0.5}) \times \{(-0.4 + 6.37C_{eq}) + (24.2 - 59C_{eq})CR^{-0.5} + 22[1 - \exp(-0.015D)]\}$ for $C_{eq} < 0.35$ $D_\alpha = (1 - 0.45\varepsilon_r^{0.5}) \times \{(22.6 - 57C_{eq}) + 3CR^{-0.5} + 22[1 - \exp(-0.015D)]$ for $C_{eq} > 0.35$ where D is the final austenite grain size after rolling and ε_r is retained strain. C_{eq} is the carbon equivalent given by Equation 11. $C_{eq} = (C + Mn)/6$	Hodgson and Gibbs (Hodgson and Gibbs 1992)
Pearlite Interlamellar Spacing	$S_o = 0.1307 + 1.027[C] - 1.993[C]^2 - 0.1108[Mn] + 0.0305CR^{-0.52}$	Kuziak and co-authors (Kuziak, Cheng and coauthors 1997)

6.6 Formulation of the cDSPs for Hot Rolling Process Chain Problem

In Step 2.1 of the method, we formulate the cDSP for the desired end mechanical properties of the product, Table 6.8. We then determine the end mechanical properties as a function of microstructure factors (D_α, X_f, S_0, Mn, Si, N) after cooling. The end mechanical property goals, e.g., maximizing YS, TS, and HV, are captured in the cDSP. The requirement for minimizing impact transition temperature is captured as a constraint. The possible achievement of these conflicting goals is characterized by solution space exploration. The upper and lower limits for the system variables and the maximum and minimum values for the mechanical properties are defined in the cDSP as bounds and constraints. The goal targets are YS_{Target}= 330 MPa, TS_{Target}= 750 MPa, HV_{Target}= 170. The requirement for ITT is to achieve the minimum value. The requirement for managing the banded microstructure is considered during solution space exploration.

On exercising the cDSP and carrying out solution space exploration a process designer is able to solve and capture the knowledge associated with the following inverse problem: *Given the end mechanical properties of a new steel product mix, what should be the microstructure factors after the cooling stage that satisfies the requirements?*

Table 6.8: The cDSP formulation for Step 2.1

Given
1) End requirements identified for the rod rolling process
• Maximize Yield Strength (Goal)
• Maximize Tensile Strength (Goal)
• Maximize Hardness (Goal)
• Minimize ITT (Requirement)

- Manage Banded Microstructure (Requirement)

2) Well established empirical and theoretical correlations, RSMs and information flow from the end of cooling to the end product mechanical properties (Details provided in Section 6.5)
3) System variables and their ranges

Find

System Variables

X_1, ferrite grain size (D_α)

X_2, the phase fraction of ferrite (X_f)

X_3, the pearlite interlamellar spacing (S_0)

X_4, manganese concentration after cooling ($[Mn]$)

X_5, the composition of Si ($[Si]$)

X_6, the composition of N ($[N]$)

Deviation Variables

d_i^-, d_i^+, *i =1,2,3*

Satisfy

System Constraints

- Minimum yield strength constraint

$$YS \geq 220 \text{ MPa} \qquad \textbf{Equation 6.13}$$

- Maximum yield strength constraint

$$YS \leq 330 \text{ MPa} \qquad \textbf{Equation 6.14}$$

- Minimum tensile strength constraint

$$TS \geq 450 \text{ MPa} \quad \textbf{Equation 6.15}$$

- Maximum tensile strength constraint

$$TS \leq 750 \text{ MPa} \quad \textbf{Equation 6.16}$$

- Minimum hardness constraint

$$HV \geq 131 \quad \textbf{Equation 6.17}$$

- Maximum hardness constraint

$$HV \leq 170 \quad \textbf{Equation 6.18}$$

- Minimum ITT constraint

$$ITT \geq -100\text{°C} \quad \textbf{Equation 6.19}$$

- Maximum ITT constraint

$$ITT \leq 100\text{°C} \quad \textbf{Equation 6.20}$$

System Goals

Goal 1:

- Maximize Yield Strength

$$\frac{YS(X_i)}{YS_{Target}} + d_1^- - d_1^+ = 1 \quad \textbf{Equation 6.21}$$

Goal 2:

- Maximize Tensile Strength

$$\frac{TS(X_i)}{TS_{Target}} + d_2^- - d_2^+ = 1 \quad \textbf{Equation 6.22}$$

Goal 3:

- Maximize Hardness

$$\frac{HV(X_i)}{HV_{Target}} + d_3^- - d_3^+ = 1$$ **Equation 6.23**

Variable Bounds

$8 \leq X_1 \leq 25$ (μm)

$0.1 \leq X_2 \leq 0.9$

$0.15 \leq X_3 \leq 0.25$ (μm)

$0.7 \leq X_4 \leq 1.5$ (%)

$0.18 \leq X_5 \leq 0.3$ (%)

$0.007 \leq X_6 \leq 0.009$ (%)

Bounds on deviation variables

$$d_i^-, d_i^+ \geq 0 \text{ and } d_i^- * d_i^+ = 0 \text{ , i} = 1,2,3$$ **Equation 6.24**

Minimize

We minimize the deviation function

$$Z = \sum_{i=1}^{3} W_i(d_i^- + d_i^+); \sum_{i=1}^{3} W_i = 1$$ **Equation 6.25**

On exercising the cDSP for different design scenarios and carrying out solution space exploration, following the steps in Concept Exploration Framework, we obtain the combinations for D_α, X_f, S_0, Mn, Si, N that satisfy the end mechanical properties and other requirements. The desired solutions identified for D_α, X_f, S_0 are then used as the target goals for the next cDSP (Step 2.2 of the goal-oriented, inverse method).

In Step 2.2 of the method, we formulate the cDSP for the cooling stage, Table 6.9. Using this cDSP, we relate the microstructure factors after cooling that best satisfy the first cDSP requirements as a function of the microstructure and composition factors (D,

C, Mn) after the rolling and the cooling stage operating factor (CR). The target values for the goals are defined as $D_{\alpha_{Target}}$, $X_{f_{Target}}$, $S_{0_{Target}}$ as the results from the first cDSP. On exercising this cDSP the process designer will be able to solve and capture the knowledge associated with the following inverse problem: *Given the microstructure after cooling that best satisfy the end mechanical properties of a new steel product mix, what should be the microstructure factors after rolling and the design and operating set points for cooling that satisfy the requirements identified?*

Table 6.9: The cDSP formulation for Step 2.2

Given

1) Target values for microstructure after cooling (the combination identified from the first cDSP as best satisfying the end goals)
2) Well established empirical and theoretical correlations, RSMs and complete information flow from the end of rolling to the end product mechanical properties (Details provided in Section 6.5)
3) System variables and their ranges

Find

System Variables

X_1, Cooling Rate (CR)

X_2, Austenite Grain Size (D)

X_3, the carbon concentration ($[C]$)

X_4, the manganese concentration after rolling ($[Mn]$)

Deviation Variables

d_i^-, d_i^+, *i =1,2,3*

Satisfy

System Constraints

- Minimum ferrite grain size constraint

$$D_\alpha \geq 8\ \mu m$$ **Equation 6.26**

- Maximum ferrite grain size constraint

$$D_\alpha \leq 20\ \mu m$$ **Equation 6.27**

- Minimum pearlite interlamellar spacing constraint

$$S_o \geq 0.15\ \mu m$$ **Equation 6.28**

- Maximum pearlite interlamellar spacing constraint

$$S_o \leq 0.25\ \mu m$$ **Equation 6.29**

- Minimum ferrite phase fraction constraint (manage banding)

$$X_f \geq 0.5$$ **Equation 6.30**

- Maximum ferrite phase fraction constraint (manage banding)

$$X_f \leq 0.9$$ **Equation 6.31**

- Maximum carbon equivalent constraint

$$C_{eq} \leq 0.35$$ **Equation 6.32**

Also included are mechanical properties constraints based on the results obtained from first cDSP solution space exploration (the acceptable ranges identified for mechanical properties)

- Minimum yield strength constraint

$$YS \geq YS_{lower\ limit}\ \text{MPa}$$ **Equation 6.33**

- Maximum yield strength constraint

$$YS \leq YS_{upper\ limit} \text{ MPa} \qquad \textbf{Equation 6.34}$$

- Minimum tensile strength constraint

$$TS \geq TS_{lower\ limit} \text{ MPa} \qquad \textbf{Equation 6.35}$$

- Maximum tensile strength constraint

$$TS \leq TS_{upper\ limit} \text{ MPa} \qquad \textbf{Equation 6.36}$$

- Minimum hardness constraint

$$HV \geq HV_{lower\ limit} \qquad \textbf{Equation 6.37}$$

- Maximum hardness constraint

$$HV \leq HV_{upper\ limit} \qquad \textbf{Equation 6.38}$$

System Goals

The target values for system goals are identified from the solution space exploration carried out for the first cDSP.

Goal 1:

- Achieve Ferrite Grain Size Target from cDSP 1

$$\frac{D_{\alpha_{Target}}}{D_{\alpha}(X_i)} + d_1^+ - d_1^- = 1 \qquad \textbf{Equation 6.39}$$

Goal 2:

- Achieve Ferrite Fraction from cDSP 1

$$\frac{X_f(X_i)}{X_{f_{Target}}} + d_2^- - d_2^+ = 1 \qquad \textbf{Equation 6.40}$$

Goal 2:

- Achieve Pearlite Interlamellar Spacing Target from cDSP 1

$$\frac{S_{o_{Target}}}{S_o(X_i)} + d_3^+ - d_3^- = 1$$ **Equation 6.41**

Variable Bounds

$11 \leq X_1 \leq 100$ (K/min)

$30 \leq X_2 \leq 100$ (μm)

$0.18 \leq X_3 \leq 0.3$ (%)

$0.7 \leq X_4 \leq 1.5$ (%)

Bounds on deviation variables

$$d_i^-, d_i^+ \geq 0 \text{ and } d_i^- * d_i^+ = 0, \text{i} = 1,2,3$$ **Equation 6.42**

Minimize

We minimize the deviation function

$$Z = \sum_{i=1}^{3} W_i(d_i^- + d_i^+);\ \sum_{i=1}^{3} W_i = 1$$ **Equation 6.43**

6.7 Integrated Solution Space Exploration of Hot Rod Rolling Process Chain Using the Proposed Method

We have exercised 19 different scenarios for both cDSPs in Steps 2.1 and 2.2, Table 6.10. These scenarios are selected based on judgement to effectively capture the design space for exploration in a ternary space with different combination of weights on goals.

Table 6.10: Scenarios with weights for goals

Scenarios	W_1	W_2	W_3
1	1	0	0

2	0	1	0
3	0	0	1
4	0.5	0.5	0
5	0.5	0	0.5
6	0	0.5	0.5
7	0.25	0.75	0
8	0.25	0	0.75
9	0.75	0	0.25
10	0.75	0.25	0
11	0	0.75	0.25
12	0	0.25	0.75
13	0.33	0.34	0.33
14	0.2	0.2	0.6
15	0.4	0.2	0.4
16	0.2	0.4	0.4
17	0.6	0.2	0.2
18	0.4	0.4	0.2
19	0.2	0.6	0.2

We explain the significance of these scenarios using the cDSP for the end product (the cDSP in Step 2.1). For the first cDSP, Scenarios 1-3 are for a situation where the designer's interest is to achieve the target of on a single goal, i.e., maximizing YS, maximizing TS or maximizing X_f as closely as possible. For example, the designer's preference in Scenario 2 (for cDSP 1) is to achieve only the tensile strength goal. Scenarios 4-6 are for a situation where two goals are given equal preference, and the third goal is not assigned any preference. For example, Scenario 4 is a situation where designer's interest is in equally maximizing YS and TS without giving any preference to the X_f goal. Scenarios 7-12 are situations where the designer gives greater preference to one goal, a lesser preference to the second goal and zero preference to the third goal. Scenario 13 is a situation where the designer gives equal preference to all the three goals. Scenarios 14-19 are situations where all the goals are assigned preferences with two of them being the same preference. The exploration of solution space is carried out by exercising the cDSPs for these scenarios and plotting the solution space obtained in a ternary space. The axes of the ternary plots are the weights assigned to each goal and the color contour in the interior is the achieved value of the specific goal that is being addressed. From these plots, we identify feasible solution regions that satisfy our requirements and the associated weights to be assigned to each goal to achieve this solution space. To read more about the creation and interpretation of ternary plots, see (Nellippallil, Song and coauthors , Nellippallil, Song and coauthors 2016)

6.7.1 Solution Space Exploration of Step 2.1 cDSP

The requirement for the process designer in Step 2.1 cDSP is to achieve the goals associated with the mechanical properties of the end rod product. For Goal 1, a process designer is interested in maximizing the yield strength. The target value of 330 MPa is specified in the cDSP. On exercising the cDSP and analyzing the solution space in Figure 6.9, we see that the red contour region identified by the blue dashed lines satisfy the requirements as closely as possible. The maximum yield strength achieved is 320 MPa and the maximum value has achieved the weight assigned to Goal 1 tends to 1. We select the region identified in Figure 6.9 as that satisfying the requirement for YS.

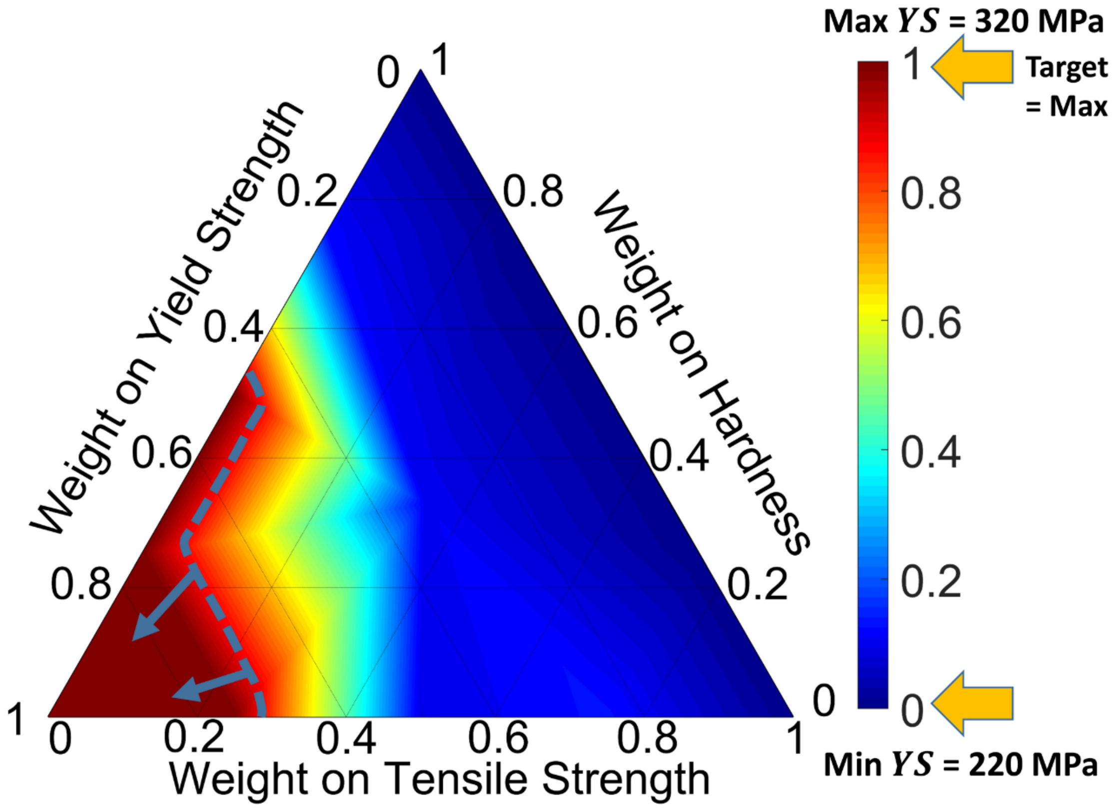


Figure 6.9: Ternary Plot for Goal 1 – Yield Strength

For Goal 2, a process designer is interested in maximizing the tensile strength of the product. A target value of 750 MPa is specified for this goal. On analyzing Figure 6.10, we observe that the red region marked with the light orange dashed lines satisfies this requirement. The target value of 750 MPa is achieved as we tend to the weight of 1 for the tensile strength goal. However, as the weight on the third goal (hardness) is increased there is an increase in tensile strength as well. We achieve a value of 750 MPa for tensile strength when the weight on the hardness goal is 1. From this, we can clearly see the forward relationship that hardness and tensile strength holds with respect to the system variables identified.

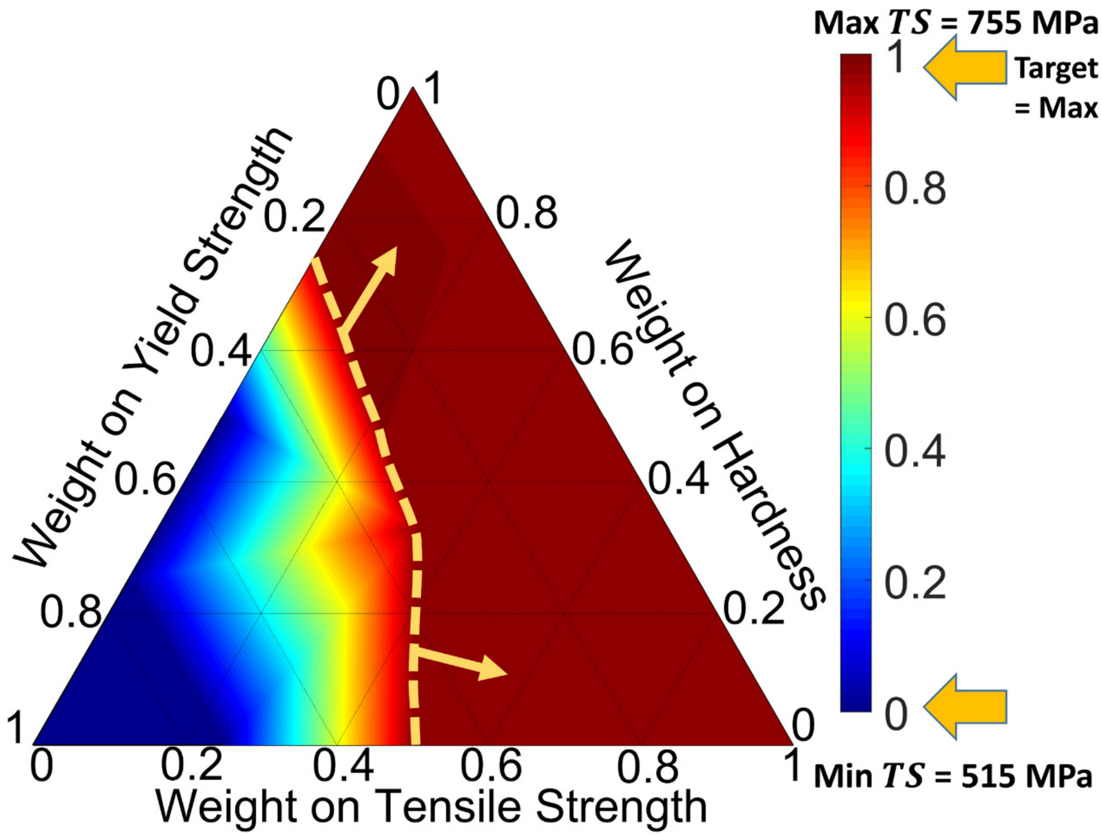


Figure 6.10: Ternary Plot for Goal 2 – Tensile Strength

For Goal 3, the process designer is interested in maximizing hardness. The hardness is a function of the ferrite fraction, silicon content and transformational temperature of austenite to ferrite. We assumed a transformation temperature of 700 ℃. From Figure 6.11, it is clear that the hardness target value of 170 is achieved in the red contour region marked by the white dashed lines. We also observe that the requirement for hardness is achieved in regions with high weights for tensile strength confirming the relationship that we saw in Figure 6.10.

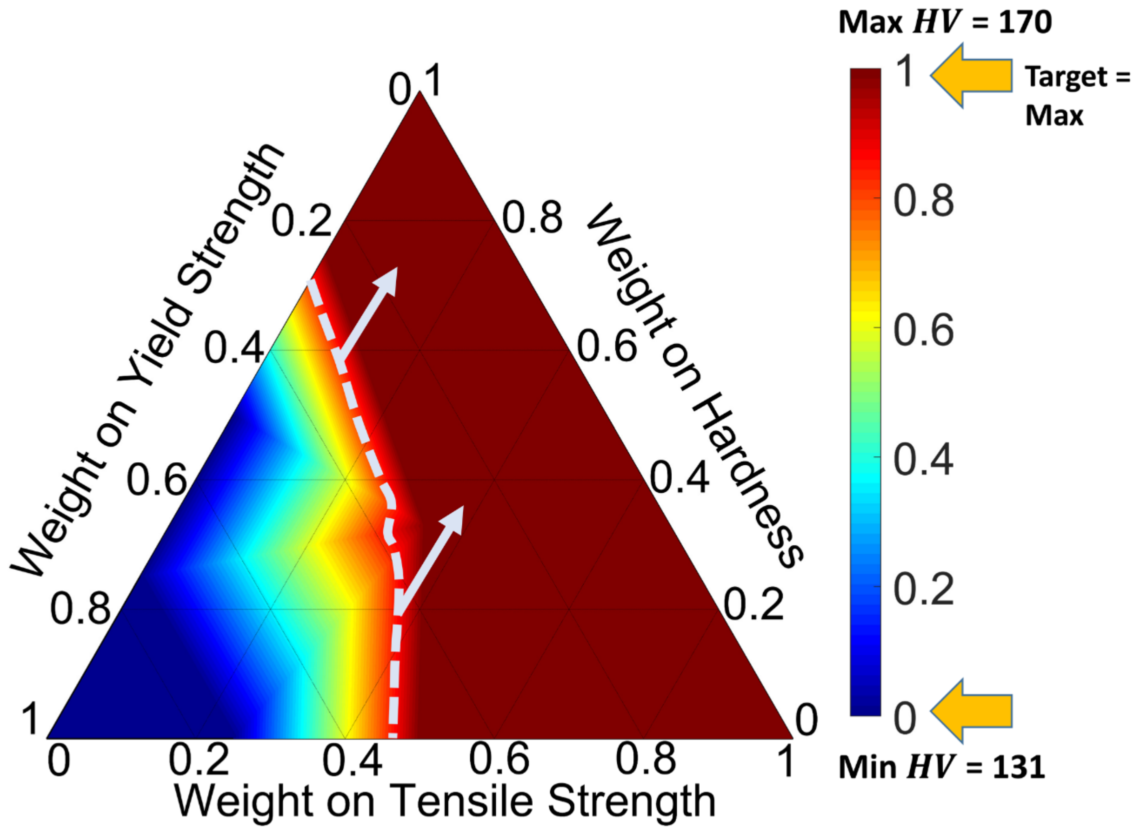


Figure 6.11: Ternary Plot for Goal 3 – Hardness

On carrying out a parametric study with the transformation temperature value, we found that the positive relationship between tensile strength and hardness holds only at high transformation temperatures. At transformation temperatures in the range of 500-550°C, we see that hardness tends to be greater where there is high yield strength.

Another requirement that must be strictly satisfied is the requirement for minimum impact transition temperature for the rod. From the solution space for the three goals for YS, TS, and HV, we check the region where this requirement is satisfied the best. In Figure 6.12, the achieved values of impact transition temperature are plotted and we see that the blue contour region marked by two red dashed lines is where the impact transition temperature is minimum. The first red dashed line corresponds to an ITT of 0

°C and the second dashed line closer to the blue contour region corresponds to an ITT of -66 °C. The minimum ITT is achieved in this region and corresponds to the same region where yield strength is maximized.

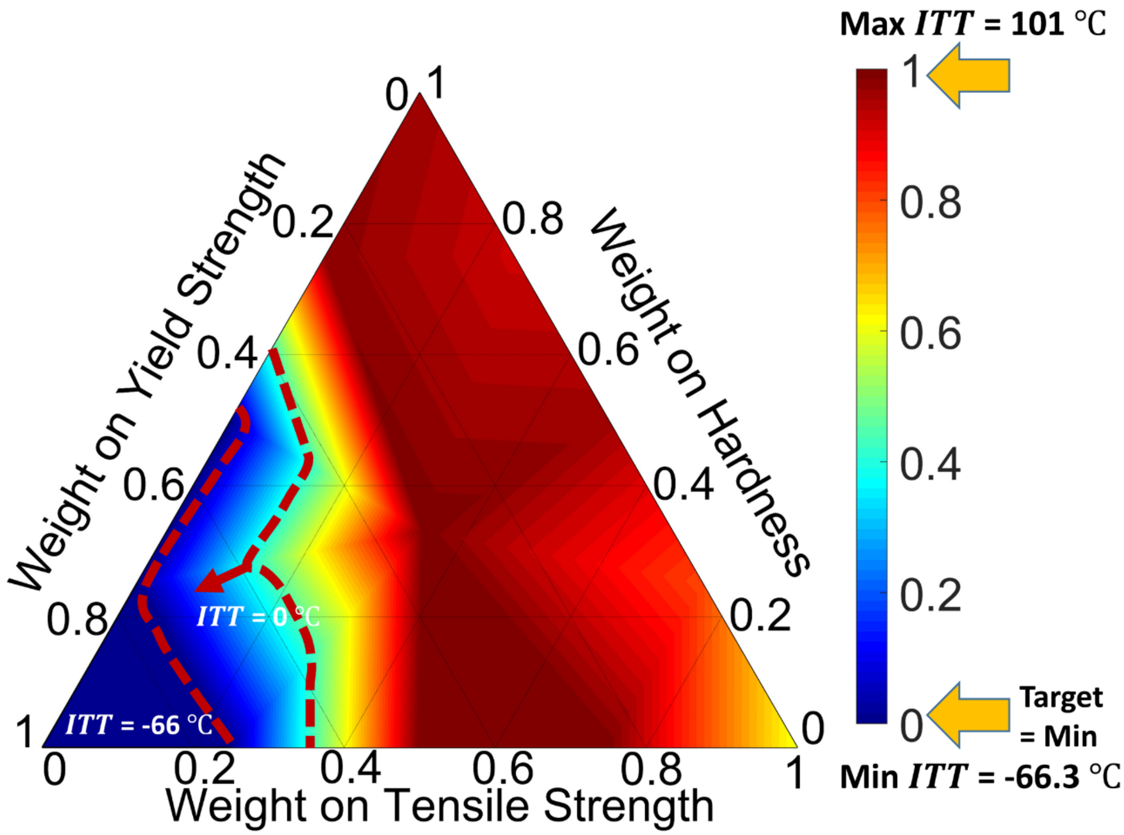


Figure 6.12: Ternary Plot – *ITT* Solution Space

On analyzing the results for the mechanical property goals and requirements, we observe that the ferrite fraction system variable plays a key role in defining the mechanical properties. A major requirement is to manage the banded microstructure. In this work, we satisfy this requirement by identifying regions with high ferrite fractions. Hence, we plot the achieved solution space for ferrite fraction with respect to the weights assigned to the three goals in Figure 6.13. We see in Figure 6.13 that the red contour region marked by the dark blue dashed lines is the region with highest ferrite fraction (near 0.899). The dark blue contour region marked by the dark yellow dashed lines is the region with highest pearlite fraction (ferrite fraction near to 0.1). The region in between these two dashed lines has both ferrite and pearlite. Also, from Figure 6.13 a high ferrite fraction supports maximizing yield strength and minimizing impact transition temperature and high pearlite fraction supports maximizing tensile strength and maximizing hardness. The banded microstructure in between satisfies these goals, however, due to the concern about distortions in gear blanks due to these banded structures, the designer must find a region that is either highly ferritic or highly pearlitic in Figure 6.13. To come to a decision, we superimpose plots as shown in Figure 6.14.

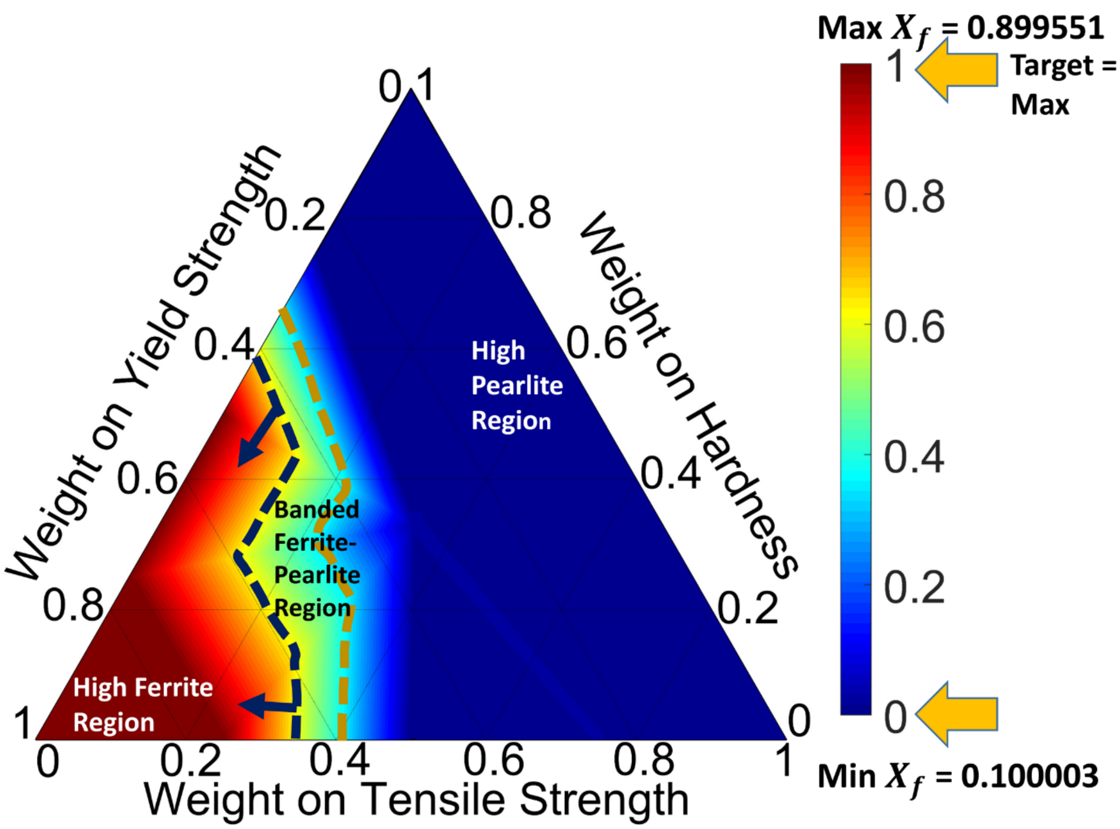


Figure 6.13: Ternary Plot – Ferrite Fraction Solution Space

In the superimposed plot, all the regions identified for the mechanical property goals, and the other requirements are combined to identify a single region that satisfies all the requirements, if it exists. If such a region doesn't exist, the designer must make trade-offs among the conflicting goals. On analyzing Figure 6.14, the requirements for maximizing tensile strength and hardness are achieved in the high pearlite fraction region while the requirements for maximizing yield strength and minimizing impact transition temperature is satisfied at the high ferrite fraction region. Hence the designer is faced with the dilemma of choosing from either the region of high ferrite or high pearlite that satisfies the goals. To make a decision, we first identify some solution points from the superimposed plot and analyze the extent to which the goals are met. We identify 8 solution points A, B, C, D, E, F, G and H from the ternary space and the results associated with each of these solution points are summarized in Table 6.11.

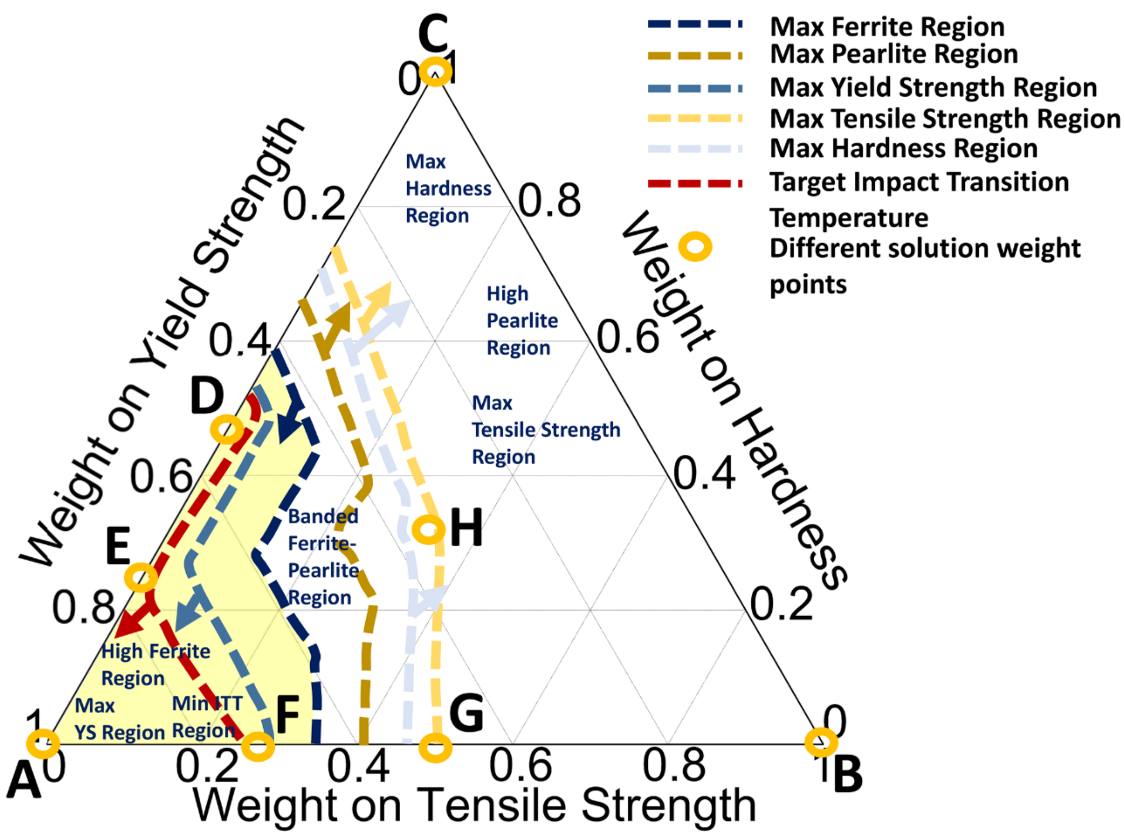


Figure 6.14: Superimposed Ternary Plot

From Table 6.11, we see that all the goals are satisfied by minimum values of ferrite grain size D_α and interlamellar spacing S_o. This is a very important information that needs to be communicated to the preceding stages as the requirements from these stages must be to produce a material having these characteristics at the end. On analyzing the impact of ferrite fraction, we see that high yield strength and minimum ITT are satisfied when the ferrite fraction is high, while low yield strength, high ITT, high tensile strength and high hardness occurs when the ferrite fraction is low (more pearlite). As the pearlite fraction increases the values of ITT achieved are very high (65-100 ℃) which is not acceptable. Hence, we identify regions (the light yellow region in Figure 6.14) with a high ferrite fraction, where both yield strength and impact transition temperature requirements are met while compromising on the requirements for tensile strength and hardness. From a design standpoint, the compromise does not severely affect either tensile strength and hardness. Therefore, we choose solution point A having the highest ferrite fraction. Point A achieves a YS of 321 MPa, TS of 516 MPa, HV of 131 and ITT of -66 ℃.

Table 6.11: Solution points selected

Sol. Pts	**Microstructure Factors After Cooling**				**Mechanical Properties of End Rod**			
	D_α μm	X_f	S_0 μm	Mn (%)	YS MPa	TS MPa	HV	ITT ℃
A	8	0.9	0.15	1.49	321	516	131	-66
B	8	0.101	0.21	0.7	220	750	169.9	35
C	8	0.1	0.15	0.7	220	749	169.9	94.8
D	8	0.89	0.15	1.5	320	516	131	-66

E	8	0.89	0.15	1.49	320	516	131	-66
F	8	0.89	0.15	1.49	320	516	131	-66
G	8	0.1	0.18	1.5	228	749	169.8	65
H	8	0.113	0.15	1.49	231	749	169.4	100

The solutions for the microstructure space after cooling identified after exploration become the goals for the next cDSP (Step 2.2). The target goals for the cDSP for cooling, therefore, is to achieve a minimum ferrite grain size, maximum ferrite fraction and minimum pearlite interlamellar spacing; target values of 8 μm, 0.9 and 0.15 μm respectively.

6.7.2 Solution Space Exploration of Step 2.2 cDSP

The requirement in Step 2.2 cDSP is to achieve the targets identified from the first cDSP as closely as possible. For Goal 1, the process designer is interested in minimizing ferrite grain size and the target value is 8 μm. On exercising the cDSP and analyzing the solution space for ferrite grain size in Figure 6.15, we see that the minimum achieved value of D_α using the current configuration is 10.06 μm. Based on literature study (Kuziak, Cheng and coauthors 1997, Pietrzyk, Cser and coauthors 1999), we determine that any value less than 15 μm is acceptable as the ferrite grain size after cooling. This updated requirement is met in the region identified by the red dashed lines in Figure 6.15. As we move closer to the dark blue contour regions the requirement for minimum D_α is closest to being satisfied.

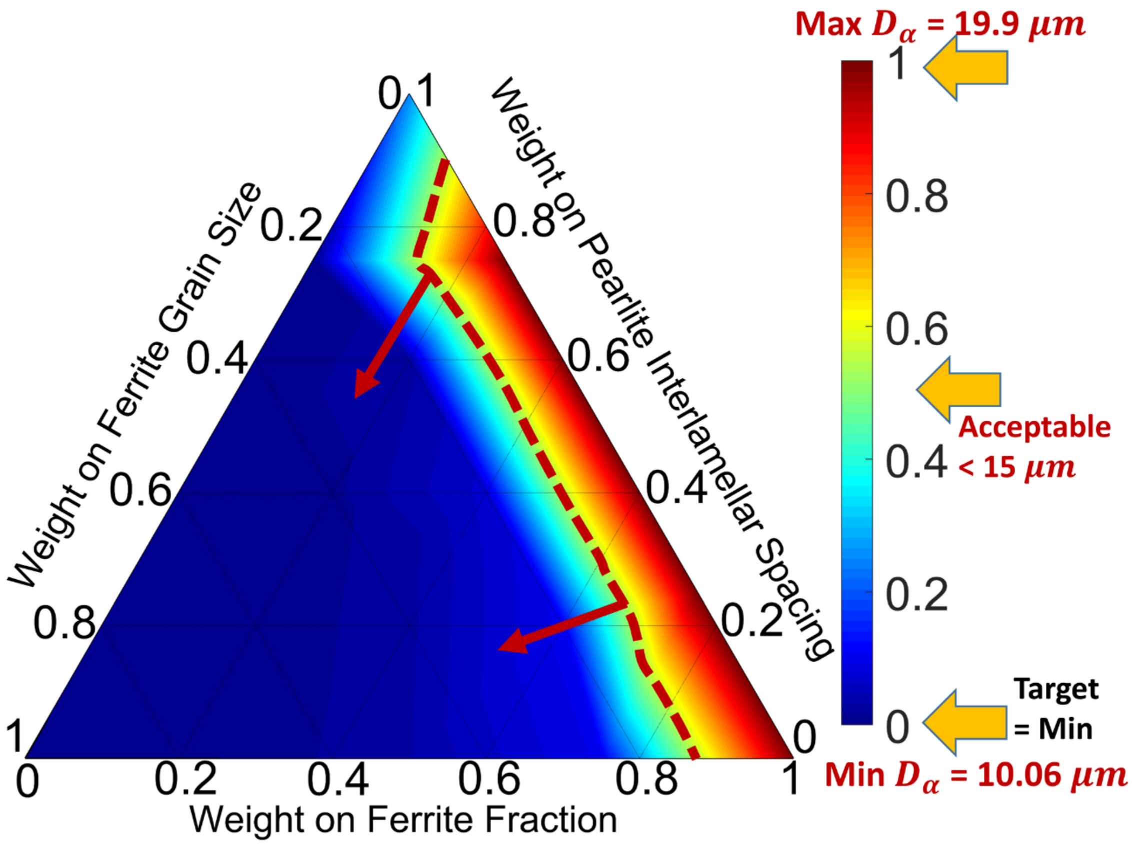


Figure 6.15: Ternary Plot – Ferrite Grain Size

For Goal 2, the process designer must maximize ferrite fraction to the target value of 0.9. In Figure 6.16, we see that the maximum ferrite fraction achieved is around 0.7149. Based on reported ferrite fractions after cooling from the literature (Kuziak, Cheng and coauthors 1997), we find that any value of the ferrite fraction above 0.68 is acceptable. The region that satisfies the requirement is marked by the dashed orange line in Figure 6.16. As we move towards the red contour region, the maximum ferrite goal is satisfied most closely.

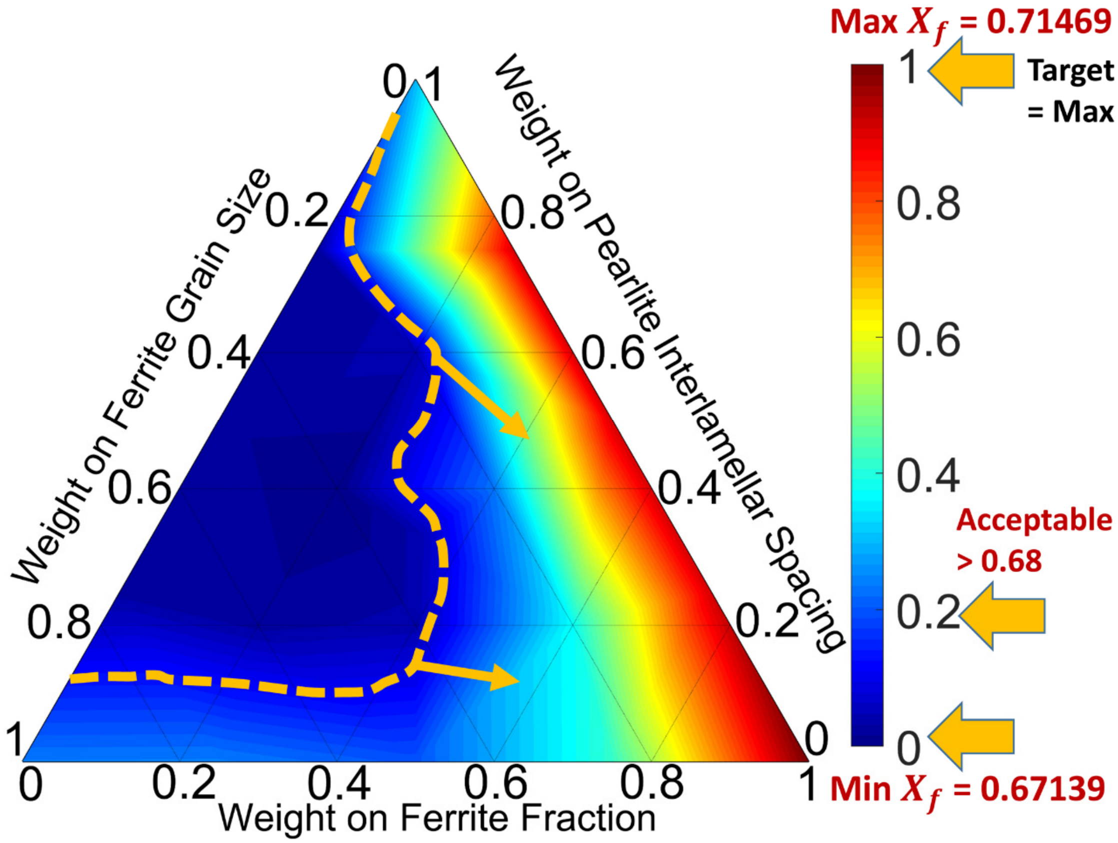


Figure 6.16: Ternary Plot – Ferrite Fraction

For Goal 3, the requirement is to minimize pearlite interlamellar spacing to a target value of 0.15 μm. On analyzing Figure 6.17, the minimum value achieved is 0.1497 marked by the blue contour region. Based on reported values of pearlite interlamellar spacing (Kuziak, Cheng and coauthors 1997), we define that any value less than 0.17 μm is acceptable. This region is marked by the dark blue dashed line in Figure 6.17.

Again, to make a design decision, we superimpose all the goals in one superimposed ternary plot, Figure 6.18.

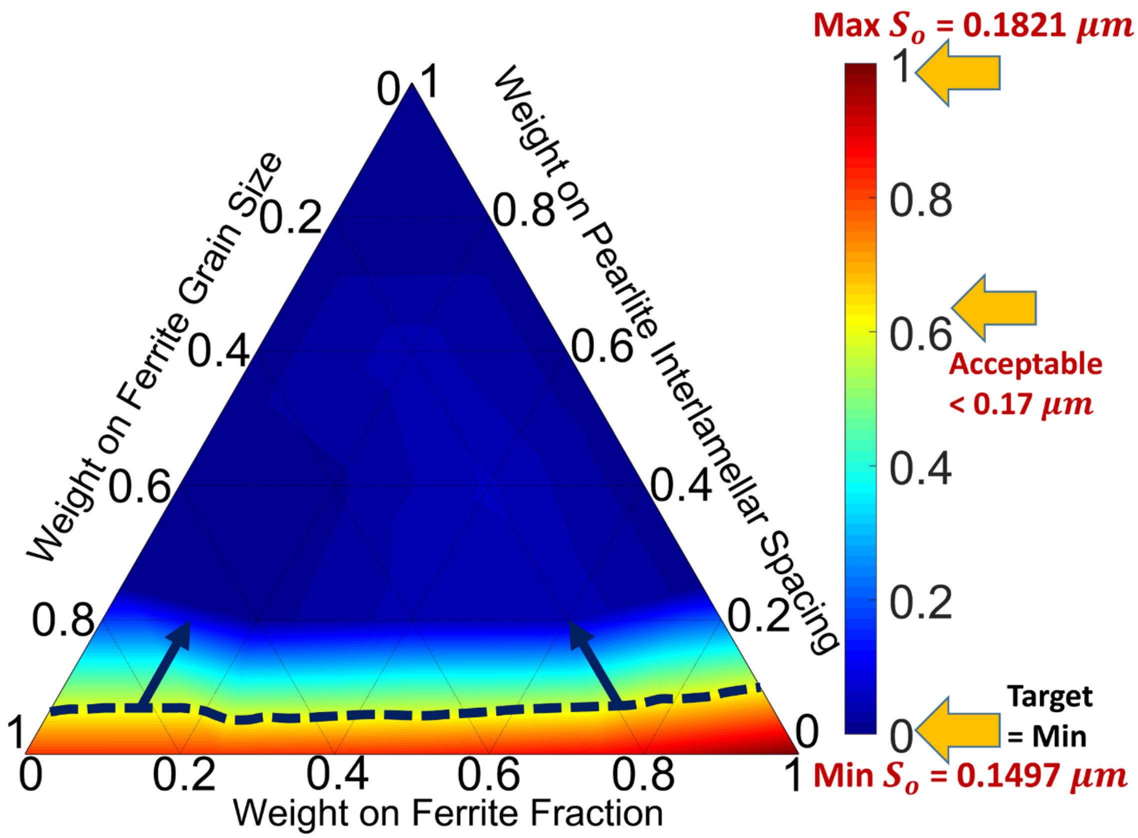


Figure 6.17: Ternary Plot – Pearlite Interlamellar Spacing

In the superimposed ternary plot, the light yellow region satisfies all the requirements. To analyze further we pick 6 solution points both from within the region identified and outside. Solution points C, D, and E lie within the region that satisfies all the goals in the best possible way. Solution points A, B and F lies outside the region. The results are summarized in Table 6.12.

On analyzing the results in Table 6.12, we see that solution point A satisfies the requirement of minimizing ferrite grain size to the greatest extent and this is achieved with a high cooling rate and low value of austenite grain size. This happens because a high cooling rate results in less time for the nuclei to grow before new nuclei are formed resulting in a decrease of average grain size (Jägle 2007).

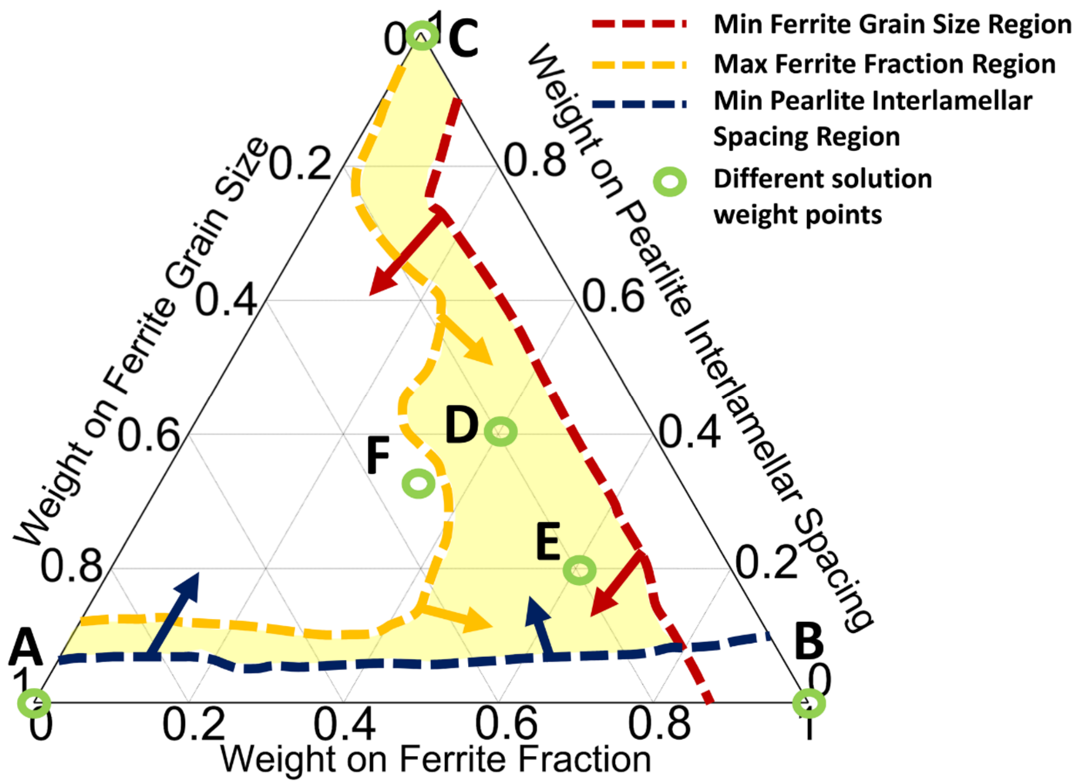


Figure 6.18: Superimposed Ternary Plot for all Goals

This means that there is an increased grain boundary area per volume available for nucleation resulting in more nuclei and thus smaller ferrite grain sizes. Solution point B satisfies the requirement for a high ferrite fraction and this is achieved with a low cooling rate, high austenite grain size and low manganese. The holds true as a low cooling rate favors the growth of allotriomorphic ferrite resulting in the overall growth of ferrite. A high austenite grain size results in an increase in Widmanstatten ferrite, while a low austenite grain size results in an increase in allotriomorphic ferrite. Both these situations need to be considered when studying the effect of austenite grain size on the ferrite fraction. Also, a low manganese content results in less banded microstructure favoring an increase in allotriomorphic ferrite. Solution point C satisfies the requirement for minimum pearlite interlamellar spacing and this is achieved with both low values of cooling rate and austenite grain size. On analyzing all solutions listed in Table 6.12, we see that solution point D satisfies all the requirements to the extent possible. In Point D the values of a D_α of 10.74 μm, X_f of 0.681 and S_0 of 0.151 μm are achieved. The values for cooling rate, austenite grain size and compositions will act as target goals for the cDSP for the last stage of rolling (cDSP in Step 2.3) following a similar format as demonstrated using cDSPs and solution space explorations in Steps 2.1 and 2.2.

Table 6.12: Solution points selected

Sol. Pts	**Processing (Cooling) and Microstructure Space after Rolling**				**Microstructure Space after Cooling**		
	$\boldsymbol{CR}$ K/min	$\boldsymbol{D}$ μm	$\boldsymbol{C}$ %	$\boldsymbol{Mn}$ %	$\boldsymbol{D_\alpha}$ μm	$\boldsymbol{X_f}$	$\boldsymbol{S_0}$ μm
A	99.9	30	0.18	0.7	10.06	0.681	0.176
B	11	74.2	0.18	0.7	19.9	0.714	0.182
C	11	30	0.19	1.02	12.5	0.684	0.149
D	44.4	30	0.18	0.94	10.74	0.681	0.151
E	33.06	30	0.18	0.95	11.05	0.687	0.151
F	70.3	30	0.18	0.93	10.33	0.673	0.151

6.8 On Verification and Validation

Empirical Structural Validation

Empirical structural validation involves accepting the appropriateness of the example problems used to verify the performance of the framework and the method. The second example problem in Chapter 5 is further improved and expanded to the comprehensive problem on vertical and horizontal integration of hot rolling process chain in this chapter. Using the comprehensive example problem in Chapter 6, the utility of the framework and the method is tested for the integrated design exploration of materials, products and manufacturing processes. In Chapter 6, the design architecture in terms of Research Question 1 and 2 developed in the dissertation are applied to a multiscale, multistage materials design problem - vertical and horizontal integration and integrated design of hot rod rolling process chain, steel and rolled rod. In this chapter, the industry inspired problem of focus in this dissertation is addressed. The bigger picture of the problem of interest and how integrated materials; product and process design can be applied at industrial scale is discussed in beginning. A discussion on the specific problem (vertical and horizontal integration of hot rolling process chain) is carried out in detail. A literature review on hot rod rolling process is carried out. The problem– impact of segregation along the rolling to forging process chain is discussed in detail. The problem is to design the material microstructure and processing paths to satisfy conflicting product and process related end performances and properties in an inverse manner. The problem is modeled as an integrated design of materials, products, and manufacturing processes. In addition to the validation of design methods, the chapter is also crucial from the standpoint of the major theme addressed in this dissertation. In this chapter, we discuss the validation of the proposed systematic method of model integration, inverse design method and concept exploration framework.

Empirical Performance Validation

Empirical performance validation consists of accepting the usefulness of the outcome with respect to the initial purpose and accepting that the achieved usefulness is related to applying the framework and method. The utility of the proposed method is demonstrated by carrying out the integrated solution space exploration of the processing and microstructure spaces of the rolling and cooling processes to identify satisficing solutions that realizes the end mechanical properties of the rod product in Chapter 6.

In this chapter, we present a goal-oriented, inverse decision-based design method supported by the Concept Exploration Framework (CEF) to achieve the vertical and horizontal integration of models for the hot rolling and cooling stages of the steel manufacturing process chain for the production of a rod with defined properties. The method is goal-oriented and inverse because we start with end mechanical properties of the product and inversely maps the requirements to microstructure and processing spaces of the product as well as the process to identify multiple solutions that satisfies the requirements. The utility of the proposed method is demonstrated by carrying out the integrated solution space exploration of the processing and microstructure spaces of the rolling and cooling processes to identify *satisficing solutions* that realizes the end mechanical properties of the rod product. The primary advantage of the proposed method is in empowering a process designer to rapidly explore the design space for manufacturing processes using simulation models by managing the uncertainty associated with models. We believe that the ability to predict the design and operating set points using models reduces the need for expensive plant trials resulting in reduced time and cost involved in the production of a new grade of steel product mix with improved properties using a new class of material. The proposed method is generic and supports the integrated decision-based design of other manufacturing stages that are connected and having a sequential flow of information by identifying the design and operating set points that best satisfies the requirements identified. Through the proposed method and demonstration carried out in this chapter using an industry-driven problem, we propose an approach for *microstructure-mediated design* by *integrating the design of the material, product and associated manufacturing processes* involved.

The method and its application are characterized by a confluence of different disciplines like engineering mechanics, materials science, manufacturing and systems engineering. The functionalities offered by the method supported by CEF as illustrated using the comprehensive example problem includes (Selected from Chapter 4 and proved based on the testing done using the comprehensive example problem in Chapter 6):

- Requirements driven, “top-down” design of system and associated subsystems by taking a goal-oriented approach which is different to the standard practice of bottom-up modeling and design of material and product systems,
- Human perception of a satisficing design space across process chains,
- augmenting the human ability to make design decisions - visualizing a solution space and making logical judgements through trade-offs to identify satisficing solution regions of interest,

- Capability to handling ‘n’ number of design variables – this is an advantage over other design exploration methods like IDEM where there is a limitation on the number of design variables,
- Propagation of end goal requirements (product performance or properties) across a process chain with the designer having the capability to check whether the end goals are actually achievable at previous spaces in their current configuration or not – designer can recommend adjustments in the design space if needed,
- Offers flexibility in design: The capability to define new goals and requirements at each level as the method uses individual cDSPs to facilitate information flow allowing to formulate a design space at each level - advantage over other design exploration methods like IDEM and pyDEM where the design space is defined by mapping from previous spaces (Choi, McDowell and coauthors 2008, Kern, Priddy and coauthors 2017),
- The capability to carry out rapid, integrated design exploration of material and products using simulation models that we accept are typically incomplete and inaccurate,
- The capability to coordinate information and human decision making,
- The CEF offers the capability to prioritize models, input factors, output responses and computational tools in terms of their value in design, and
- ensuring feasible design solutions that allows to invest on new complex material systems with confidence.

The proposed method and the concept exploration framework are generic and supports the integrated decision-based design of similar manufacturing processes involving the material and product. Given any complex systems problem that involve sequential flow of information across processes/levels, the proposed method has the potential to be applied to support information flow and human decision making across the processes/levels in order to realize an end goal. The verification and validation aspects are shown in Figure 6.19.

Theoretical Structural Validity (TSV)

Validity of the constructs of the systems-based architecture

- Arguing the validity of constructs of the systems-based design architecture (Chapters 3, 4)

Theoretical Performance Validity (ESV)

Usefulness of the architecture beyond examples

- Generalizing Findings (Chapters 9, 10)
- Arguing the validity of the systems-based design architecture developed beyond the example problems used in different domains (Chapter 10)

Empirical Structural Validity (ESV)

Appropriateness of the examples chosen to verify the architecture

- Vertical and Horizontal Integration of Hot Rod Rolling Process Chain (Chapter 6)
- ✓ Problem modeled as an integrated design of materials, products, and manufacturing processes.
- ✓ Design microstructure and processing paths to satisfy product related end performances in an inverse manner

Empirical Performance Validity (EPV)

Usefulness of the architecture in examples

- Function-based Approach
- ✓ Usefulness for systematic model integration and information flow generation
- Concept Exploration Framework
- ✓ Usefulness of the framework for systematic integrated concept exploration of materials, products and processes
- Goal-oriented Inverse Design Method
- ✓ Usefulness of the method for systematic inverse design exploration material, product and processes

Figure 6.19: Verification and validation aspects discussed in Chapter 6

6.9 Role of Chapter 6 and connection with Other Chapters in this Dissertation

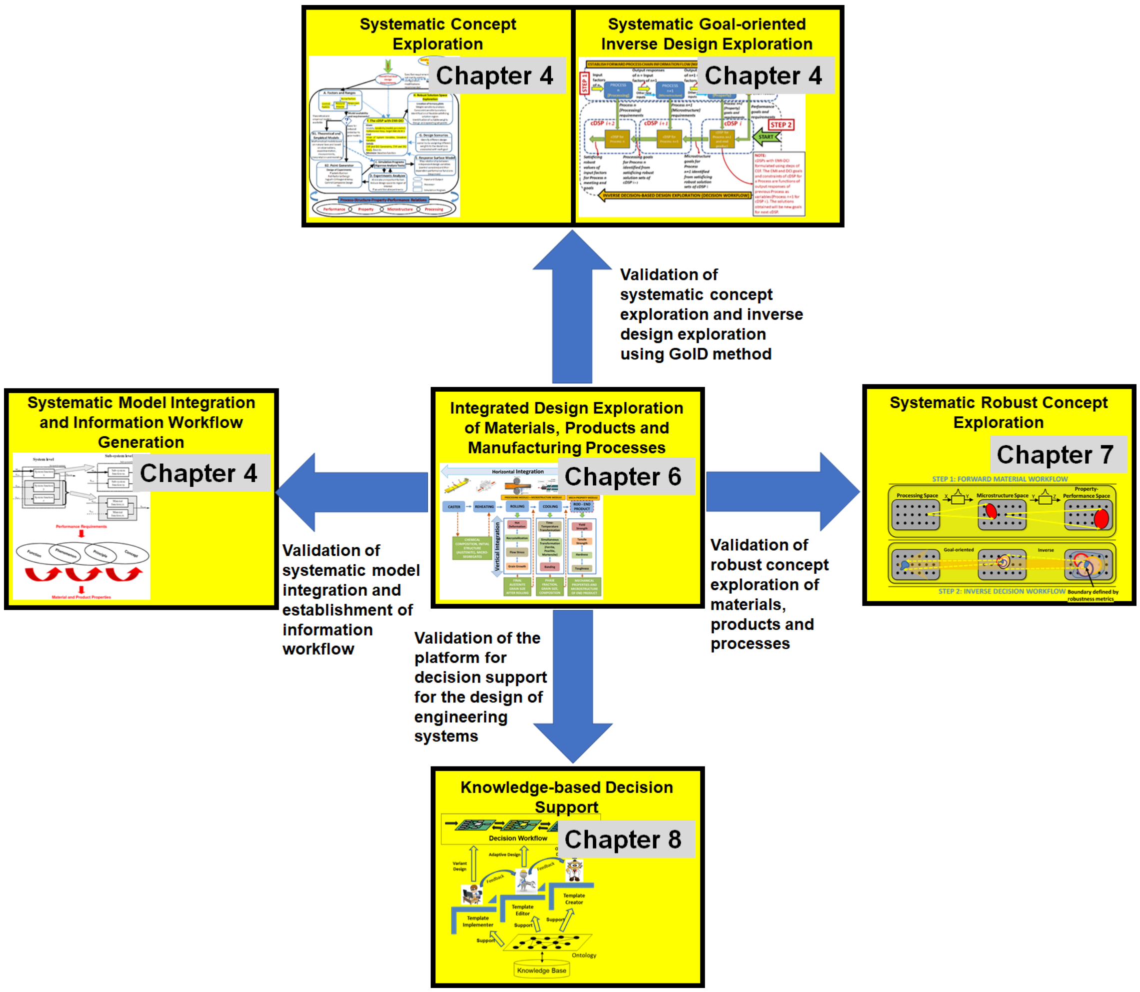


Figure 6.20: Chapter 6 and connections with other chapters in this dissertation

In Chapter 6, the design architecture in terms of Research Question 1 and 2 developed in the dissertation are applied to a multiscale, multistage materials design problem - vertical and horizontal integration and integrated design of hot rod rolling process chain, steel and rolled rod. In this chapter, the industry inspired problem of focus in this dissertation is addressed. The bigger picture of the problem of interest and how integrated materials, product and process design can be applied at industrial scale is discussed in beginning. A discussion on the specific problem (vertical and horizontal integration of hot rolling process chain) is carried out in detail. A literature review on hot rod rolling process is carried out. The problem– impact of segregation along the rolling to forging process chain is discussed in detail. The problem is to design the material microstructure and processing paths to satisfy conflicting product and process related end performances and properties in an inverse manner. The problem is modeled as an integrated design of materials, products, and manufacturing processes. In addition to the validation of design methods, the chapter is also crucial from the standpoint of the major theme addressed in this dissertation. In this chapter, we discuss the validation of the proposed systematic method of systematic model integration (Chapter 4), concept exploration framework and goal-oriented inverse design method (Chapter 4). Further, the problem discussed in this chapter is reformulated and utilized to demonstrate robust concept exploration of materials, products and processes in Chapter 7. The example is also reformulated and used in Chapter 8 to test the utility of the platform PDSIDES to support different users for original, adaptive and variant designs. In Figure 6.20, the validation tasks for which the example problem in Chapter 6 are used is shown along with the connectivity with other chapters of this dissertation.

Chapter 7: Robust Concept Exploration of Materials, Products and Associated Manufacturing Processes

7.1 Frame of Reference – Answering Research Question 3

Several challenges associated with top-down, goal-oriented approach of materials design have been highlighted, see (McDowell, Choi and coauthors 2007, McDowell, Panchal and coauthors 2009, McDowell 2018). Among these are the challenges arising due to i) uncertain material models (that includes input factors, parameters, responses, etc.) due to simplification/idealization or a lack of complete knowledge and ii) the propagation of uncertainty due to hierarchical information dependence in a multiscale model chain or in Olson's processing-structure-property-performance relations. An effective top-down, goal-oriented systems approach for materials design must be able to manage the uncertainty with regard to all relevant information ensuring feasible designs that meets specified ranges with high confidence. McDowell (McDowell 2018) asserts that such an approach must address uncertainty of models and experiments at each scale, as well as uncertainty propagation through a chain of models and/or experiments at different levels of hierarchy with the ability to provide decision support through rapid design space exploration.

In this chapter, we introduce a variation to the existing goal-oriented, inverse decision-based design method proposed in Chapter 6 (Nellippallil, Rangaraj and coauthors 2018) to bring in robustness for multiple goals from the stand-point of Type I to III robust design across process chains. The variation embodies the introduction of specific robust design goals, constraints and metrics to determine ''*satisficing robust design*'' specifications for given performance requirement ranges using the goal-oriented, inverse design method. The primary mathematical construct used in the enhanced inverse method is the compromise Decision Support Problem with Error Margin Index and Design Capability Index (cDSP with EMI-DCI) supported by the Concept Exploration Framework (CEF) to generate satisficing Type I, II and III robust design solutions across process chains. The design of a hot rolling process chain for the production of a rod is used as an example.

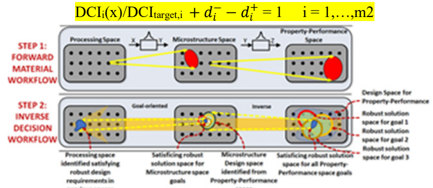
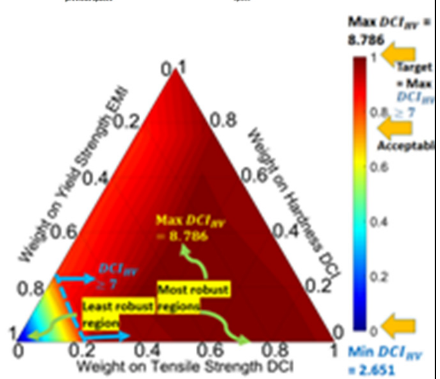
We revisit Secondary Research Question 3 and the Research Hypotheses in Table 7.1.

The constructs of the systems-based design architecture developed to address these requirements are highlighted in Table 1.6. A portion of Table 1.6 that is relevant to this chapter is reproduced in Table 7.2.

Table 7.1: Research Question 3 and Research Hypotheses

Secondary Research Question 3	Research Hypothesis 3
RQ3. What are the requirements for an ***inverse, goal-oriented design approach*** for realizing the ***robust design exploration*** of the material, product and process as a system by managing the associated uncertainties?	***H3.1.*** Introduction of specific robust design goals and constraints anchored in the mathematical constructs of error margin indices and design capability indices to determine "satisficing robust design" specifications for given performance requirement ranges using the goal-oriented, inverse design method can bring in robustness for multiple conflicting goals across process chains.

Table 7.2:Requirements, constructs of the robust concept exploration using GoID, and associated hypothesis validated in Chapter 8

Requirements	Constructs of the Systems-based Design Architecture developed in this Dissertation	Research Hypotheses	Validation Examples
Robust concept exploration of process chains in an inverse manner under uncertainty for multiple conflicting goals	System Constraints: $EMI_{constraints,i}(x)$ or $DCI_{constraints,i}(x) \geq 1$ $i = 1,\ldots,q$ $EMI_i(x) \geq 1$ $i = 1,\ldots,m1$ $DCI_{,i}(x) \geq 1$ $i = 1,\ldots,m2$ **Robust solution constraints:** New constraints defined to ensure robust solutions under multiple conflicting goals System Goals: $EMI_i(x)/EMI_{target,i} + d_i^- - d_i^+ = 1$ $i = 1,\ldots,m1$ $DCI_i(x)/DCI_{target,i} + d_i^- - d_i^+ = 1$ $i = 1,\ldots,m2$   **Robust Concept Exploration**	**R.H3.1.** Introduction of specific robust design goals and constraints anchored in the mathematical constructs of error margin indices and design capability indices to determine ''satisficing robust design'' specifications for given performance requirement ranges using the goal-oriented, inverse design method can bring in robustness for multiple conflicting goals across process chains	1. Steel Manufacturing Process Chain Problem - **Focus on robust exploration across process chains** 

In Section 7.2, we describe the Concept Exploration Framework (CEF) and the cDSP-EMI-DCI construct for robust concept exploration. In Section 7.3, the enhanced inverse decision-based design method for inverse design exploration is described. In Section 7.4, we describe the integrated design of materials, products and processes for the hot rod rolling process chain problem. The empirical models and the response surface models for computational analysis of the problem are presented in Section 7.4.1. The cDSP formulated for the property-performance space is also described in Section 7.4.2. The inverse exploration of the solution space to identify satisficing robust design specifications is covered in Sections 7.4.3 and 7.4.4. In Section 7.5, we discuss the ability of EMI and DCI to design systems under MPU and MSU. We close the chapter with our remarks in Section 7.6.

7.2 The Concept Exploration Framework for Types I, II, III Robust Design

The Concept Exploration Framework (CEF) is a mathematical framework that includes systematic steps to generate design alternatives by exploring the solution space and identify satisficing design specifications. However, the idea of robustness is not captured in the CEF in its current form as defined in (Nellippallil, Rangaraj and coauthors 2018) and is therefore a limitation. We recognize that a framework that supports robust concept exploration in integrated material, product and process design should satisfy three requirements: i) computational efficiency, ii) generic enough to be applicable to various levels of material design hierarchy and iii) incorporation of Type I, II and III robust design formulations.

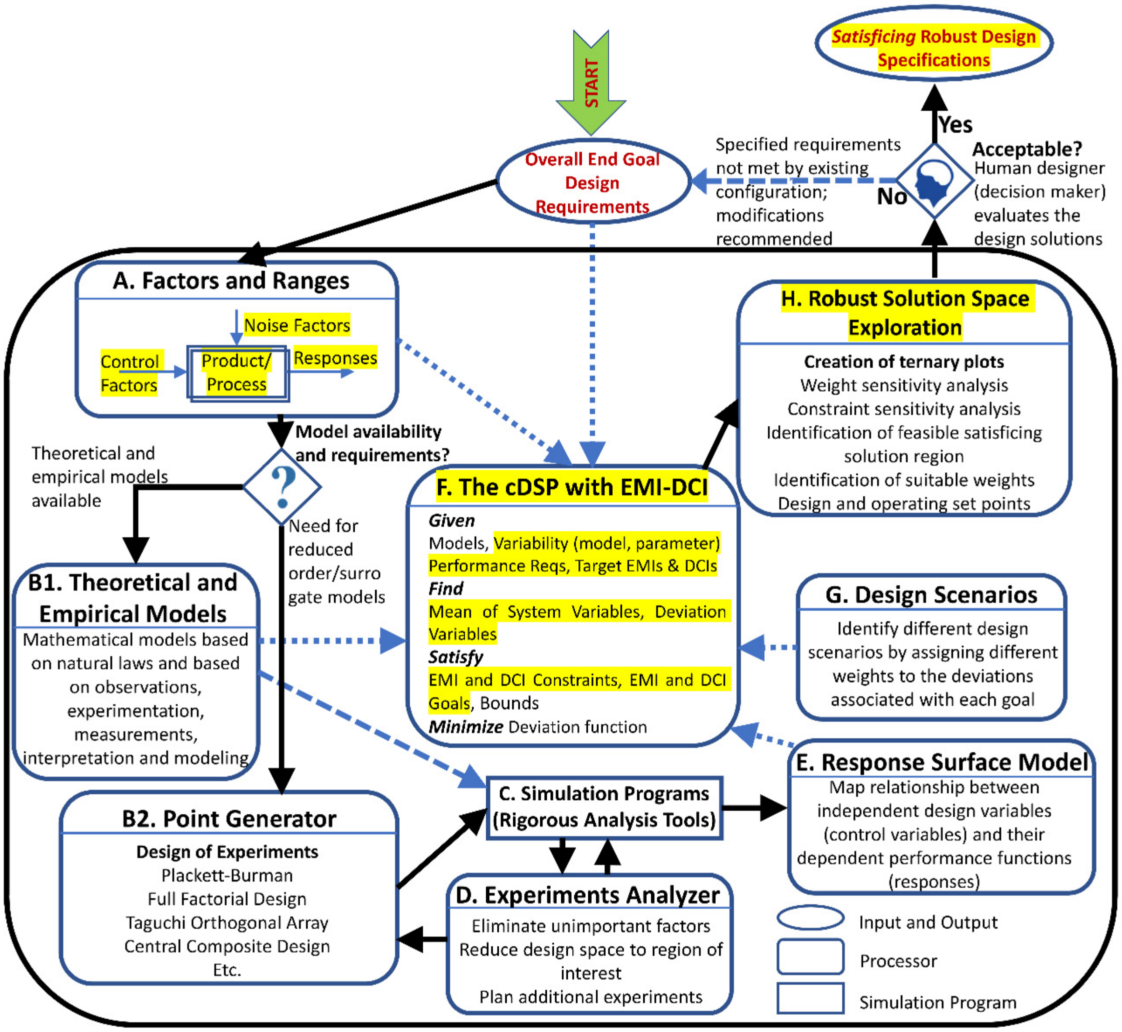


Figure 7.1: The modified (highlighted in yellow) Concept Exploration Framework for Types I, II, III Robust Design

In this chapter, we update the CEF to include the compromise Decision Support Problem with Error Margin Index and Design Capability Index together in a single formulation to take into account complex material and product design problems that require combination of Type I, II and III robust designs. In Figure 7.1, we show the modified CEF with incorporation of robust design goals and constraints in the cDSP using the EMIs and DCIs. The systematic steps associated with the CEF to generate satisficing design specifications remains the same as defined in (Nellippallil, Allen and coauthors 2017, Nellippallil, Rangaraj and coauthors 2018) and hence will not be discussed here. In this chapter, we address robust concept exploration for instantiating Type I, II, and III robust designs and therefore focus on the portions highlighted in yellow in processors A, F and H of the CEF shown in Figure 7.1. The formulation of a cDSP with EMI and DCI using the CEF involve: a) quantification of variability and model parameter uncertainty, b) formulation of error margin indices and design capability indices and incorporating them in the cDSP, and c) robust decision making by exploration of solution space by executing the cDSP with EMI-DCI. Choi and coauthors (Choi, Austin and coauthors 2005) explain in detail on quantifying variability and model parameter uncertainty. They use response modeling approach for quantifying response variability due to parameterizable noise factors and location and dispersion modeling approach for quantifying unparameterizable variability. We adopt the approach by Choi and coauthors in our work for quantifying variability associated with response functions that are developed from raw data.

However, we observe that for problems related to complex manufacturing processes involving materials and products like hot rolling and cooling, several studies are already carried out and different models defining material/process behavior are available in the literature (Gladman, McIvor and coauthors 1972, Gladman, Dulieu and coauthors 1977, Yada 1987, Majta, Kuziak and coauthors 1996, Kuziak, Cheng and coauthors 1997, Pietrzyk, Cser and coauthors 1999, Phadke, Pauskar and coauthors 2004). These models are either based on natural laws or based on experiments/modeling. Such available theoretical and empirical models when directly used to formulate the cDSP does not require the approach followed by Choi and coauthors as the variability can be assessed directly using the function relations.

7.2.1 Formulation of Design Capability Indices (DCIs) and Error Margin Indices (EMIs)

DCIs and EMIs are metrics for system performance and robustness. DCIs represent the amount of safety margin against system failure due to uncertainty in the system variables while EMIs represent the margin against failure due to uncertainty in both model and design variables. Both are dimensionless. The EMIs support Type I, II and III robust designs while DCIs support Type I and II robust designs. We hypothesize that the EMIs and DCIs when used together in search algorithms are capable of helping the designer in designing the system robust to both model parameter and model structure uncertainty. We briefly describe the steps involved in formulating and calculating DCIs and EMIs for two types of systems respectively.

DCIs for systems having variability in design variables only

Step 1: Using a first order Taylor series expansion, estimate the response variation due to variation in the design variable vector $\mathbf{x} = \{\boldsymbol{x_1}, \boldsymbol{x_2}, \dots, \boldsymbol{x_n}\}$. The response variation (ΔY) for small variations in design variables is

$$\Delta Y = \sum_{i=1}^{n} \left|\frac{\partial f}{\partial x_i}\right| \cdot \Delta x_i \qquad \textbf{Equation 7.1}$$

Step 2: Using the mean response (μ_y) obtained from the mean response model ($f_0(x)$) and the response variation due to variation in design variables (ΔY), calculate the DCIs. For a 'Larger is Better' case, the DCI is calculated as

$$\text{DCI} = \frac{\mu_y - LRL}{\Delta Y} \qquad \textbf{Equation 7.2}$$

where, LRL is the lower requirement limit. A DCI ≥ 1 means that the ranged set of design specifications satisfies a ranged set of design requirements and the system is robust against model parameter uncertainty. Higher the value of DCI, higher is the measure of safety against failure due to model parameter uncertainty.

EMIs for systems having variability in both models and design variables

Step 1: Assuming a system model has k uncertainty bounds, calculate the response variation (ΔY_j) for each of them for small variation in design variables is

$$\Delta Y_j = \sum_{i=1}^{n} \left|\frac{\partial f_j}{\partial x_i}\right| \Delta x_i \qquad \textbf{Equation 7.3}$$

where j = 0, 1, 2, …, k (number of uncertainty bounds).

In Figure 7.2a (adopted from (Choi, Austin and coauthors 2005)) we show a mean response model (solid red curve) with two uncertainty bounds (the dotted curves). In left side of Figure 7.2a, we show the response variations of mean function and uncertainty bound functions with respect to the variations in design variables.

Step 2: After evaluating the multiple response variations of mean response function and the k uncertainty bound functions for variations in design variables, calculate the minimum and maximum responses by considering the variability in design variables and uncertainty bounds around the mean response as

$$Y_{max} = Max\left[f_j(x) + \Delta Y_j\right] \text{ and} \qquad \textbf{Equation 7.4}$$

$$Y_{min} = Min\left[f_j(x) - \Delta Y_j\right] \qquad \textbf{Equation 7.5}$$

where j = 0, 1, 2, …, k (number of uncertainty bounds), $f_0(x)$ is the

mean response function, and $f_1(x)\ldots.f_k(x)$ are the uncertainty bound functions

Step 3: Calculate the upper and lower deviation of response at x as

$$\Delta Y_{upper} = Y_{max} - f_o(x) \text{ and} \qquad \textbf{Equation 7.6}$$

$$\Delta Y_{lower} = f_o(x) - Y_{min} \qquad \textbf{Equation 7.7}$$

Step 4: Using the mean response (μ_y) obtained from the mean response model ($f_0(x)$) and the upper and lower deviations (DY_{upper} and DY_{lower}), calculate the EMIs. For a 'Larger is Better' case, the EMI is calculated:

$$\text{EMI} = \frac{\mu_y - LRL}{\Delta Y_{lower}} \qquad \textbf{Equation 7.8}$$

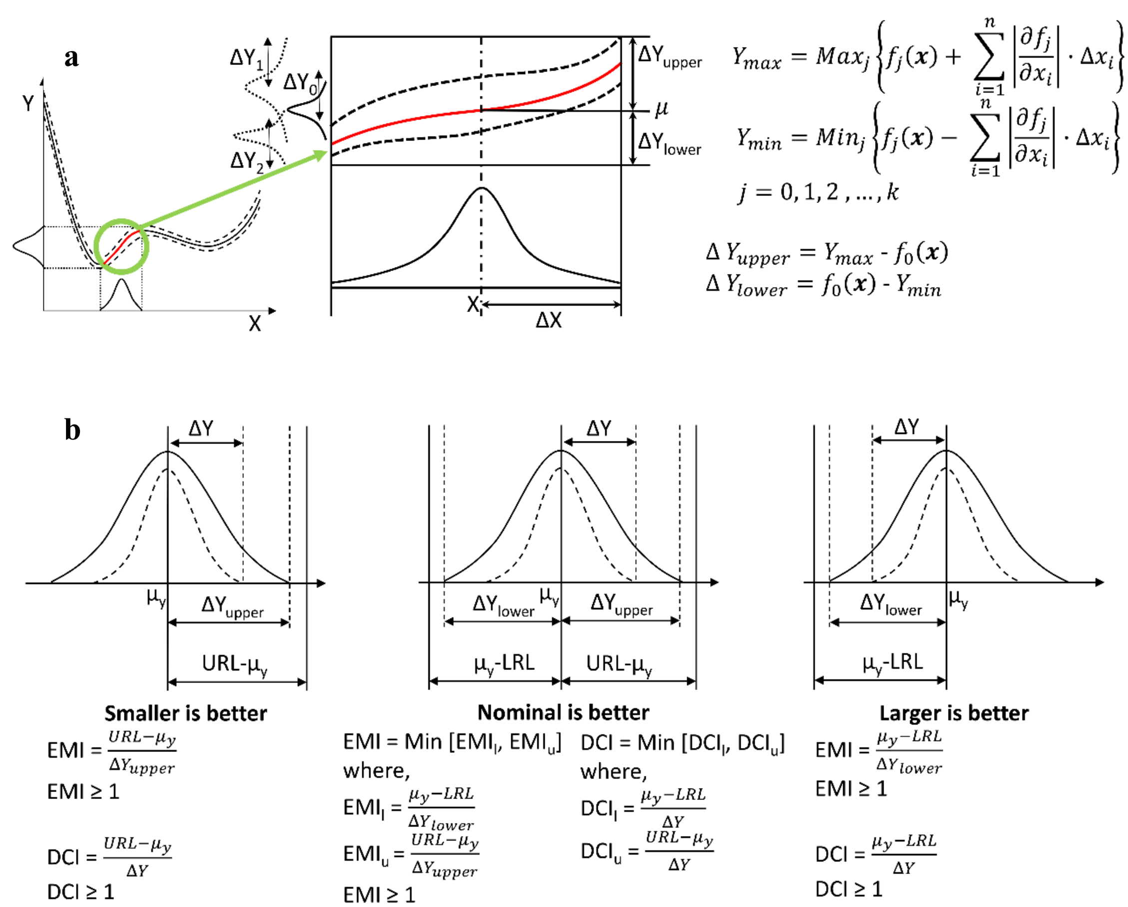


Figure 7.2: a -Uncertainty bound formulation for variability in design variable and model, b – Mathematical constructs of EMIs and DCIs (adopted from (Choi, Austin and coauthors 2005))

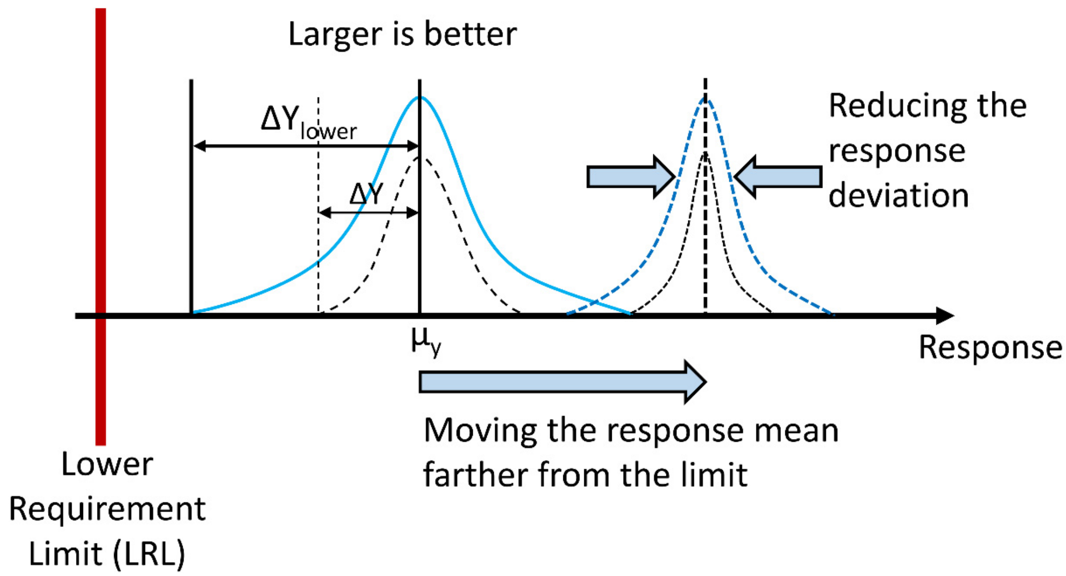


Figure 7.3: Achieving a larger value of EMI and DCI

The EMI thus calculated for 'Larger is Better' case will be larger when the location of μ_y is farther away from the LRL and/or when the ΔY_{lower} gets smaller, as shown in Figure 7.3. An EMI = 1 means that the uncertainty bound just meets the requirements limit. An EMI ≤ 1 means that the requirement limit may get violated due to the uncertainty in the model and design variables. The same can be derived for other cases shown in Figure 7.2.b for both EMI and DCI.

7.3 The cDSP with EMI-DCI for Robust Design Type I, II, III

Core to the CEF is the foundational mathematical construct – the compromise Decision Support Problem (cDSP). The cDSP construct is anchored in the robust design paradigm first proposed by Taguchi. The fundamental assumption here is that the models are not complete, accurate and of equal fidelity (Mistree, Hughes and coauthors 1993). The cDSP is a hybrid of mathematical programming and goal programming. Target values for each goal are defined in a cDSP and the emphasis of the designer is to satisfy these target goals as closely as possible. This is achieved by seeking multiple solutions through trade-offs among multiple conflicting goals. The solutions obtained are further evaluated by solution space exploration to identify solution regions that best satisfy the requirements identified. There are four keywords in the cDSP – Given, Find, Satisfy and Minimize. The overall goal of the designer using the cDSP is to minimize a deviation function – a function formulated using the deviations (captured using deviation variables) that exists from the goal targets. The details regarding formulating and solving the cDSP are available (Bras and Mistree 1993, Mistree, Hughes and coauthors 1993) and are not explained here. The mathematical formulation of the cDSP with EMI and DCI goals, constraints to achieve robust design Types I, II and III is shown in Table 7.3.

7.3.1 The modified cDSP formulation for robust design Types I, II and III for multiple goals

In the cDSP formulation, mean response functions for different multiple performance goals $f_{0,i}(x)$, the upper and lower uncertainty bound functions for those goals with model uncertainty, $f_{1,i}(x)$ and $f_{2,i}(x)$ are captured. These could be either through the method presented by Choi and coauthors, if we are developing response functions from raw data or by directly using the different functions for certain performances available in literature that captures model variability related to complex manufacturing processes (for example, yield strength functions for a hot rolled product defined by different researchers predicting the yield strength at different ranges). System constraints and goals in terms of EMI and DCI are formulated in the cDSP to capture the designer's requirements and the functionalities desired in the material-product system. The LRLs and URLs denote the lower and upper requirements limits for the system. The uncertain system constraints are captured as EMI $_{constraints,i}$ (x) or DCI$_{constraints,i}$ (x) ≥ 1 using $g_i(x)$ functions depending on type of variability. We have defined new constraints (highlighted in yellow in box in Table 7.3) in our cDSP formulation to ensure the identification of robust solutions always when preferences are changed for the different goals.

While dealing with multiple conflicting goals, there is a tendency to achieve a high robust solution (high values of EMI or DCI) for one goal when a high preference is assigned to the goal, but probably resulting in a non-robust solution for the other conflicting goal (EMI or DCI < 1). To ensure such a situation won't happen for all the different conflicting goals, we introduce the '***robust solution constraint***' for multiple conflicting goals. By assigning this constraint, we achieve a solution having EMI and DCI ≥ 1 always while different preferences are assigned to the goals during solution space exploration.

This approach will result in a solution space of only robust solutions to be explored– we define it as '***robust solution space exploration***' for multiple conflicting goals. From these robust solutions the designer chooses the range of solutions that best satisfices his/her interest. We define this as '***satisficing robust solutions***' for multiple conflicting goals under uncertainty.

Table 7.3: Mathematical form of the cDSP with EMI-DCI

cDSP with EMI-DCI for RD Type I, II, III for multiple goals
Given   n, number of system variables   m, total number of system goals   m1, number of system goals for robust design Type I, II, and III   m2, number of system goals for robust design Type I, and II   m= m1+ m2   q, number of inequality constraints $f_{0,i}(x)$, multiple mean response functions $f_{1,i}(x)$, multiple upper uncertainty bound functions $f_{2,i}(x)$, multiple lower uncertainty bound functions $g_{0,i}(x)$, multiple mean constraint functions $g_{1,i}(x)$, multiple upper constraint bound functions $g_{2,i}(x)$, multiple lower constraint bound functions URL_i and LRL_i, performance requirements $\Delta \boldsymbol{x}$, deviations of system variables $EMI_{target,i}$, $EMI_{targets}$ $DCI_{target,i}$, $DCI_{targets}$ ***Find*** μ_x (mean of system variables) d_i^+,d_i^- (deviation variables)   ***Satisfy***

System Constraints:

EMI $_{constraints,i}$ (x) or DCI$_{constraints,i}$ (x) ≥ 1 i = 1,…,q

EMI$_i$ (x) ≥ 1 i = 1,…,m1 DCI$_{,i}$ (x) ≥ 1 i = 1,…,m2	**Robust solution constraints:** New constraints defined to ensure robust solutions under multiple conflicting goals

System Goals:

EMI$_i$(x)/EMI$_{target,i}$ + $d_i^- - d_i^+ = 1$ i = 1,…,m1

DCI$_i$(x)/DCI$_{target,i}$ + $d_i^- - d_i^+ = 1$ i = 1,…,m2

(Assuming there will be at least one goal for EMI and DCI)

Bounds:

$x_i^{min} \leq x_i \leq x_i^{max}$ i =1,…,n

$d_i^-, d_i^+ \geq 0$ and $d_i^+ \cdot d_i^- = 0$ i = 1,…,m

Minimize

Z = $[f_1(d_i^-, d_i^+), \ldots, f_k(d_i^-, d_i^+)]$ Preemptive

Z = $\sum W_i\,(d_i^- + d_i^+), \sum W_i = 1$ Archimedean

7.4 The Inverse Decision-Based Design Method for Robust Design Across Process Chains

7.4.1 Generic Form of the Inverse Design Method

The approach followed in this method for finding robust satisficing solutions in a multi-level, multi-stage process chain that involves the Processing-Structure (PS), Structure-Property (SP) relations is the passing of robust satisficing solution ranges in an inverse manner, from given final performance range to the design space of the previous space (defined by model input and output) with designer having the flexibility to choose robust solution of preference. We explain the method using the information flow diagram shown in Figure 7.4.

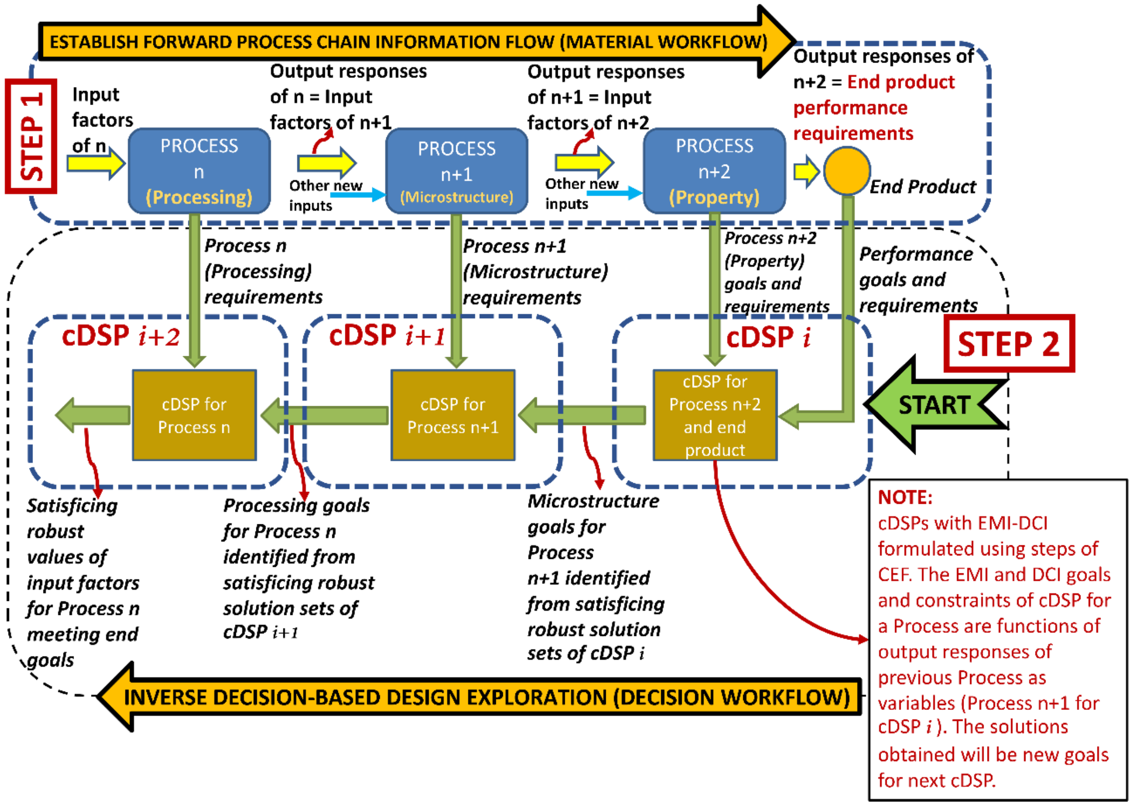


Figure 7.4: Generic form of Inverse Decision-Based Design Method

The method is goal-oriented because we start with the end goals for the product as well as process and then design the preceding processes to satisfy these end goals as closely as possible by exploring the design space. The design decisions that are made for the end requirements of the product/process after exploration are communicated to the processes that precede to make logical decisions there that satisfy the requirements identified thereby carrying out an inverse design space exploration process, as described by Steps 1 and 2, Figure 7.4. The method uses the cDSP construct with EMI-DCI along with the CEF to formulate the decision workflow and generate and propagate robust design solutions across the process chains in an inverse manner. To demonstrate the generic nature of the method we are naming the different sequential processes as ‘n’ to ‘n+2’ and the decision support constructs as ‘i' to ‘i+2’.

Step 1: Establish forward modeling and information flow across the process chain (forward material workflow)

Step 1 of the proposed method involves establishing the forward modeling and information flow across models. In Step 1, the designer makes sure that there is proper flow of information as models are connected across different ‘Processes’. These processes could be different manufacturing processes that are sequentially connected to produce the product with information passing across processing-microstructure-property-performance spaces. Mathematical models are either identified or developed to establish the information flow. The Steps 1 and 2 of the Concept Exploration Framework are used to identify factors, ranges, responses, and models for the specific materials design problem under study. In Figure 7.4, Step 1 we see that the output of a Process serves as the input to the next Process with the final output being the end product. We can imagine these ‘Processes n, n+1 and n+2’ as Processing, Microstructure and Property Spaces respectively as shown in Figure 7.4 to understand the method clearly. Thus, Process n (Processing Space) generates output that serves as input for Process n+1 (the Microstructure Space). The output of Process n+1 (the microstructure identified) serves as the input for Process n+2. The output of Process n+2 defines the Property Space and this directly defines the final performance characteristics of the end product. From a design standpoint the input to a Process are design variables and the output response from the Process serves as input variables to next Process.

Step 2: Carry out inverse decision-based design exploration starting from performance space and sequentially identifying robust regions of interest in previous spaces in an inverse manner

We start the inverse decision-based design exploration from Process n+2 (Property-Performance space). The cDSP for the last space is formulated with EMI and DCI goals that captures both property and performance requirements for the end product. The design variables for this cDSP will be the output responses from Process n+1 (Microstructure space) which forms the input for Process n+2 along with other new inputs for Process n+2, see Figure 7.4 (Process n+2 and cDSP for Process n+2). The output of cDSP i after solution space exploration will be the target ranges of microstructure factors that satisfies the properties and performances defined for the product taking into consideration the uncertainty in the models and design variables. The target ranges for microstructure identified is passed as goals in the form of EMI or DCI to next cDSP i+1 for Process n+1. The design variables for cDSP i+1 are the output responses from Process n that serves as input to Process n+1. Executing this cDSP and exploring the solution space using CEF, the designer is able to identify the ranges for processing space that best satisfies the target goals defined after considering the uncertainty associated. The process can be repeated to identify the inputs for Process n by formulating the cDSP for Process n, if needed as shown in Figure 7.4. An explanation of the solution space exploration part is provided in Section 7.4.2.

7.4.2 Robust solution space exploration across process chain in an inverse manner (Inverse Decision Workflow)

We define a workflow as a sequence of computational tasks in which information flows from one process/space to another. For the integrated design of materials, products and associated manufacturing processes, we define two types of workflows, namely, the workflows associated with simulating the behavior of the material through process-structure-property-performance hierarchy (material workflow) and the workflows associated with the process of design in an inverse manner across process chains (inverse decision workflow). Our focus in this chapter is on the uncertainty associated with the inverse decision workflows and the analysis models embodied therein.

In Figure 7.5, we show the robust solution space exploration across process chain considering model structure and model parameter uncertainty. In Step 1, we map models from space to another and a rough design space is thus generated. This is defined as forward modeling and defines the material workflow using models. We start the exploration from the rough design space for Property-Performance. In the rough design space, we formulate the actual decision-based design space for Property-Performance using the cDSP construct supported by CEF. The actual decision-based design space is identified by the light blue region in Figure 7.5. On exercising the cDSP for the different conflicting goals by assigning preferences, we obtain different solution regions that satisfy individual goals identified by the three circles (red, orange and gold color in Property-Performance space, Figure 7.5).

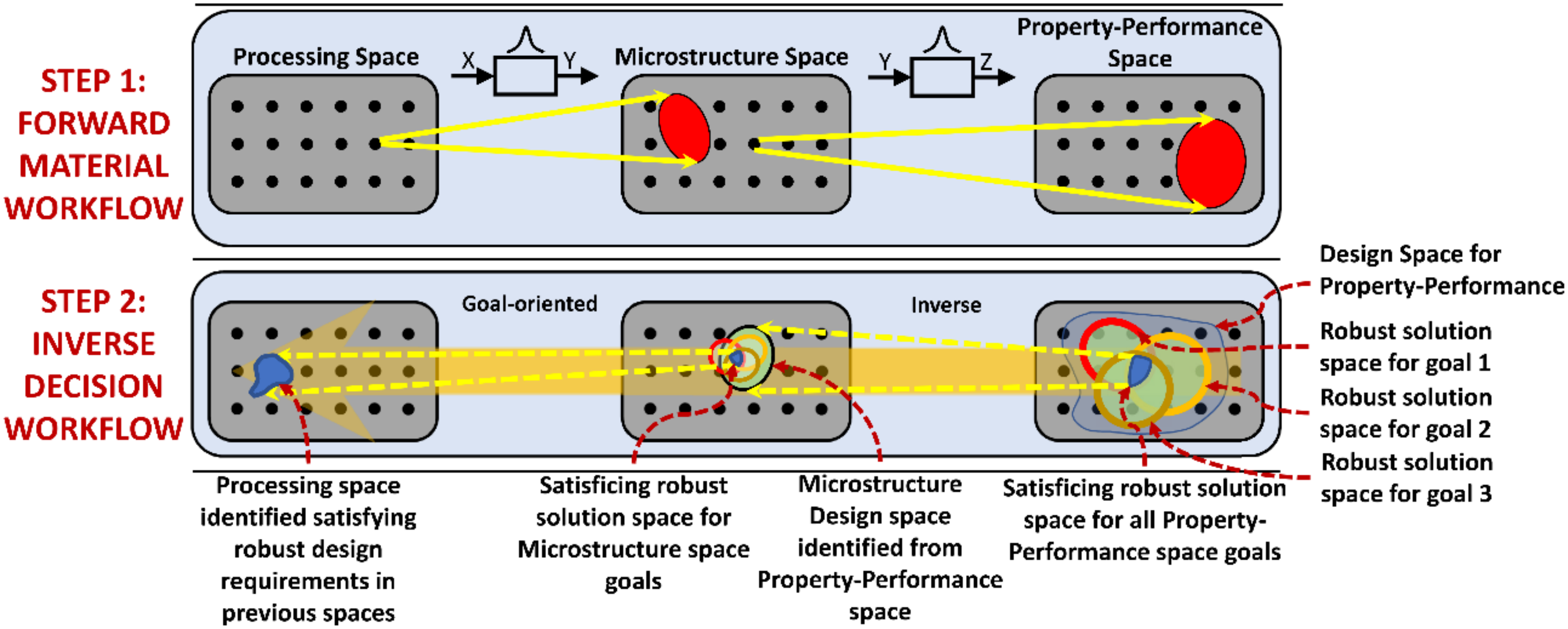


Figure 7.5: Robust solution space exploration across process chain in an inverse manner (Inverse decision workflow)

If the cDSP is formulated with the robust solution constraint defined in Section 7.3.1 (EMI_i (x) ≥ 1 and $DCI_{,i}$ (x) ≥ 1), then the regions inside the circle denote the regions with EMI or DCI greater than 1 depending on the type of goal formulation. Any region inside the circle satisfies the robust design requirement of that particular goal and there will be regions with highest robustness and lowest robustness within the circle. The designer can pick solutions that achieve maximum robustness for the goal. Now, since the cDSP is formulated with the defined robust design constraint, such a solution is never reached that gives a high value of EMI or DCI for one goal but an EMI or DCI < 1 for another goal, thus ensuring a robust solution space for all the goals. The designer can then explore the robust solution space of all the conflicting goals and identify common robust regions that satisfy all the goals in the best possible manner – satisficing robust solution region for all goals, if it exists. This region is identified as the dark blue region inside the circles in Property-Performance decision-based design space, Figure 7.5.

Once the first cDSP is executed and satisficing robust solution region is identified, the next cDSP for microstructure design space is formulated. This cDSP is formulated with design variable values identified from first cDSP as the microstructure goal requirements and is formulated in terms of EMI or DCI depending on the type of uncertainty present (the circle with the green region in Microstructure space represents the region identified from previous cDSP and is the design space for the new cDSP, Figure 7.5). On solving the cDSP with EMI-DCI for microstructure and exploring the solution space, we obtain the robust solution regions that satisfies each goal (represented by the three circles inside the green region in microstructure space, Figure 7.5). From these robust solutions, the designer identifies the satisficing robust region for all goals – the blue region within the circles. The processing space region/values that gives this robust microstructure region is identified from the design variables values of the cDSP (the blue region in the Processing space, Figure 7.5). Thus, using this proposed method, the designer is able to carry out top-down driven, simulation-supported, decision-based robust design exploration of processing paths and material microstructure to satisfy a ranged set of product-level performance requirements. The method is generic and can be applied to similar problems with information flow from one process to another.

7.5 Robust Concept Exploration of Material (Steel), Product (Rod) and Associated Manufacturing Processes (Hot Rolling and Cooling)

Developing new grades of steels with improved properties and performance is the focus for steel manufacturers. Developing steels with a range of mechanical properties resulting in improved performance of products is possible by carefully managing the material processing and thereby tailoring the microstructure generated. Several manufacturing processes such as casting, reheating, rolling and cooling are involved in the processing of a steel rod. This round rod produced is further used for gear production after forging into gear blanks. The end properties of the rolled product are influenced by the chemical composition of the steel including the segregation of alloying elements, the deformation history during rolling, the cooling after rolling and the microstructure generated after rolling and cooling processes. The steel rod making process chain is highly complex due to large numbers of design variables, constraints and bounds, conflicting goals and sequential information/material flow during material processing. Many plant trials that are usually expensive and time-consuming are required to produce a new steel grade with desired properties and performance. An alternative therefore is to carry out simulation-based, integrated design exploration of the different manufacturing processes involved by exploiting the advances in computational modeling and identifying ranged set of robust solutions satisfying the requirements of the processes and product.

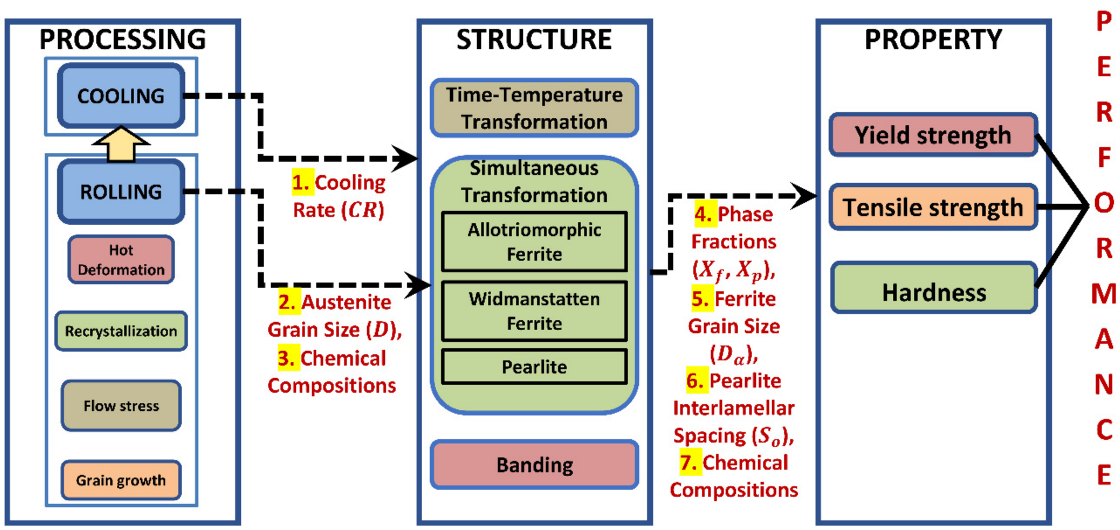


Figure 7.6: Process-Structure-Property-Performance hierarchy for the integrated design of hot rolling and cooling processes to produce a steel rod – forward material workflow

In Figure 7.6, we show the process-structure-property-performance hierarchy for the integrated design of hot rolling and cooling processes to produce the steel rod. Using Figure 7.6, we capture the forward material workflow for the problem. The processing stage involves the two manufacturing processes, namely hot rolling and cooling. During hot rolling, the thermo-mechanical processing of the material happens. The modeling of hot rolling process involves a hot deformation module, recrystallization module, grain growth module and flow stress module (Nellippallil, De and coauthors). The input to the rolling process are the chemical composition, initial austenite grain size after reheating, and the rolling schedule (strain, strain rate, interpass time, number of passes). Using these inputs we predict the temperature evolution, flow stress and calculate the final austenite grain size (AGS, D) after rolling, see (Nellippallil, De and coauthors). In our design problem, we are interested in the final the final AGS and it forms the input from rolling side to the microstructure space. The microstructure space is generated in the cooling process. Depending on the cooling rate (CR) and the final AGS from rolling and the chemical composition of the incoming steel, time-temperature transformations and simultaneous transformations take place resulting in the phase transformation of austenite to different steel phases like Allotriomorphic ferrite, Widmanstatten ferrite, pearlite, etc. Also, alternate layers of banded microstructure of ferrite and pearlite can form depending on the micro segregates that are present and the cooling conditions.

In our study, we consider the transformations of austenite to ferrite and pearlite. The output after cooling process from the microstructure space as shown in Figure 8 is the phase fractions of ferrite and pearlite ($X_f and\ X_p$), ferrite grain size after transformation (FGS, D_α), pearlite interlamellar spacing (S_o) and the chemical composition of the material. These are input for the property space to predict mechanical properties, yield strength, tensile strength, and hardness which are measures of performance for the final rod product. This completes the forward material workflow for the problem and establishes the process-structure-property-performance hierarchy for the material system. Next, we begin the design exploration process.

7.5.1 Step 1: Establish forward modeling and information flow across the process chain (Material Workflow)

Identifying factors (input) and responses across process chain (see steps of CEF): For the hot rod rolling process chain problem addressed in this chapter, the mechanical property goals and requirements are for yield strength (YS), tensile strength (TS) and hardness (HV). These mechanical properties are dependent on the final microstructure after cooling: the ferrite grain size after cooling (FGS, D_{α}), the phase fractions of ferrite (X_f) and pearlite ($1 - X_f$), the pearlite interlamellar spacing (S_0) and the composition variables like silicon $[Si]$, nitrogen $[N]$, phosphorous $[P]$ and manganese $[Mn]$. These microstructure factors are defined by the rate (CR) at which cooling is carried out and the final austenite grain size after rolling (AGS, D) and composition variables like carbon $[C]$ and manganese $[Mn]$.

Identify models and relationships that map from Processing space to final Performance space across the process chain taking into account the uncertainty in models and design variables

Microstructure-Mechanical Property Correlation Models

The mechanical properties for the end rod produced are represented by yield strength (YS), tensile strength (TS) and hardness (HV). Gladman and co-authors (Gladman, McIvor and coauthors 1972, Gladman, Dulieu and coauthors 1977) were instrumental in predicting the mechanical properties of plain carbon steel products as a function of the microstructural parameters of ferrite-pearlite microstructure. Models were later developed by Hodgson and Gibbs (Hodgson and Gibbs 1992), Majta and co-authors

(Majta, Kuziak and coauthors 1996) and Kuziak and co-authors (Kuziak, Cheng and coauthors 1997).

Models for Yield Strength and the variability associated

Over the years, several researchers have predicted yield strength as a function of different microstructural parameters. These models predict values at different ranges for a given input and hence have variability associated with them in the prediction of the yield strength. In this chapter to demonstrate our method for inverse design and managing uncertainty, we assume the yield strength model by Gladman and coauthors (Gladman, McIvor and coauthors 1972, Gladman, Dulieu and coauthors 1977) as the mean response model $f_0(x)$ for our problem. The upper uncertainty bound function $f_1(x)$ for yield strength is the model by Hodgson and Gibbs (Hodgson and Gibbs 1992) that always predicts yield strength higher than the model by Gladman and coauthors for a given input. The lower uncertainty bound function $f_2(x)$ for yield strength is the model by Kuziak and co-authors (Kuziak, Cheng and coauthors 1997) which predicts yield strength at a lower level than the mean response model for a given input. The models thus identified for yield strength are included in Table 7.4. The mean response function and prediction interval models are plotted in Figure 7.7. The models are depicted as a function of the ferrite grain size (FGS, D_α) and ferrite fraction (X_f) for a value of pearlite interlamellar spacing of 0.15 (μm), manganese concentration of 1.5 (%), nitrogen of 0.007 (%), silicon of 0.36 (%), phosphorous of 0.019 (%) and copper of 0.08 (%).

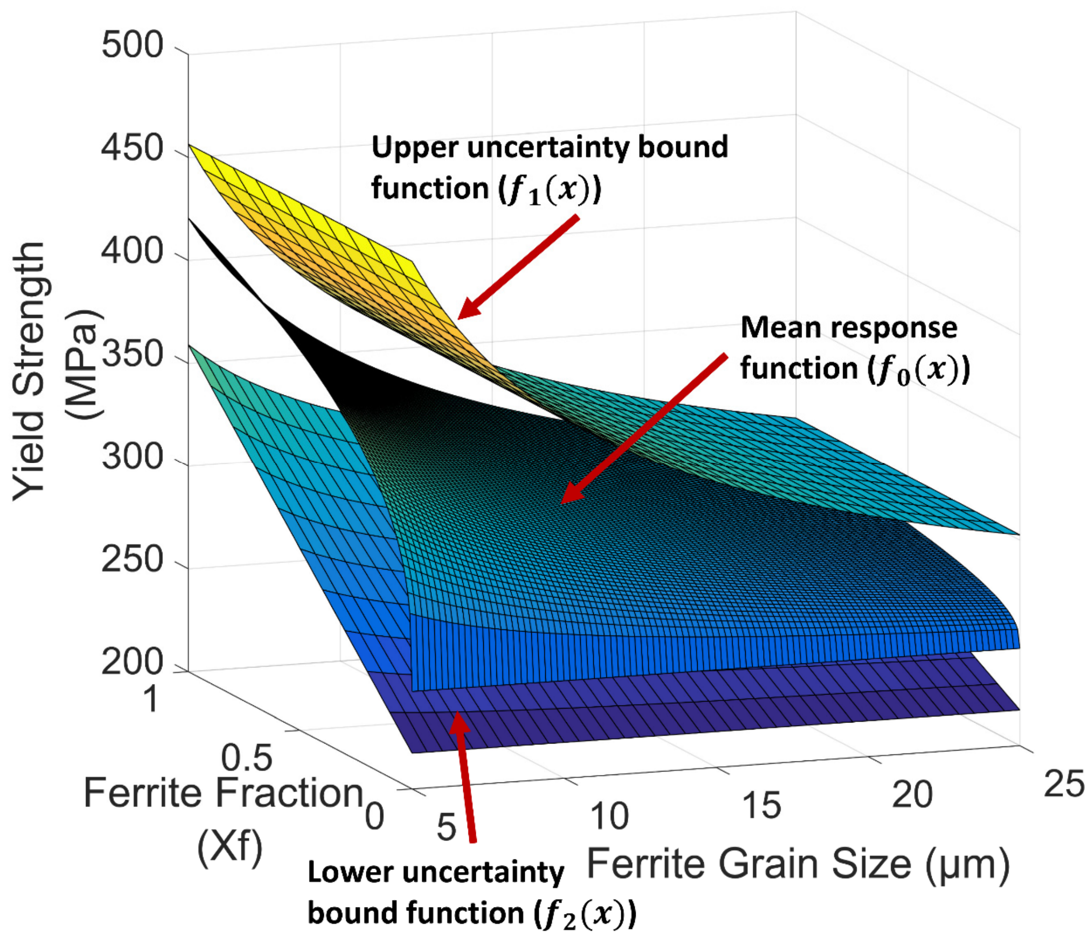


Figure 7.7: The mean response function and the upper and lower uncertainty bound functions for Yield Strength

Model for Tensile Strength

We have selected the model by Kuziak and co-authors that describes the tensile strength TS, of carbon-manganese steels as a function of ferrite grain size after cooling D_α, cooling rate CR, ferrite fraction X_f, the pearlite interlamellar spacing S_o, and the composition elements in the steel (Kuziak, Cheng and coauthors 1997). The model is included in Table 7.4.

Model for Hardness

Hardness (HV) is represented as a function of ferrite and pearlite fractions, average austenite to ferrite transformation temperature (T_{mf}) and weight percentage of silicon (Si) as depicted in Table 7.4 based on the investigation by Yada (Yada 1987).

Processing-Microstructure Correlation Models

Model for Ferrite Fraction

We are selecting the response surface model developed by Nellippallil and coauthors (Nellippallil, Allen and coauthors 2017) for ferrite fraction, Table 7.4. The model is developed by carrying out design of experiments using the program STRUCTURE developed by Jones and Badeshia to predict the simultaneous transformation of austenite (and, H. K. D. H and coauthors Last accessed 4, February 2017.). For more details on the development of the response surface model and the validation of the same, see Chapter 6 (Nellippallil, Allen and coauthors 2017).

Model for Ferrite Grain Size

We are adopting the models by Hodgson and Gibbs (Hodgson and Gibbs 1992) for defining ferrite grain size, see Table 7.4. The factors affecting ferrite grain size D_{α} are final austenite grain size after rolling D, retained strain ε_r, and the composition both related to the deformation history of the material from rolling side and cooling rate from cooling side.

Model for Pearlite Interlamellar Spacing

We are adopting the model by Kuziak and co-authors (Kuziak, Cheng and coauthors 1997) where pearlite interlamellar spacing S_o is defined as a function of carbon C, manganese Mn and cooling rate CR, see Table 7.4.

Table 7.4: Models establishing forward material workflow

Response	Model	
Yield Strength (Mean Response Function)	$YS = 63[Si] + 425[N]^{0.5} + X_f^{1/3}(35 + 58[Mn] + 17(0.001D_\alpha)^{-0.5}) + (1 - X_f^{1/3})(179 + 3.9S_0^{-0.5})$	**Equation 7.9**
Yield Strength (Upper uncertainty bound function)	$YS = 62.6 + 26.1[Mn] + 60.2[Si] + 759[P] + 212.9[Cu] + 3286[N] + 19.7(.001D_\alpha)^{-0.5}$	**Equation 7.10**
Yield Strength (Lower uncertainty bound function)	$YS = X_f(77.7 + 59.9 \times [Mn] + 9.1 \times (0.001D_\alpha)^{-0.5}) + 478[N]^{0.5} + 1200[P] + (1 - X_f)[145.5 + 3.5S_0^{-0.5}]$	**Equation 7.11**
Tensile Strength	$TS = X_f(20 + 2440 \times [N]^{0.5} + 18.5 \times (0.001D_\alpha)^{-0.5}) + 750(1 - X_f) + 3(1 - X_f^{0.5})S_0^{-0.5} + 92.5 \times [Si]$	**Equation 7.12**
Hardness	$HV = X_f(361 - 0.357T_{mf} + 50[Si]) + 175(1 - X_f)$	**Equation 7.13**
Ferrite Fraction	$X_f = 1 - (0.206 - 0.117[Mn] - 0.0005CR - 0.00113D + 0.248[C] + 0.00032[Mn]CR + 0.000086[Mn]D + 0.9539[Mn][C] - 4.259 \times 10^{-6}CR * D + 0.00726CR[C] + 0.0023D[C] - 0.0305[Mn]^2 - 0.0000056CR^2 + 4.859 \times 10^{-6}D^2 + 0.79[C]^2)$	**Equation 7.14**
Ferrite Grain Size	$D_\alpha = (1 - 0.45\varepsilon_r^{0.5}) \times \{(-0.4 + 6.37C_{eq}) + (24.2 - 59C_{eq})CR^{-0.5} + 22[1 - \exp(-0.015D)]\}$ where $C_{eq} = (C + Mn)/6$	**Equation 7.15**
Pearlite Interlamellar Spacing	$S_o = 0.1307 + 1.027[C] - 1.993[C]^2 - 0.1108[Mn] + 0.0305CR^{-0.52}$	**Equation 7.16**

7.5.2 Step 2: Carry out inverse decision-based design exploration starting from performance space

We start the inverse decision-based design exploration from Property-Performance space. The cDSP for the last space is formulated with EMI and DCI goals that captures both property and performance requirements for the end product. The design variables for this cDSP will be the output responses from Microstructure space which forms the input for Property-Performance space, see Figure 8. On exercising the cDSP the process designer will be able to solve and capture the knowledge associated with the following inverse problem: *Given the end mechanical properties of a new steel product mix, what should be the microstructure factors after phase transformation that satisfies the requirements identified taking into account the uncertainty associated with models and parameters associated?* The cDSP is shown below.

cDSP for Property-Performance (Larger is Better)
Given End requirements identified for the rod rolling process • Maximize Yield Strength • Maximize Tensile Strength • Maximize Hardness $f_{0,i}(x)$, multiple mean response functions $f_{1,i}(x)$, multiple upper uncertainty bound functions $f_{2,i}(x)$, multiple lower uncertainty bound functions LRL_{YS} = 200 MPa

LRL_{TS} = 450 MPa

LRL_{HV} = 130

$EMI_{target,YS}$ = 3	EMI Target for EMI goal for YS considering Type I, II and III RD
$DCII_{target,TS}$ = 8	DCI Target for DCI goal for TS considering Type I and II RD
$DCII_{target,HV}$ = 8	DCI Target for DCI goal for HV considering Type I and II RD

System variables, their ranges and variability

Table 7.5: System variables, ranges and variability

Sr. No	**System Variables (X)**	**Ranges**	**Variability (Δx)**
1	X_1, ferrite grain size (D_α)	5-25 μm	[±3]
2	X_2, the phase fraction of ferrite (X_f)	0.1-1	[±0.1]
3	X_3, the pearlite interlamellar spacing (S_0)	0.15-0.25 μm	[±0.01]
4	X_4, manganese concentration after cooling ($[Mn]$)	0.7-1.5 %	[±0.1]

Fixed parameters

Parameter	**Value**
C (Carbon)	0.18 (%)
Si (Silicon)	0.36 (%)
V (Vanadium)	0.003 (%)

Cu (Copper)	0.08 (%)
N (Nitrogen)	0.007 (%)
P (Phosphorous)	0.019 (%)
ε_r (Retained strain)	0
T_{mf} (Austenite to ferrite transformation temperature)	700 ℃

Find

μ_x, (Mean location of system variables)

Deviation Variables

d_i^-, d_i^+, *i =1,2,3*

Satisfy

System Constraints

- Robust solution constraint for YS

  EMI_{YS} (x) ≥ 1

- Robust solution constraint for TS

  DCI_{TS} (x) ≥ 1

- Robust solution constraint for HV

  DCI_{TS} (x) ≥ 1

System Goals

Goal 1:

- Maximize EMI for Yield Strength

$$\frac{EMI_{YS}\text{ (x)}}{EMI_{Target,YS}} + d_1^- - d_1^+ = 1$$

where EMI(x) = $\{f_0(x) - \text{LRL}\}/\{Y_{min} - f_0(x)\}$

where $Y_{min} = \text{Min}\left\{\left(f_j(x) - \sum_{i=1}^{n}\left|\frac{\partial f_j}{\partial x_i}\right| \cdot \Delta x_i\right)\right\}$

Goal 2:

- Maximize DCI for Tensile Strength

$$\frac{DCI_{TS}\text{ (x)}}{DCI_{Target,TS}} + d_2^- - d_2^+ = 1$$

Goal 3:

- Maximize DCI for Hardness

$$\frac{DCI_{HV}\text{ (x)}}{DCI_{Target,HV}} + d_1^- - d_1^+ = 1$$

where DCI(x) = $\{f_0(x) - LRL\}/\Delta Y$

where $\Delta Y = \sum_{i=1}^{n}\left|\frac{\partial f_0}{\partial x_i}\right| \Delta x_i$

Variable Bounds

Defined in Table 7.5

Bounds on deviation variables

$$d_i^-, d_i^+ \geq 0 \text{ and } d_i^- * d_i^+ = 0\text{ , i} = 1{,}2{,}3$$

Minimize

We minimize the deviation function

$$Z = \sum_{i=1}^{3} W_i(d_i^- + d_i^+);\ \sum_{i=1}^{3} W_i = 1$$

On exercising the cDSP for different design scenarios and carrying out robust solution space exploration, following the steps in Concept Exploration Framework, we obtain the combinations for D_{α}, X_f, S_0, Mn that best satisfy the end mechanical properties in the presence of model structure and model parameter uncertainty. The desired solution ranges identified for D_{α}, X_f, S_0 are then identified as the target goals for the next cDSP (cDSP for microstructure space).

7.6 Robust Solution Space Exploration

7.6.1 Robust Solution Space Exploration of Property-Performance Space

We have exercised 13 different scenarios for the cDSP formulated in Section 7.5.2. Different weights are assigned to each goal in these scenarios, Table 7.6.

Table 7.6: Scenarios and achieved values of goals

Scenarios	w1	w2	w3	Goal 1 - EMI YS	Goal 2 - DCI TS	Goal 3 - DCI HV
1	1	0	0	2.635	1	2.65
2	0	1	0	1.202	8.11	8.663
3	0	0	1	1.226	7.45	8.278
4	0.5	0.5	0	1.57	6.818	8.691
5	0.5	0	0.5	1.663	5.852	7.748
6	0	0.5	0.5	1.188	8.154	8.64
7	0.25	0.75	0	1.408	7.277	8.786
8	0.25	0	0.75	1.663	5.847	7.744
9	0.75	0	0.25	1.673	5.769	7.668
10	0.75	0.25	0	1.584	6.72	8.596
11	0	0.75	0.25	1.202	8.11	8.663
12	0	0.25	0.75	1.192	8.146	8.647
13	**0.34**	**0.33**	**0.33**	1.562	6.917	8.786

These scenarios are selected based on judgement to effectively capture the design space for exploration in a ternary space with different combination of weights on goals. Next, we explain the significance of each of these scenarios and identify robust satisficing solutions from the solution space generated in Table 7.6. We explain the significance of the scenarios using the cDSP for the Property-Performance space.

Scenarios 1-3 are for a situation where the designer's interest is to achieve the target of one of the goals, maximizing EMI_{YS}, maximizing DCI_{TS} or maximizing DCI_{HV} as close as possible. For example, the designer's preference in Scenario 3 is to achieve only the DCI goal for hardness. Scenarios 4-6 are for a situation where two goals are given equal preference, while the third goal is not given any preference. For example, Scenario 5 is a situation where designer's interest is in equally maximizing EMI_{YS} and DCI_{HV} without giving any preference to the DCI_{TS} goal. Scenarios 7-12 are situations where the designer gives greater preference to one goal, a lesser preference to second goal and zero preference to third goal. Scenario 13 is a situation where the designer gives equal preference to all the three goals considered.

The exploration of solution space is carried out by exercising the cDSPs for these scenarios and plotting the solution space obtained in a ternary space. In the context of our work, the axes of the ternary plots are the weights assigned to each goal and the color contour in the interior is the achieved value of the specific goal that is being addressed. From these plots, we identify feasible solution regions that satisfies our requirements and the associated weights to be assigned to each goal to achieve this solution space. To read more about the creation and interpretation of ternary plots, see (Nellippallil, Song and coauthors 2016, Nellippallil, Rangaraj and coauthors 2018).

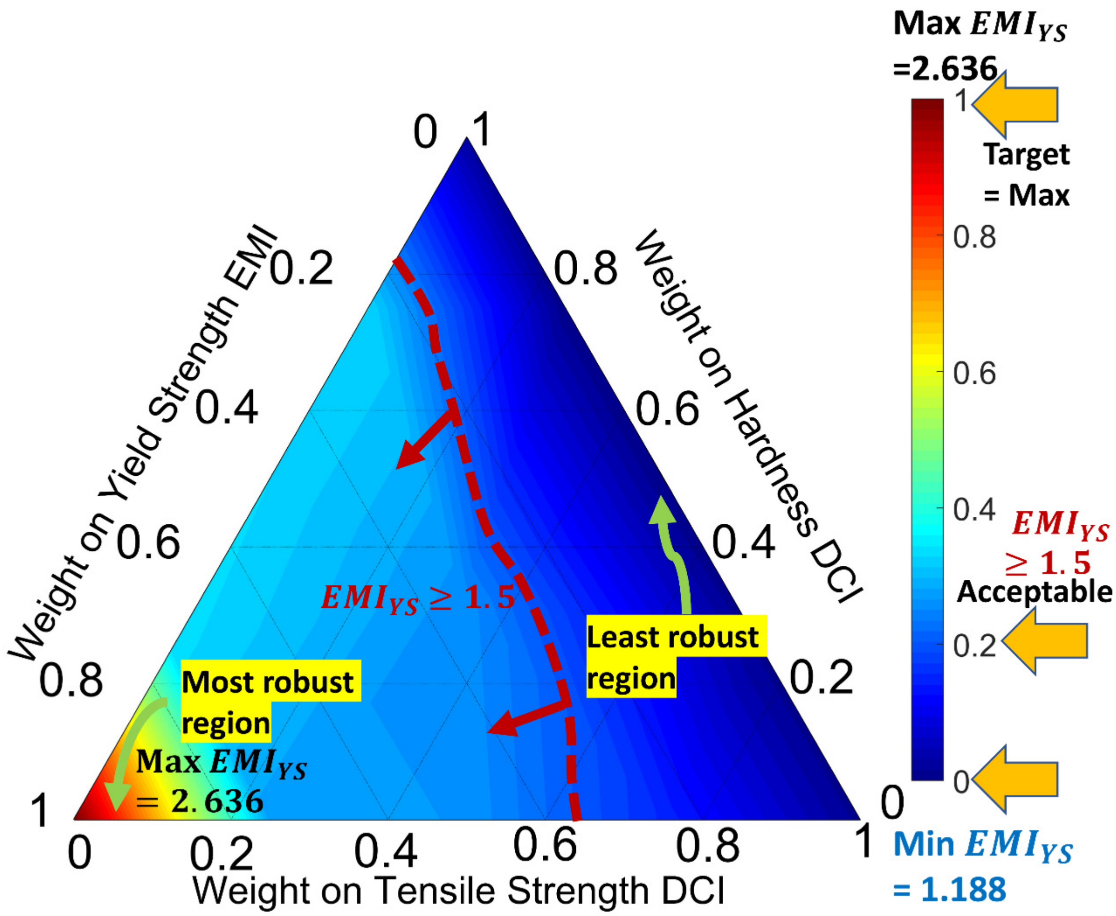


Figure 7.8: Robust solution space for YS

For Goal 1, we are interested in achieving a high value of EMI_{YS}. We see from Figure 7.8 that the solution space is composed of solutions with $EMI_{YS} \geq 1$ ensuring robust solutions under both model structure and model parameter uncertainty. The maximum EMI_{YS} is achieved in the red region and this region is therefore the most robust region for Yield Strength for the given design scenario and the dark blue region is the least robust in this solution space. We define an acceptable robust region within the solution space as $EMI_{YS} \geq 1.5$ identified by the red dashed lines. Any solution points lying within this region is acceptable for us as it satisfies the requirement for yield strength under uncertainty.

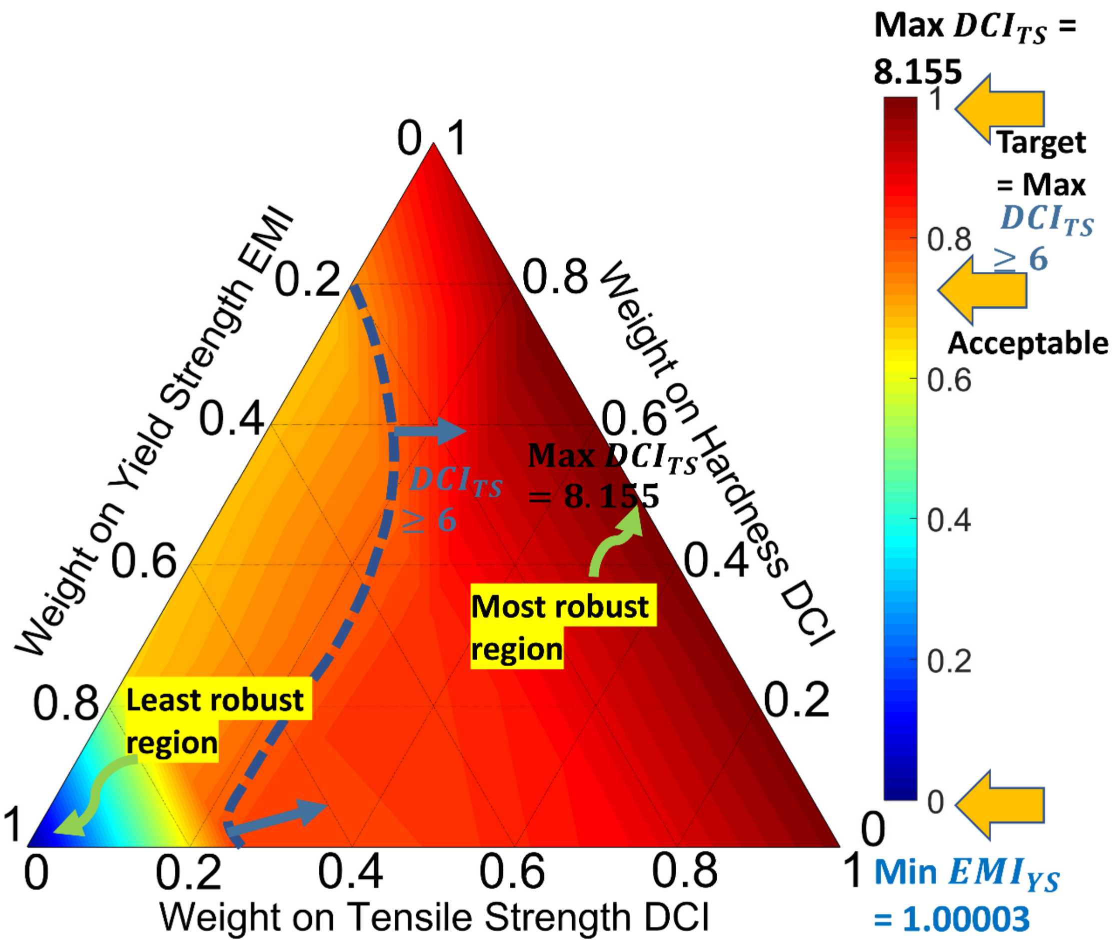


Figure 7.9: Robust solution space for TS

For Goal 2, we are interested in achieving a high value of DCI_{TS}. We see from Figure 7.9 that the solution space is composed of solutions with $DCI_{TS} \geq 1$ ensuring robust solutions under model parameter uncertainty for TS. The maximum DCI_{TS} is achieved in the red region and this region is therefore the most robust region for Tensile Strength and the dark blue region is the least robust in this solution space. We define an acceptable robust region within the solution space as $DCI_{TS} \geq 6$ identified by the blue dashed lines.

Any solution points lying within this region is acceptable for us as it satisfies the requirement for tensile strength under model parameter uncertainty.

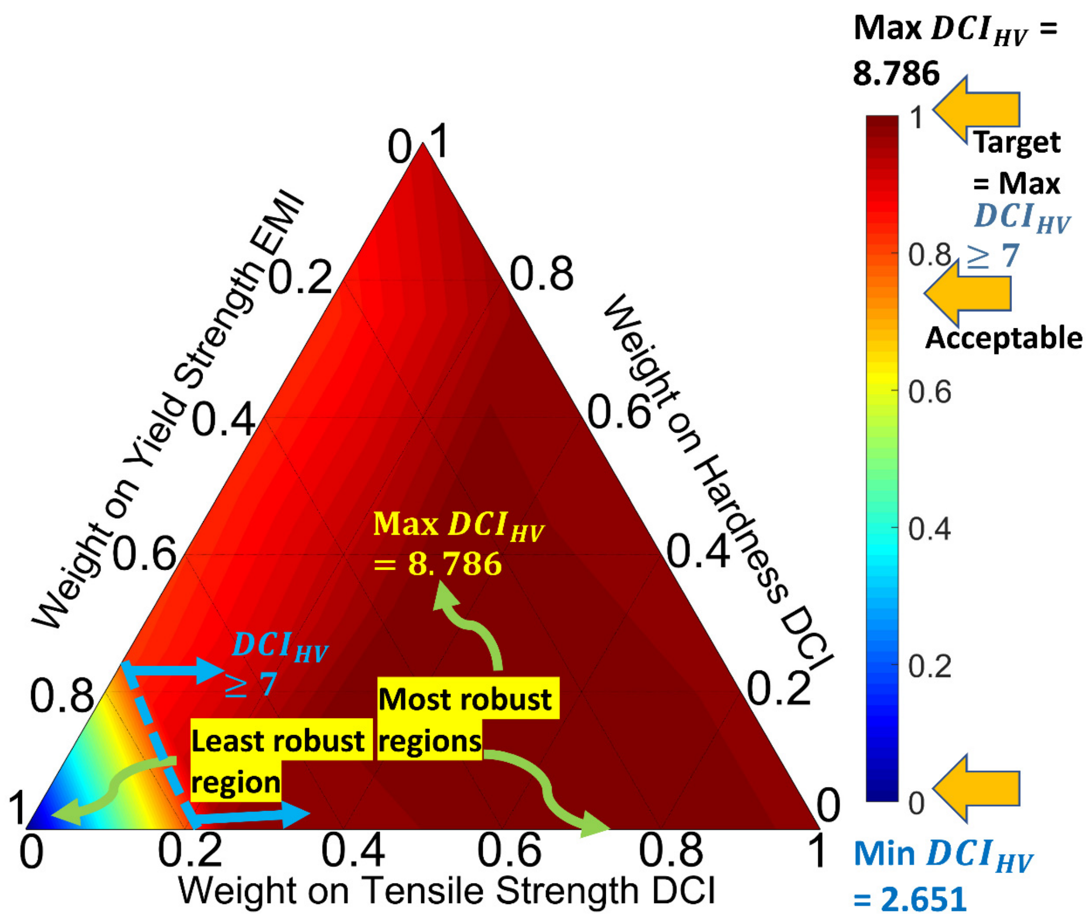


Figure 7.10: Robust solution space for HV

For Goal 3, we are interested in achieving a high value of DCI_{HV}. We see from Figure 7.10 that the solution space is composed of solutions with $DCI_H \geq 1$ ensuring robust solutions under model parameter uncertainty for HV. We identify the red region with $DCI_{HV} \geq 7$ as the robust region that satisfies the requirement for hardness under model parameter uncertainty.

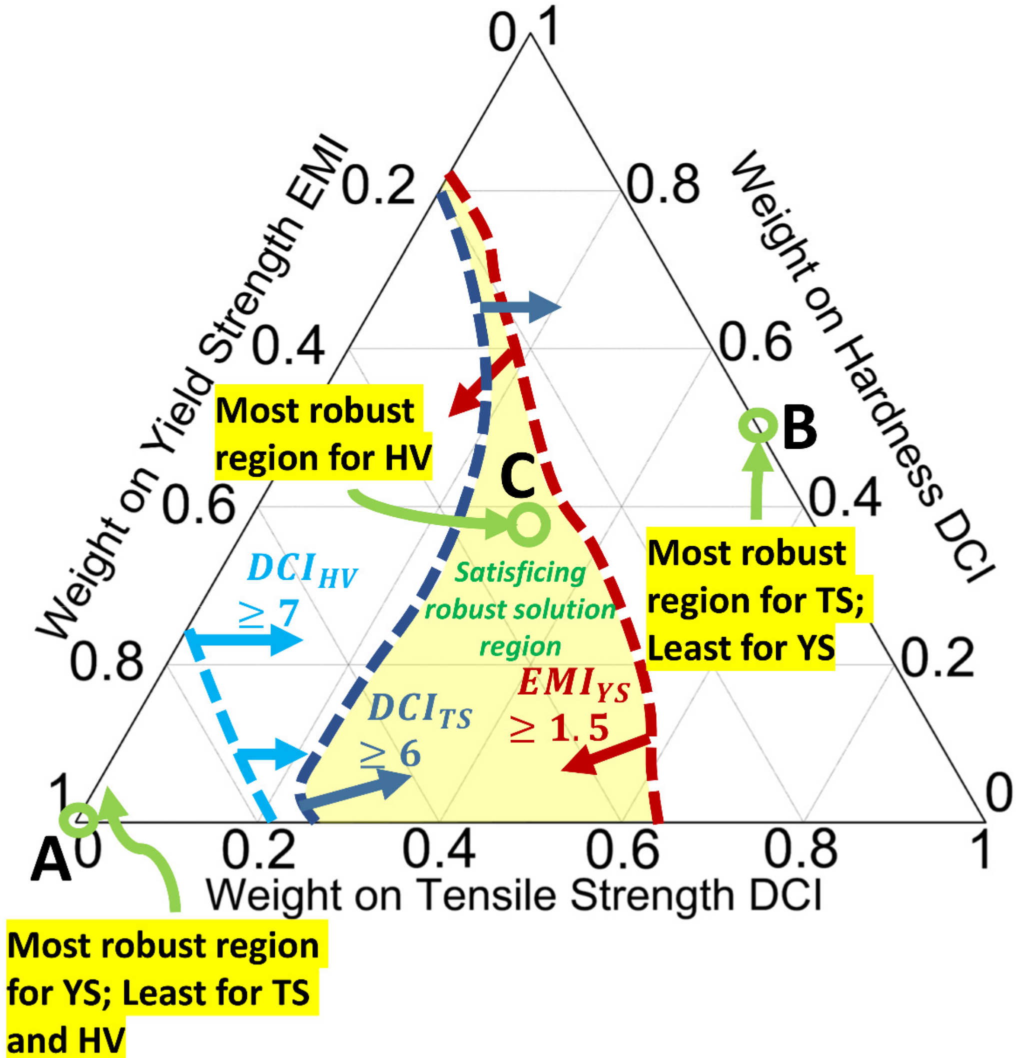


Figure 7.11: Superposed robust solution spaces

Since we are interested in identifying *satisficing robust solution* regions for the multiple conflicting goals, we plot the superposed plot with all the robust solution spaces of interest as shown in Figure 7.11. The light-yellow region identified in Figure 7.11, satisfies the robust design requirements identified for the conflicting mechanical property goals. In Figure 7.11, we highlight three points A, B and C. A is the most robust region for YS with high EMI but lowest for TS and HV with low DCIs. Similarly, B is the most robust region for TS with high DCI_{TS} but lowest for YS with low EMI_{YS}. Point C

(Scenario 13 in Table 7.6) lying inside the satisficing robust solution space achieves the highest DCI_{HV} and is the most robust region for HV goal satisfying the robust design requirements of other goals. We select Point C and the solution region around it as the robust solution of interest and this information is passed to the cDSP for microstructure space, Table 7.7.

Table 7.7: Microstructure information for next cDSP

Sol. Pt	Microstructure Factors (Solutions identified are passed as microstructure requirements to next cDSP)				Mechanical Properties of Rod (Achieved robust values)		
	X_f	D_α μm	S_0 μm	Mn (%)	YS MPa	TS MPa	HV
C	0.1 [±0.1]	24.7 [±3]	0.15 [±0.01]	0.7 [±0.1]	245	747	170

7.6.2 Robust Solution Space exploration of Microstructure Space

We carry out the inverse exploration of Microstructure space with information coming from the first cDSP as our requirements. The cDSP for the microstructure space is formulated with EMI and DCI goals capturing microstructure requirements identified under uncertainty. The design variables for this cDSP is the output responses from Processing space which forms the input for Microstructure space, see Figure 8. In this example, we will be looking only at the model parameter uncertainty associated with the microstructure responses, namely X_f, D_α, and S_0. The cDSP with DCI reads as follows:

cDSP for Microstructure Space (Smaller is Better), RD I&II

Given

End requirements identified for the rod rolling process

- Minimize Ferrite Fraction
- Minimize Ferrite Grain Size
- Minimize Pearlite Interlamellar Spacing

$f_{0,i}(x)$, multiple mean response functions

$URL_{X_f} = 0.75$

$URL_{D_\alpha} = 30\ \mu$m

$URL_{S_O} = 0.2\ \mu$m

(assigned based on the results from previous cDSP)

$DCI_{target},\ X_f = 10$

$DCII_{target},\ D_\alpha = 10$

$DCII_{target},\ S_O = 200$

System variables, their ranges and variability

Table 7.8: System variables, ranges and variability

Sr. No	System Variables (X)	Ranges	Variability (Δx)
1	X_1, Cooling Rate (CR)	11-100 K/min	[±10]
2	X_2, Austenite Grain Size (D)	30-100 μm	[±10]

Find

μ_x, (Mean location of system variables)

Deviation Variables

d_i^-, d_i^+, *i =1,2,3*

Satisfy

System Constraints

- Robust solution constraint for Ferrite Fraction

$$DCI_{X_f}\,(\mathrm{x}) \geq 1$$

- Robust solution constraint for Ferrite Grain Size

$$DCI_{D_\alpha}\,(\mathrm{x}) \geq 1$$

- Robust solution constraint for Pearlite Interlamellar Sp.

$$DCI_{S_O}\,(\mathrm{x}) \geq 1$$

System Goals

Goal 1:

- Maximize DCI for Ferrite Fraction

$$\frac{DCI_{X_f}\,(\mathrm{x})}{DCI_{Target,X_f}} + d_1^- - d_1^+ = 1$$

Goal 2:

- Maximize DCI for Ferrite Grain Size

$$\frac{DCI_{D_\alpha}\,(\mathrm{x})}{DCI_{Target,D_\alpha}} + d_2^- - d_2^+ = 1$$

Goal 3:

- Maximize DCI for Pearlite Interlamellar Spacing

$$\frac{DCI_{S_O}\text{ (x)}}{DCI_{Target,S_O}} + d_1^- - d_1^+ = 1$$

where DCI(x) = $\{URL - f_0(x)\}/\Delta Y$

where $\Delta Y = \sum_{i=1}^{n} \left|\frac{\partial f_0}{\partial x_i}\right| \Delta x_i$

Variable Bounds

Defined in Table 7.8

Bounds on deviation variables

$$d_i^-, d_i^+ \geq 0 \text{ and } d_i^- * d_i^+ = 0 \text{ , i} = 1,2,3$$

Minimize

We minimize the deviation function

$$Z = \sum_{i=1}^{3} W_i(d_i^- + d_i^+);\ \sum_{i=1}^{3} W_i = 1$$

On exercising the cDSP for different design scenarios and carrying out robust solution space exploration, following the steps in Concept Exploration Framework, we obtain the combinations for CR and D, the variables from Processing space that best satisfy the microstructure requirements in the presence of model parameter uncertainty. The cDSP formulated for microstructure space is exercised for 13 different scenarios (same Scenarios as in Table 7.6) by assigning weights to the goals. In Figure 7.12, we show the robust solution space Goal 1. Our interest in Goal 1 is to achieve high DCI value for X_f. The ternary space is made of $DCI_{X_f} \geq 1$ ensuring robust solutions under model parameter uncertainty associated with the design variables. We identify the region with $DCI_{X_f} \geq 7$ as the robust region of interest under uncertainty as shown in Figure 7.12.

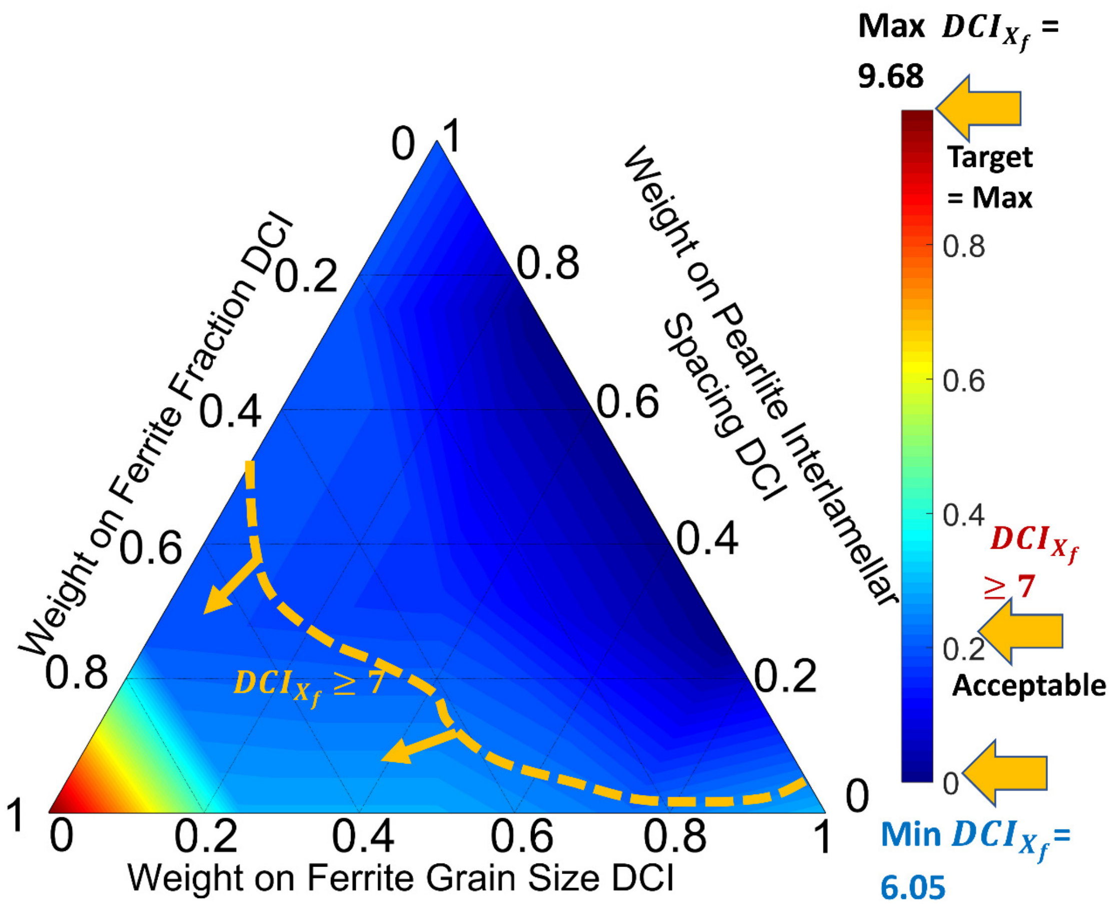


Figure 7.12: Robust solution space for X_f

For Goal 2, our interest is to achieve high DCI value for D_α. The ternary space obtained after executing the cDSP for different scenarios is made with $DCI_{D_\alpha} \geq 1$ ensuring a robust solution region, see Figure 7.13. From this space we define a region with $DCI_{D_\alpha} \geq 9.5$ as our robust region of interest. It can also be seen that the DCI target of 10 is achieved very closely by D_α for the given design configuration.

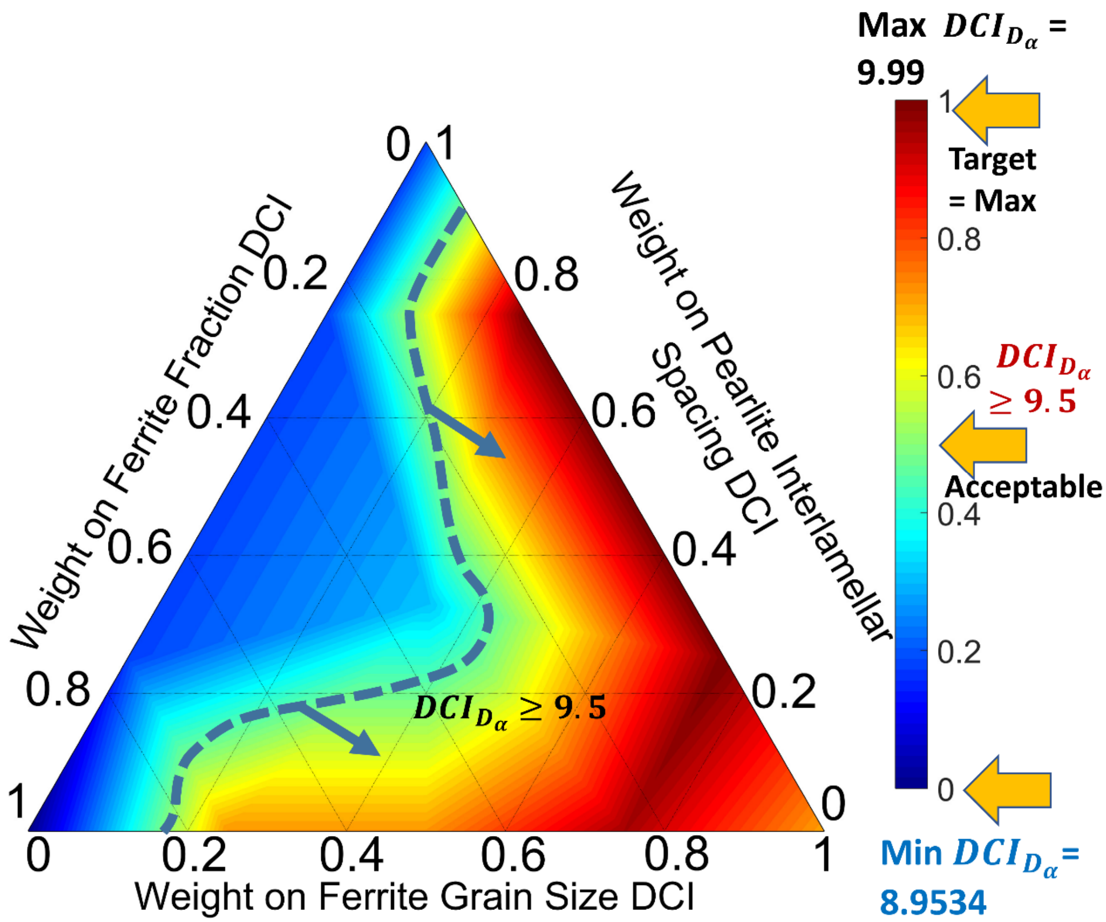


Figure 7.13: Robust solution space for D_α

Similarly, we identify the region with $DCI_{S_O} \geq 150$ as our robust region of interest for Goal 3 on Pearlite Interlamellar Spacing as shown in Figure 7.14.

To identify satisficing robust solution regions for microstructure, superimpose the plots in Figure 7.15 with the all the robust solution spaces of interest. In the superposed ternary plot, we see that the light-yellow region satisfies all the identified microstructure requirements under model parameter uncertainty. To analyze further we pick 3 solution points from the region identified, solution points A, B and C. The results associated with the selected points are summarized in Table 7.9.

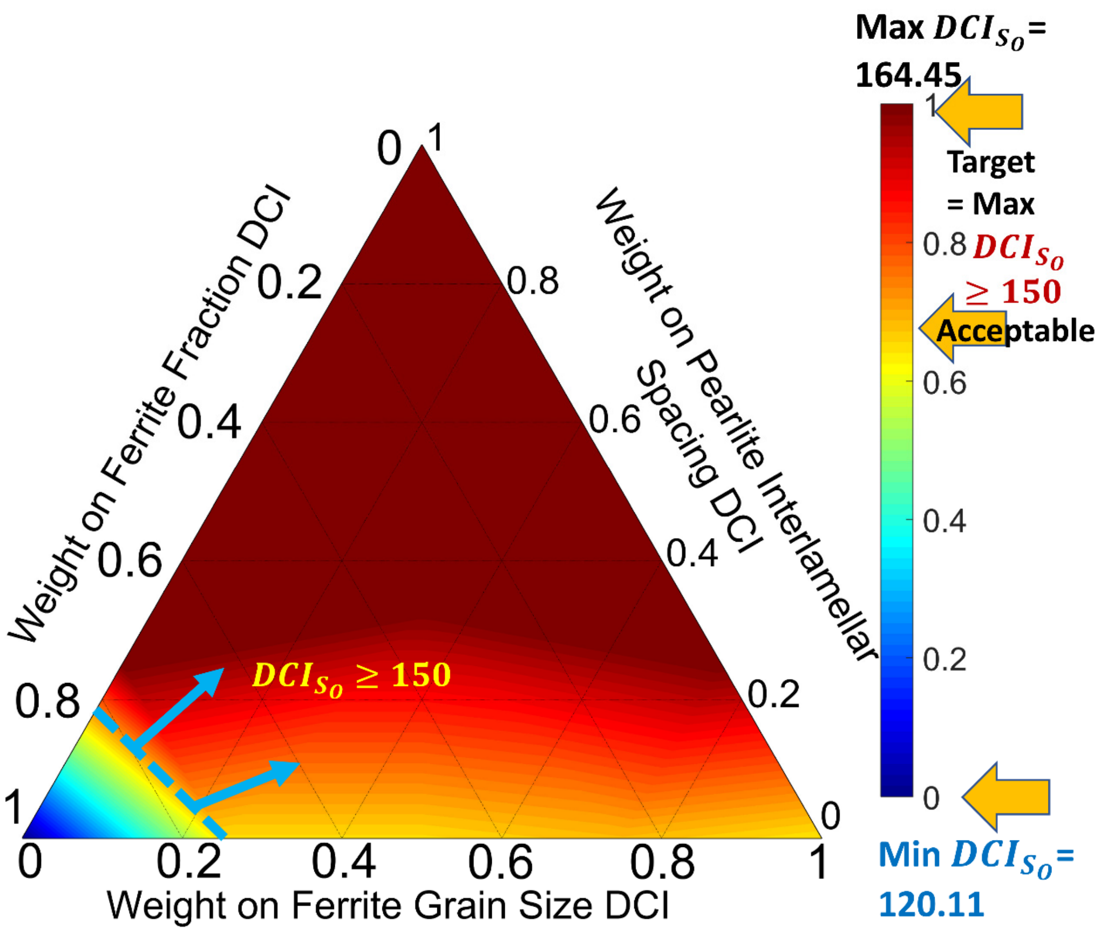


Figure 7.14: Robust solution space for S_O

Table 7.9: Solution Points Selected

Sol. Pts	**Factors from Processing Space**		**Microstructure Space**		
	CR K/min	***D*** μm	X_f	D_α μm	S_0 μm
A	94	46	0.69147	13.1038	0.176
B	93.9	46.	0.691	13.103	0.1763
C	93.7611	45.7	0.69125	13.0554	0.1763

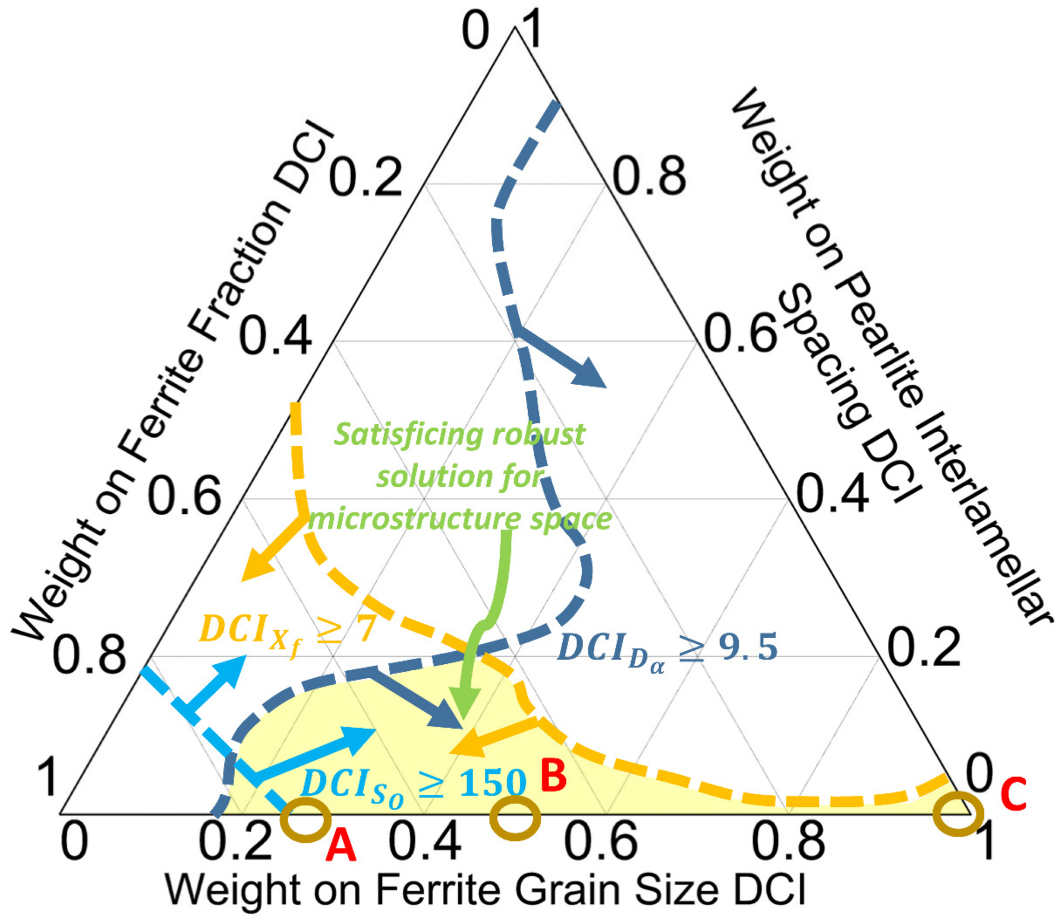


Figure 7.15: Superposed robust solution space

On analyzing the results in Table 7.9, we see that the solutions identified from the satisficing robust region in the ternary space show very little deviation in performance from each other. The processing variable values associated with the solution points in this region will give robust solutions of microstructure under the model parameter uncertainty considered in this design problem.

Thus, using this proposed inverse method, the designer is able to carry out top-down driven, decision-based robust design exploration of processing paths and material microstructure to satisfy a ranged set of product-level performance requirements. The inverse method proposed is generic and can be applied to similar problems with information flow from one process to another to design the system under different types of uncertainty classified in this dissertation.

7.7 Discussion: Robustness Under Model Structure and Model Parameter Uncertainty Using EMI and DCI

In this section, we discuss the usefulness of the robust design metrics EMI and DCI used in this chapter for designing a system under model structure and model parameter uncertainty. To illustrate the same, we use the Yield Strength model proposed by Gladman and coauthors (Equation 7.9), which we used as the mean response function for YS in the cDSP formulated for Property-Performance space. We explore three formulations: In the first, we formulate a single goal cDSP with EMI for the Yield Strength mean model with the uncertainty bounds defined by the yield strength models by Hodgson and Gibbs (Equation 7.10) and Kuziak and coauthors (Equation 7.11; the formulation is same as in first cDSP, expect there is only one goal which is for maximizing the EMI for Yield Strength). In second, we formulate a single goal cDSP with DCI goal for the Yield Strength mean model with consideration of only model structure uncertainty defined in first cDSP. Third, we formulate a single objective optimization problem for maximizing the mean Yield Strength function. The results associated with this comparative study are plotted in Figure 7.16 with Ferrite Fraction and Ferrite Grain Size as the input factors for the Yield Strength model. We see that the cDSP with EMI predicts a mean response value of 288.755 MPa. The corresponding EMI value for the solution point is 2.63568. The formulation with DCI predicts yield strength at 306.08 MPa and is higher than the EMI prediction.

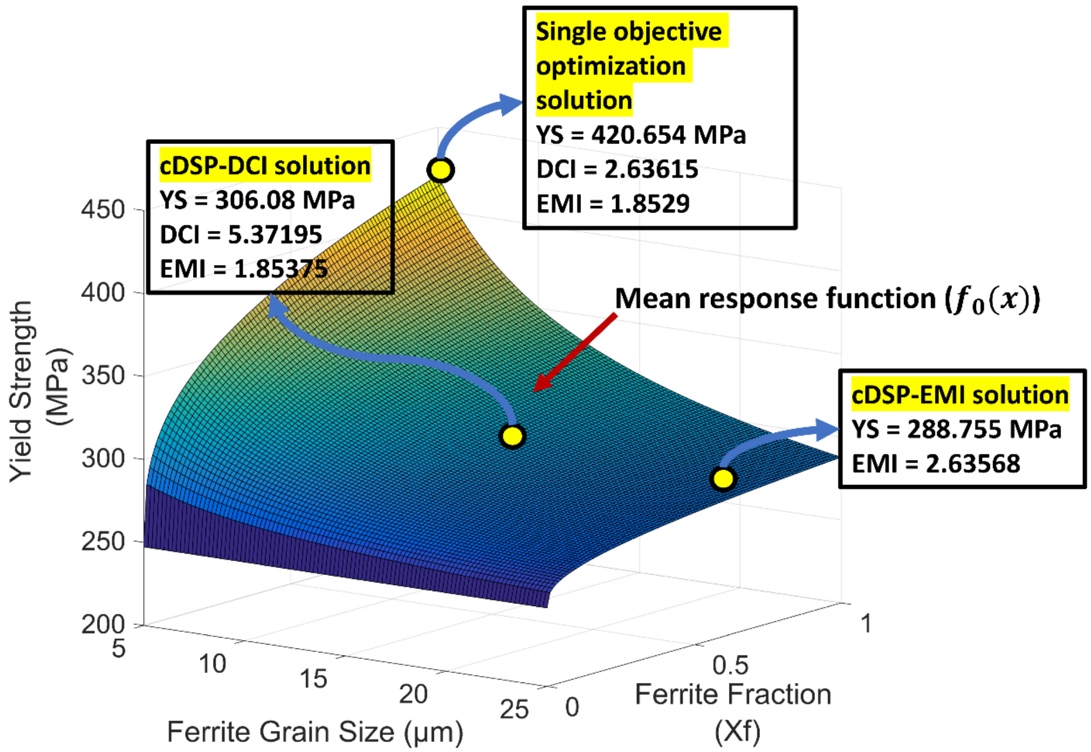


Figure 7.16: Solutions obtained for Yield Strength as single goal using different formulations – a comparative study

The DCI value at this point is 5.37195. However, the EMI value when calculated is only 1.85375. This means that the EMI is less for the solution point that is identified using DCI formulation compared to the solution point identified using an EMI formulation. The reason here is because the DCI formulation overlook the uncertainty associated with the model and thus achieve a lower EMI values for the design solutions. Next, on analyzing the solution obtained via the single objective optimization formulation, we see that optimal solution predicts the highest response for yield strength (YS=420.654 Mpa). However, both the DCI and EMI values are low for the optimization solution point when calculated meaning the optimal solution points obtained are prone to both model structure and model parameter uncertainty and are less robust compared to the solutions obtained via cDSP-DCI and cDSP-EMI.

As discussed in this section, the advantage of EMI and DCI formulations for complex material-product and process systems is because the design solutions will be more robust against model structure uncertainty and model parameter uncertainty thus ensuring the propagation of robust solutions across process chains. The limitation here with the EMI and DCI would be the inability to capture the designer's preference since the EMI and DCI are calculated as a combination of mean and response variations. This limitation can be overcome by separating the mathematical combinations of mean and performance variance and formulating them as two individual goals in the cDSP and repeating the same for multiple goals.

7.8 On Verification and Validation

Theoretical Structural Validation

Theoretical structural validation refers to accepting the validity of individual constructs of error margin index and design capability index and accepting the internal consistency of the way the constructs are put together with the concept exploration framework and the goal-oriented inverse design method. Theoretical structural validation involves systematically identifying the scope of the two construct's application, reviewing relevant literature and identifying the research gaps that is existing, identifying the strengths and limitations of the constructs used based on literature review, determining the constructs and approaches that can be leveraged for robust concept exploration, reviewing literature on the advantages, disadvantages and accepted domains of application, and checking the internal consistency of the constructs both individually and when integrated.

In Chapter 3, robust design is reviewed in detail. Robust design from the perspective of materials and products is reviewed first in Section 3.4. This is followed by reviewing the different classification of uncertainty – from the perspective ICME, multiscale modeling and engineering systems design. A detailed review of robust design is then carried out starting with the work of Taguchi in Section 3.4.2. The significance of Taguchi's work is emphasized, and the associated criticisms and limitations are highlighted. Work carried out by other researcher's on addressing the limitations of Taguchi's approach is reviewed further. A review of Suh's axiomatic design and how the axioms by Suh tie to robust design is addressed next in Section 3.4.3. In this review, the association of robust design to Suh's information axiom is explored and the connection to Shannon's information theory is established. Further review is carried out on Robust Design Type II proposed by Wei Chen in Section 3.4.4. The Design Capability Index (DCI) is introduced and reviewed in detail along with the Robust Concept Exploration Method (RCEM). The utility of the index in Robust Design Type II for a single goal is addressed. This is followed by the review of Robust Design Type III in Section 3.4.5. The Error Margin Index (EMI) is reviewed further, along with RCEM-EMI for robust design type III of systems with a single goal. The capabilities of EMI for type III robust design is reviewed and the limitations associated are discussed. In Section 3.4.6, robust design across process chains is discussed. The Inductive Design Exploration Method is reviewed in this section as a method that facilitates robust design during propagation of uncertainty. The limitations associated with IDEM is reviewed here and the need for an approach for robust design across process chains is established. In Chapter 7, robust concept exploration of materials, products and manufacturing processes is proposed.

The proposed robust concept exploration approach is shown in Figure 7.5. The modified concept exploration Framework and the goal-oriented inverse design method that supports robust concept exploration is shown in Figure 7.1 and 7.4 respectively. The details of the framework and the design method with description of each steps to be performed to formulate, exercise and explore a complex systems design problem in a robust manner using the metrices of EMI and DCI are provided in Chapter 7. The input needed, and the output generated is clarified, the internal information flow is checked to ensure sufficient information availability to execute next steps. Through critical evaluation of each step and the way individual constructs are put together, internal consistency of the concept exploration framework and the inverse design method is verified and accepted.

The theoretical structural validity of the robust concept exploration of process chains is accepted by the logical procedure of literature review, gap analysis and development and evaluation individual and integrated constructs like the DCI, EMI and modified CEF. Empirical studies need to be carried out to establish the usefulness and effectiveness of the framework and the method.

Empirical Structural Validation

Empirical structural validation involves accepting the appropriateness of the example problems used to verify the performance of the framework and the method. In Chapter 7, the robust concept exploration of process chains using the cDSP-EMI-DCI constructs and GoID method is illustrated using the comprehensive example problem discussed in Chapter 6. The example problem is reformulated using robustness metrics of EMI and

DCI. Specific robust design constraints and goals are defined to achieve Type I, II, and III robust across process chains for multiple conflicting goals.

Empirical Performance Validation

Empirical performance validation consists of accepting the usefulness of the outcome with respect to the initial purpose and accepting that the achieved usefulness is related to applying the robust design metrics, goals and constraints. Key functionalities of the cDSP with EMI-DCI combination metrics and corresponding robust design goals and constraints include:

- Type I, II, III Robust Design across process chains for multiple conflicting goals
- Design a complex system insensitive to the different types of uncertainty and provide decision support
- Managing uncertainty in the system without removing the sources
- "*Satisficing*" robust design solutions through solution space explorations and trade-offs
- Goal-oriented, inverse, design exploration of production stages to achieve end performance goals and requirements of products – Generic - can be applied to achieve robust product development.

The verification and validation aspects discussed in this Chapter 7 are summarized in Figure 7.17.

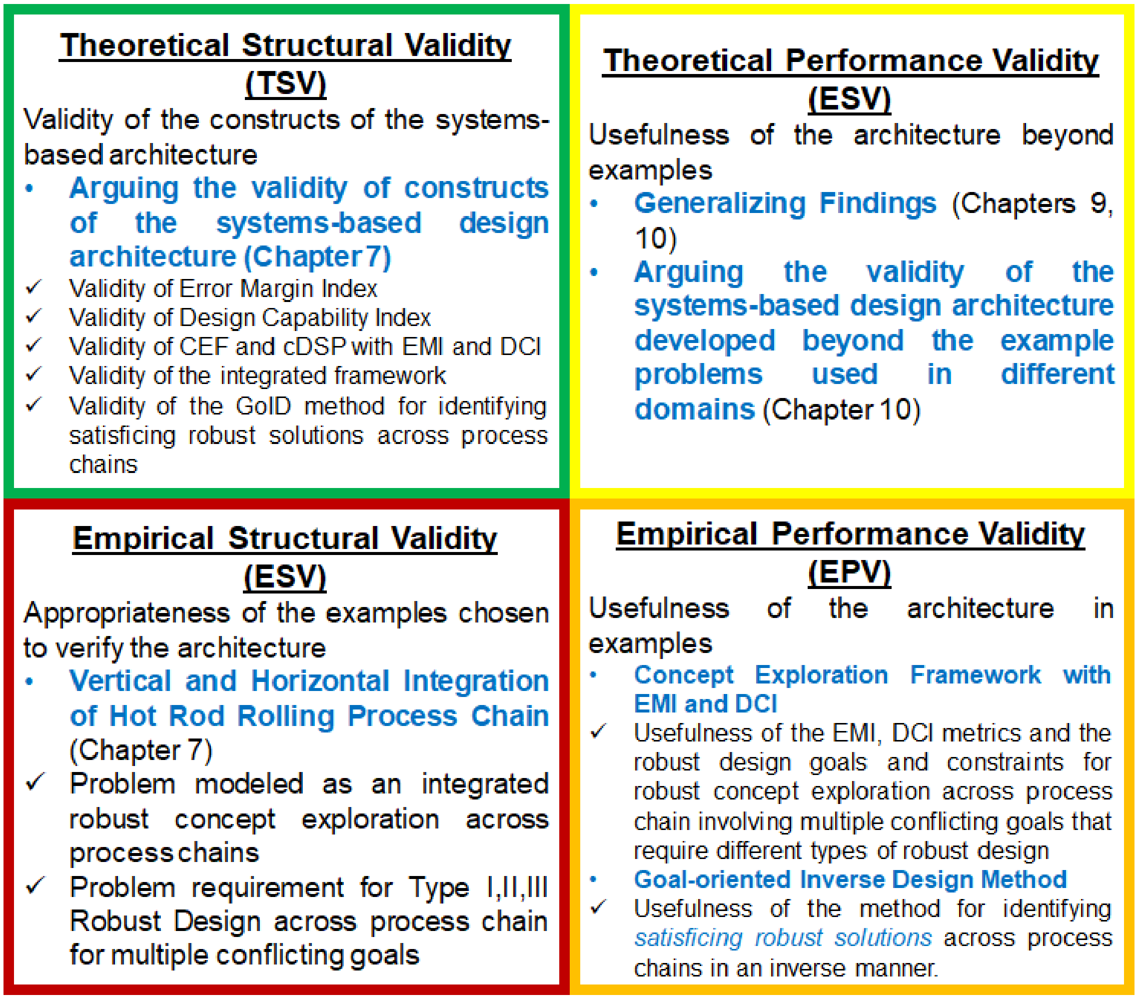


Figure 7.17: Verification and validation aspects addressed in Chapter 7

7.9 Role of Chapter 7 in this Dissertation – Remarks based on robust concept exploration using comprehensive example problem

In this chapter, we present robust concept exploration using a goal-oriented, inverse decision-based design method to carry out the integrated design of material, product and associated manufacturing processes by managing the uncertainty involved. The method is goal-oriented and inverse because we start with the end mechanical properties of the product and inversely maps the requirements to microstructure and processing spaces of the material to identify *satisficing robust solutions* across process chains. We introduce a variation to the inverse decision-based design method to bring in robustness for multiple goals from the stand-point of Type I to III robust design across process chains. The variation embodies the introduction of specific robust design goals, constraints and metrics to determine ‘‘*satisficing robust design*’’ specifications for given performance requirement ranges using the goal-oriented, inverse design method. The utility of the proposed method is demonstrated by carrying out the solution space exploration of the processing and microstructure spaces of the rolling and cooling processes to identify satisficing robust solutions that realize the end mechanical properties of the rod product. Functionalities of the method supported by the CEF include:

- rapid, concurrent "robust" design exploration of material and products using simulation models that are typically incomplete, inaccurate and not of equal fidelity,
- supporting the systems-based inverse robust design exploration of material microstructures and processing paths to meet multiple performance/property requirements,
- coordination of information and human decision making,
- capability to prioritize models, input factors, output responses and their associated variabilities with consideration of robustness, and
- ensuring feasible robust satisficing solutions by managing uncertainty.

Functionalities of the cDSP with EMI-DCI combination metrics and corresponding robust design goals and constraints include:

- Supporting a human designer under complex material system's random variability and/or model parameter uncertainty and/or model structure uncertainty in making decisions that satisfies multiple conflicting goals,

- Managing uncertainty in the system without removing the source and supporting in identifying robust design solutions across process chains, and
- Ensuring the identification of robust solution space using robust solution constraints. The designer can explore this space to further identify satisficing robust design specifications.

The functionalities offered by GoID with robustness compared to other top-down design methods like IDEM is listed in Table 7.10 based on the work carried out in this chapter. The limitations of IDEM is identified by testing the utility of IDEM for a hot rolling design problem. The testing carried out is included in Appendix B of this dissertation.

Table 7.10: IDEM vs GoID with Robustness

Limitations of IDEM **(See Appendix B for details)**	**Functionalities offered by Goal-oriented Inverse Design Method with Robustness**
• Error due to discretization of design space – IDEM uses discretization of design space and further inductive discrete constraints evaluation for mapping from one space to another – this leads to discretization errors and also inability to capture the feasible boundary accurately – resulting in	• Specific robust design goals and constraints anchored in the mathematical constructs of Error Margin Indices (for Type I, II, III RD) and Design Capability Indices (for Type I, II RD) are introduced to determine ‘‘*satisficing robust solutions*’’ for **multiple conflicting goals** across

loss of information affecting system performance. • Increasing accuracy by increasing the resolution of discrete points results in highly computationally expensive IDEM runs for evaluating feasible spaces. • There is limitation in terms of the number of design variables that can be used in IDEM for a design problem under study. The number of design variables increases the discrete points to be evaluated in the order of power – virtually impossible to evaluate beyond 9 variables for an IDEM study. • Limitation in terms of exploration and visualization – IDEM uses a three dimensional visualization space using HD-EMI metric for exploration where only a maximum of 3 design variables can be studied at a time with the	process chains (for Type I, II, III across process chains). • No limitation in terms of design variables that can be studied. • Perception of a robust design space – augmenting the human ability to make design decisions - visualize a solution space and make logical judgements through trade-offs to identify satisficing robust solution regions that are further propagated as goals and requirements to next cDSPs to establish the process chain. • Propagation of end goal requirements (product performance or properties) across a process chain with the designer having the capability to check whether the end goals are actually achievable at previous spaces in their current configuration or not – designer can recommend

others variables taking defined values – this limits the scope of the simulation study and results. • Issue of flexibility in design – IDEM do not allow designers to incorporate new goals or requirements at different levels during the process of design as the method is based on mapping to feasible spaces of 'Y' and 'X' for a given 'Z' space.	adjustments in the design space if needed. Capability to define new goals and requirements at each level as the method uses individual cDSPs to facilitate information flow allowing to formulate a design space at each level – flexibility in design

Chapter 8: PDSIDES – A Knowledge-Based Platform for Decision Support in the Design of Engineering Systems

8.1 Frame of Reference – Answering Research Question 4

This section was briefly discussed in Chapter 1. We discuss in detail here. Design is increasingly recognized as a decision-making process (Daskilewicz and German 2012, Afshari, Peng and coauthors 2016, Berg and Vance 2016, Soria, Colby and coauthors 2017). We believe that the principal role of a human designer is to make decisions. Providing decision support is of critical importance for augmenting this role, by speeding up the design process and generating quality designs. One of the challenges in providing decision support in the design of engineering systems, especially complex systems that are, by definition, made up of inter-related subsystems (Kuppuraju, Ganesan and coauthors 1985), arises because of the complexity embodied in the decision workflows that embody multiple coupled decisions networked in various degrees of complexity. The networked decision workflows may include different types of decisions, e.g., selection of design alternatives and improvement of an alternative considering multiple goals. The decisions are coupled together due to the dependency existing among systems and subsystems. The different types of decisions and their associated dependencies in the decision workflows make it difficult to provide appropriate decision support.

Decision making is a knowledge-intensive process, with knowledge playing a significant role in speeding up and affecting decisions. Design knowledge representation for conceptual and detailed design have been areas of interest in knowledge-based design and engineering for many decades. However, most of the works on knowledge representation deal with design in general (CAD oriented), not in the context of supporting decisions. For example, Shah and Mäntylä (Shah and Mantyla 1995) introduced the parametric and feature-based methods which has specific data structures and algorithms embedded to facilitate rapid and reusable 3D geometric model generation. While, the parametric, feature-based procedure knowledge representations introduced in (Shah and Mantyla 1995) cannot be (at least not directly be) applied to represent the human decision-making processes in design. Coyne and coauthors (Coyne, Rosenman and coauthors 1990) propose a prototype-centric framework for the development of knowledge-based design systems. In their framework, prototypes can be generated, refined and adapted to create novel designs. However, the design decision-making processes are not addressed in their work. Figer and Dixon (Finger and Dixon 1989) reviewed many descriptive, prescriptive, and computer-based models of design processes in the late 1980s with the aim to create intelligent CAD expert systems. Human decision-making process is not emphasized and well analyzed but just lightly mentioned as "concept selection" with no detailed information in their review. Verhagen and coauthors (Verhagen, Bermell-Garcia and coauthors 2012) analyzed a total of 50 research contributions in the area of Knowledge-Based Engineering (KBE), pointed out the challenges and suggested some future research opportunities in the field. However, the goal of the total 50 KBE research contributions, as stated by the authors, is to automate the product design and development process, but not support designers making better decisions. Similarly, Rocca (Rocca 2012) provided an extensive review of KBE from a language-based technological perspective, the aim being to understand what the technological fundamentals of KBE are and how it can be used to automate large portions of the design process. One thing in this paper that is related to decision-making is that

KBE is used to develop multi-model generators in MDO, but the compromise decision (i.e., the tradeoff) among multidisciplinary models is not discussed. Jakiela and Papalambros (Jakiela and Papalambros 1989) from University of Michigan introduced a prototype "intelligent" CAD system, in which decision-making process during the conceptual design is programmed using production rules to automatically generate 3D models. While this system provides knowledge-based automatic decision making in design, the limitation is that it only accounts for geometrical modeling. Sapuan (Sapuan 2001) presented a knowledge-based system for material selection. However, the decision process and associated knowledge representation language are domain specific thus not reusable and extensible.

Despite the fact that many knowledge-based systems have been developed to support engineering design, the challenge of supporting the decision workflow in the design of complex engineering systems is not yet well addressed, mainly, for the following reasons:

1) Lack of a both reusable and executable decision knowledge representation schemes. Knowledge reusability is critical for adaptive and variant design wherein only a small portion of the original decision workflows need to change while the rest remains the same and can be reused. Some authors have proposed to represent decision knowledge as ontologies (e.g., (Rockwell, Grosse and coauthors 2010)), but they mainly focus on capturing the semantic information of design decisions while failing to represent the execution process information which is necessary for effecting new decisions, especially in a computational environment whereby some degree of automation is realized.

2) Lack of a classification of users for decision support. The needs of designers for decision support vary according to how much novelty is involved in the design and how much knowledge they have about the design process. For example, an expert has much knowledge about design and can perform the decision-making process independently, thus the support this designer needs from the computer system is very different from a novice designer who only has the basic knowledge about design and needs to get most of the knowledge from the system. Very few of knowledge-based systems recognized this difference and provide appropriate decision support.

To address the aforementioned needs, we propose a Knowledge-Based Platform for Decision Support in the Design of Engineering Systems (PDSIDES). The new contributions embodied in this work are summarized as follows:

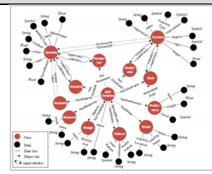
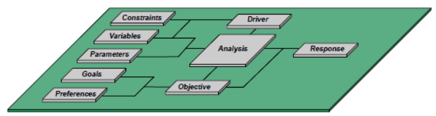
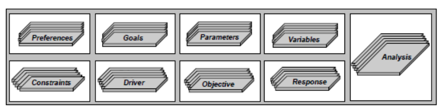
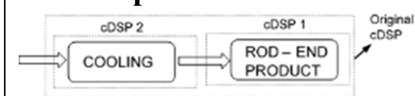
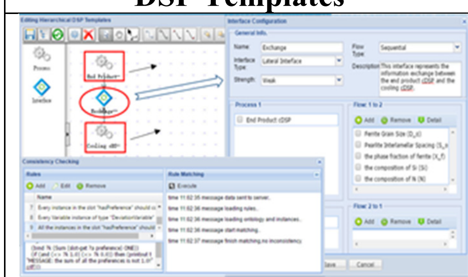
- We integrate the decision-related knowledge that is modeled as Decision Support Problem (DSP) templates and represented using ontologies in our earlier works (Ming, Yan and coauthors 2016, Ming, Wang and coauthors 2017, Ming, Wang and coauthors 2017) into a computational platform (PDSIDES) to facilitate extensive reuse and execution. Thus, in this chapter the focus is on platformization.
- We define three types of users, namely *Template Creators, Template Editors*, and *Template Implementers*, who perform *Original Design, Adaptive Design,* and *Variant Design* respectively in PDSIDES.
- We provide customized decision support for human *Template Creators, Template Editors*, and *Template Implementers* during their design of engineering systems in PDSIDES.

Chapter 8 is organized as follows. In Section 8.2 we introduce the primary constructs used in PDSIDES by referencing our previous work to provide the context. In Section 8.3 we describe the design of PDSIDES, including platform overview, users and working scenarios, knowledge-based decision support. The technical implementation of PDSIDES is introduced in Section 8.4. In Section 8.5 we illustrate the efficacy of PDSIDES using a Hot Rod Rolling System (HRRS) design example. In Section 8.6 we offer some closing remarks and enumerate future research opportunities. A portion of Table 1.6 that is relevant to this chapter is reproduced in Table 8.1. We revisit the research question and research hypotheses in Table 8.2.

Table 8.1: Research Question and Research Hypotheses 4 addressed in Chapter 8

Secondary Research Question 4	Research Hypothesis 4
RQ4. What are the foundations needed for maintaining ***structural consistency*** of the decision-based design workflow for the manufacturing process chain involving the material and product, ensuring ***robust, flexible and modifiable*** decisions while incorporating newer ***data, information and knowledge*** associated with the system?	***H4.1.*** Using ontology to represent decision-related knowledge that is modeled as Decision Support Problem (DSP) templates can capture, analyze, archive and update the decision-based design workflow as per the needs of the individual decision-maker. Separation of declarative (problem specific) knowledge and procedural (process specific) knowledge in the information flow scheme can help in generalizing the decision models in the design workflow (To address **G6**). ***H4.2.*** Defining three types of users, namely Template Creators, Template Editors, and Template Implementers, and providing customized decision support to these users during the design of engineering systems can help perform original design, adaptive design, and variant design respectively (To address **G7**).

Table 8.2: Requirements, constructs of PDSIDES, and associated hypothesis validated in Chapter 8

Requirements	Constructs of the Systems-based Design Architecture developed in this Dissertation	Research Hypotheses	Validation Examples
1.Knowledge capture and reuse 2.Facilitation of original, adaptive and variant designs .	   **Ontology to represent decision-related knowledge modeled as DSP Templates**	**RH4.1.** Ontology to represent decision-related knowledge that is modeled as Decision Support Problem (DSP) templates can capture, analyze, archive and update the decision-based design workflow	1. Steel Manufacturing Process Chain Problem – **Focus on cooling process and end rod product** 
	 **Editing Design Templates in PDSIDES**	**RH4.2.** Defining three types of users, namely Template Creators, Template Editors, and Template Implementers, and providing customized decision support to these users during the design of engineering systems can help perform Original Design, Adaptive Design, and Variant Design respectively.	

8.2 Primary Constructs used in PDSIDES

8.2.1 Decision Support Problem

PDSIDES is designed from a Decision-Based Design (DBD) perspective, wherein decisions serve as markers to identify the progression of a design from initiation to implementation to termination (Mistree, Smith and coauthors 1990). We recognize that the implementation of DBD can take many forms, such as (Hazelrigg 1998); our implementation being the Decision Support Problem (DSP) Technique (Muster and Mistree 1988). Key to the DSP Technique is the notion that there are two types of decisions, namely, selection and compromise, and that a complex design can be represented by modeling a workflow of compromise and selection decisions. The selection DSP (sDSP) (Mistree, Lewis and coauthors 1994) involves making a choice among a number of alternatives taking into account a number of measures of merit or attributes, while the compromise DSP (cDSP) (Mistree, Hughes and coauthors 1993) involves the improvement of an alternative through modification by making a trade-off among multiple design objectives. The sDSP and the cDSP are two fundamental decision-making constructs in PDSIDES.

The design of complex systems may require the formulation and resolution of a series of coupled decisions, in which case the hierarchical DSP construct based on the sDSP and the cDSP is used as the model to support hierarchical decision making, for the detailed mathematical model see (Smith 1985, Bascaran, Bannerot and coauthors 1987). Key to the hierarchical DSP is the combination of all the DSPs (including sDSPs and cDSPs) simultaneously by reformulating the DSPs into a single cDSP. Hierarchical DSPs are generally multiobjective, nonlinear, mixed discrete-continuous problems. A tailored computational system known as DSIDES (Reddy, Smith and coauthors 1996) is integrated into PDSIDES to solve such problems.

8.2.2 Decision Template

One of our primary goals in designing PDSIDES is that designers can rapidly create decision models for the specific design problems they have by using the DSP constructs, and making decisions, and finally the produced decision knowledge can be stored and reused by other users for similar designs. To achieve this goal, the DSPs are represented as computational decision templates in PDSIDES. Decision templates, originally proposed by Panchal and co-authors (Panchal, Fernández and coauthors 2004), make it possible to model the compromise DSP so that the template is reusable and computer interpretable. We extend the idea to model the selection DSP and hierarchical DSP as templates in our earlier work (Ming, Wang and coauthors 2017, Ming, Wang and coauthors 2017). Key to the computational DSP templates is the modularization of the DSP constructs and the separation of declarative and procedural knowledge, which allows both to be reused across problems.

In PDSIDES, all the DSP template modules including the sDSP template modules such as alternatives, attributes, etc., the cDSP template modules such as constraints, variables, etc. and the hierarchical DSP template modules are managed in the module repository, as shown in Figure 8.1. It is noted that the sDSP template and the cDSP template are also defined as a particular type of module since they comprise the key "building blocks" of a decision hierarchy and can be linked together using the *interface* and *process* modules, see (Ming, Wang and coauthors 2017) for details. Template modules represent the declarative knowledge in PDSIDES, which embodies problem specific information and can be reused in the instantiation of DSP templates (the wired "boards") to support a designer making selection, compromise, and hierarchical decisions. The procedural knowledge denotes how specific information is processed to reach a decision and is archived in the templates (the printed "wiring" between different modules) for the execution of decisions. The separation of these two types of knowledge makes it fairly easy for designers to reconfigure existing templates, which is critically important in adaptive and variant designs where design consideration changes and the original decision model needs to be modified. Template modification is discussed in Section 8.3.

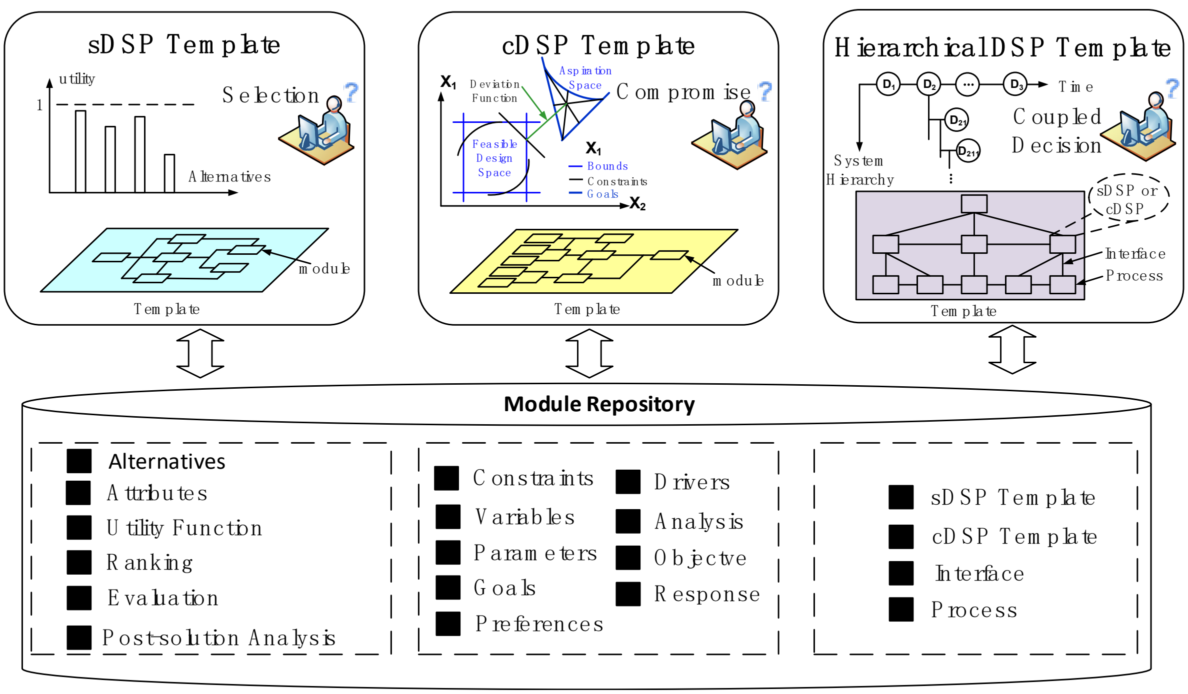


Figure 8.1: DSP Templates And their Associated Modules

8.2.3 Ontology

In order to store and reuse the knowledge archived in the DSP templates in a computational environment, there needs to be a formal representation scheme. Ontologies are defined by Gruber (Gruber 1993) as explicit formal specifications of terms and relations among them, are increasingly used for knowledge modeling in engineering design, such as (Rockwell, Grosse and coauthors 2010, Zhan, Jayaram and coauthors 2010). In PDSIDES, ontology is used to formally represent the knowledge (including declarative and procedural knowledge) archived in the DSP templates. Key elements of an ontology are terms and relations. Terms represent the components of a domain, which refers to the modules of the DSP templates. According to Li and co-authors (Li, Raskin and coauthors 2008), the grain sizes of terms in an ontology are determined by the consideration of the need for an application or computational complexity. In PDSIDES, to comprehensively capture the semantics of the DSPs, we introduce some additional terms, such as *coefficient, utility calculation* to the sDSP template ontology (Ming, Wang and coauthors 2017) and *quantity, function* to the cDSP template ontology (Ming, Yan and coauthors 2016). Relations in an ontology represent the connections of a term to other terms (e.g., the connecting a *goal* to a *variable* using relation *function-of*), that provide the context of the terms and make them easy-to-comprehend and facilitate communication. The terms and relations in an ontology capture the declarative knowledge which is domain-specific, while some attached elements such as rules, axioms, or Java function calls capture the procedural knowledge which is domain-independent. There are two popular paradigms for ontology formalism, namely, Web Ontology Language (OWL) and Frame (Wang, Noy and coauthors 2006). The Frame paradigm is chosen because it is based on a closed-world assumption wherein everything is prohibited until it is permitted, which is suitable for modeling the highly constrained DSPs. In Frame-based ontology, terms are defined as Classes and relations are defined as Slots. With Classes and Slots, ontologies in PDSIDES are defined as shown in Figure 8.2. On the left-hand side and right-hand side are the cDSP and the sDSP ontologies respectively, which are integrated by the hierarchical DSP ontology in the middle for capturing knowledge related to hierarchical decision workflows. For detailed specification of the Classes and Slots, see our earlier works (Ming, Yan and coauthors 2016, Ming, Wang and coauthors 2017, Ming, Wang and coauthors 2017).

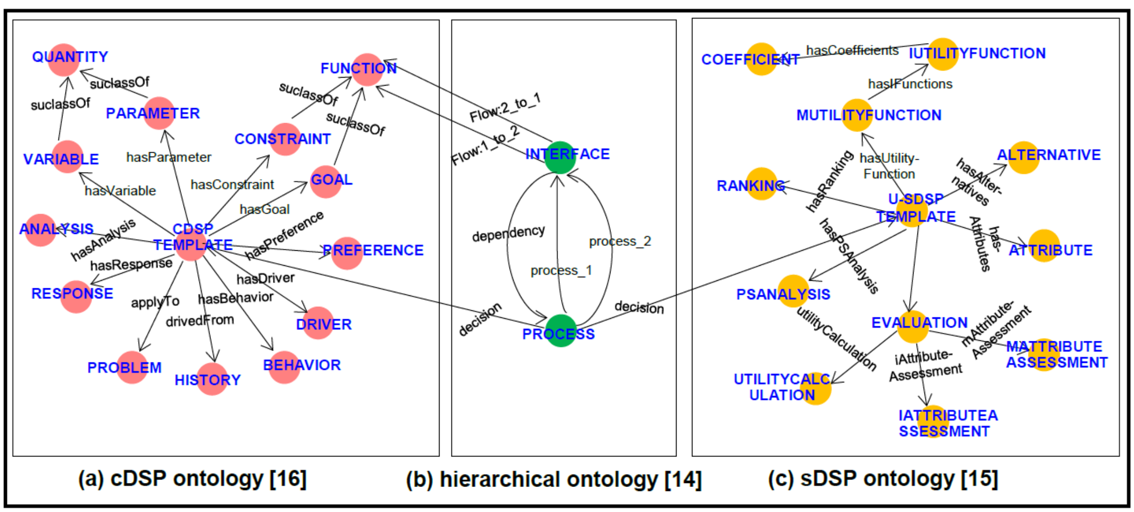


Figure 8.2: Ontologies in PDSIDES

The advantages of the use of ontology in PDSIDES are summarized as follows.

- ***Facilitate knowledge sharing***. This is embodied in two aspects, namely, knowledge sharing among different users in PDSIDES and knowledge sharing between PDSIDES and other Product Lifecycle Management (PLM) platforms. The DSP ontologies represent the common language used for design decision making in

PDSIDES, and thus users from different design disciplines (e.g., thermal, structural, dynamic, etc.) can easily understand, communicate knowledge such as *variables, goals, constraints*, etc., with each other. Meanwhile, the explicit, formal specifications of the terms of the DSP ontologies enables PDSIDES the ability to exchange knowledge with other PLM platforms such as product data management systems and simulation-based analysis systems.

- ***Facilitate knowledge population***. In order for the computational templates defined in Section 8.2.2 to execute and effect real decisions, the modules of the templates must be populated with specific knowledge (or information). The DSP ontologies are the abstractive representations of the templates, which is very convenient for instantiating different instances with specific information.
- ***Facilitate knowledge retrieval***. One of the prerequisites for the reuse of templates and the associated modules is that they can be retrieved from the repository (knowledge base) when needed. The DSP ontologies capture the complex semantic relationships among the modules and templates, which allows it to support semantic based retrieval that can respond to comprehensive query needs. For detail about semantic retrieval, see (Mocko, Rosen and coauthors 2007).
- ***Facilitating consistency maintaining***. Modification of the original templates usually happens in adaptive or variant design, which may lead to inconsistency of the modified templates since the arrangement or values of the modules are changed. The DSP ontologies support rule-based reasoning and appropriately handle the inconsistency, which is discussed in Section 8.3.3.

8.3 Design of Platform PDSIDES

Based on the primary constructs introduced in Section 8.2, the design of Platform PDSIDES is introduced in this section. First, an overview of PDSDES is presented, and then the platform users and their associated working scenarios are defined and described. Finally, we discuss how knowledge-based decision support is provided for different types of users.

8.3.1 Platform Overview

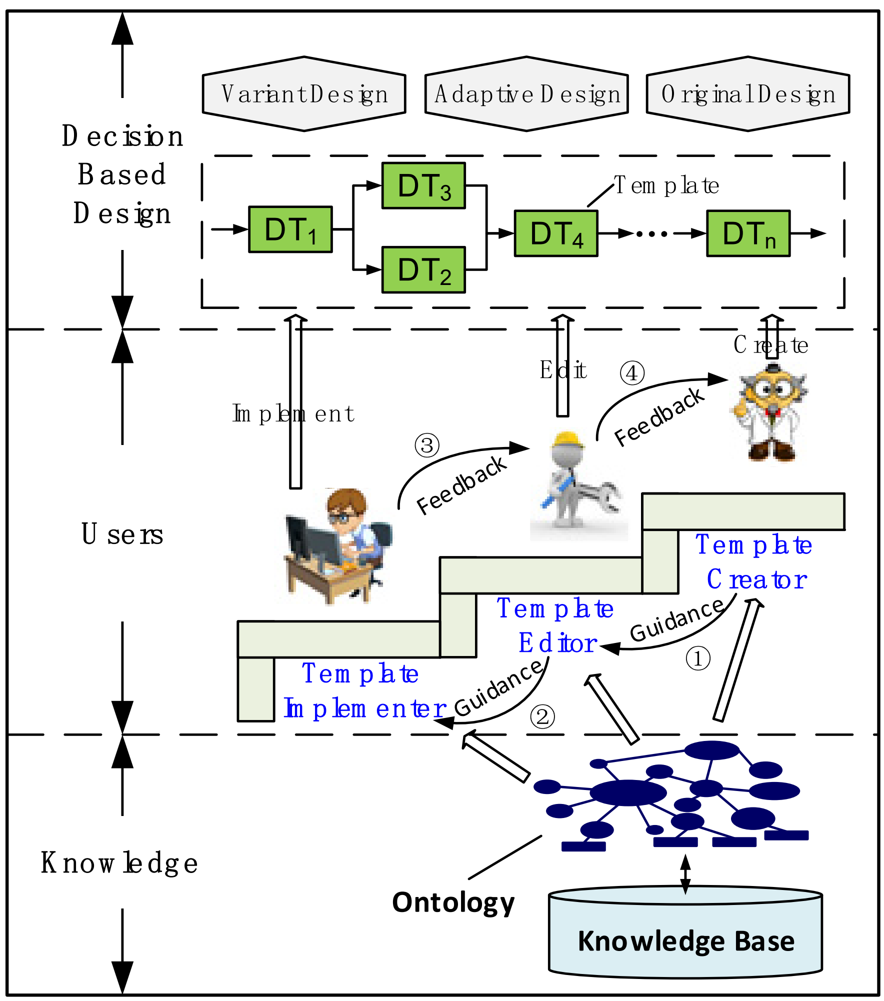


Figure 8.3: PDSIDES Overview

An overview of PDSIDES is illustrated in Figure 8.3. PDSIDES is divided into three parts: knowledge, users, and decision-based design. What follows is the description of the platform from the bottom-up that includes how these three parts are connected to enable the functionalities.

At the bottom of PDSIDES, decision-related knowledge is stored in the knowledge base. The knowledge including declarative knowledge such as *problem statement, alternatives, attributes, variables, parameters, constraints*, etc., and procedural knowledge such as consistency rules and computing codes (for calculating, e.g., expected utility of a sDSP template), are organized by a holistic ontology which is the combination of the three ontologies shown in Figure 8.2. In the middle part are the three types of users, namely, the Template Creator, Template Editor, and Template Implementer, which will be formally defined in Section 8.3.2. The three types of users embody three different levels of knowledge (represented by the stairs in Figure 9.3). The top level is the Template Creator who is responsible for creating the DSP templates, the middle level is the Template Editor who is responsible for editing DSP templates, and the bottom level is the Template Implementer who is responsible for implementing the DSP templates. The interactions among the three types of users are a closed loop, where the template operational guidance is passed downwards from the Creator to the Editor then to the Implementer and the feedback of operating the templates is sent upwards from the Implementer to the Editor and then to the Creator. The creation, edit, and implementation of the DSP templates are all facilitated using the holistic ontology. The top part of PDSIDES is about decision-based design. In PDSIDES design is classified into three types, namely, original design, adaptive design, and variant design; all are realized from a decision-based perspective using the DSP templates. In specific design cases, the underlying decision workflow is represented by networked DSP templates that can be exercised by three types of users through creating, editing, and implementing.

8.3.2 Users and Working Scenarios

The definitions of three types of users are introduced and their associated working scenarios are described in detail in this section.

Template Creator: Template Creators are domain experts and are responsible for creating DSP templates for original design that calls for new concepts. Original design usually needs the working principle of the system to be set up. In PDSIDES, to do original design Template Creators first need to determine what type of decision needs to be made since different types of decisions require different knowledge. For selection decisions, Creators need to come up with the alternatives for selection, attributes to evaluate the alternatives, and utility functions to measure the performance of the alternatives, etc. For compromise decisions, Creators need to identify the variables that represent the features of the system, constraints and bounds that confine the feasible design space, and goals and preferences that determine the aspiration space etc. For hierarchical decisions, in addition to the determination of the “nodes” (which may be selection or compromise) in the decision workflow, Creators also need to identify the dependency and the associated information flows between different “nodes”. The knowledge can be of the Creators’ previous experience, prediction, or results from simulation analysis, etc. With this knowledge, template modules are created and assembled to form decision templates that then are tested and stored for reuse.

Template Editor: Template Editors are senior designers who have sufficient knowledge and experience in a specific domain and are responsible for editing (or tailoring) existing decision templates in adaptive design, this requires the original templates to be adapted for new applications. Adaptive design stands for those design cases in which the working principle of the system remains the same while some design consideration varies due to the evolution of the requirements. For example, a pressure vessel may need to be redesigned to adapt to a new goal of minimizing the economic cost because of the intensive market competition. In PDSIDES, to perform adaptive design Template Editors need to modify existing DSP templates to reflect the change of design consideration. For the sDSP templates, the modification includes adding/removing *alternatives* and *attributes*, reconfiguration of the *utility functions*, etc. For the cDSP templates, the modification includes adding/removing *variables, constraints, goals,* etc. For the hierarchical DSP templates, modification includes three aspects: the first is about modifying the modules within the DSP templates in a decision workflow, the second is about modifying the number DSP templates (adding/removing sDSP or cDSP templates), the third is about modifying the arrangement (sequence, information flow, etc.) of the DSP templates. The editor's knowledge related to the modification is captured in the newly modified DSP templates, which are stored and used for new applications.

Template Implementer: Template Implementers are designers who have basic knowledge and typically little knowledge or interest in the analysis embodied in the template, they are responsible for executing existing decision templates that result in variant designs that require only parametric changes to the original decision templates. Variant design usually happens when the values of some original design parameters vary.

For example, assuming that the original material of a pressure vessel is replaced by some new materials with different *density* and *strength*, the values of parameters *density* and *strength* of the original design model (e.g., the cDSP) need to be updated to reflect the change that will result in a different dimension of the pressure vessel. In PDSIDES, to perform variant design Template Implementers can change the values of the DSP template parameters including: 1) bounds of the sDSP *attributes* or cDSP *variables*, 2) cDSP parameters and targets, 3) relative importance of the sDSP *attributes* and cDSP *goals*. With the change of parameters values, Template Implementers can execute the DSP templates and get variant designs.

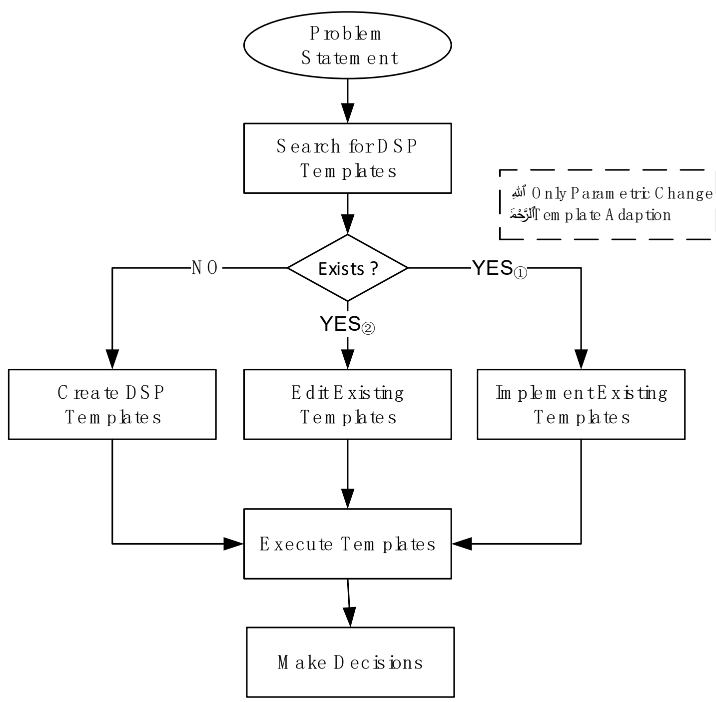


Figure 8.4: Flowchart of Decision Based Design in PDSIDES

It is noted that in PDSIDES users with access to higher knowledge levels also have the access to perform the operations that are defined for users of lower knowledge levels. For example, a Template Creator can be an Editor or Implementer, an Editor can also be an Implementer. With decisions modeled as DSP templates and users classified into three types, the process of decision-based design in PDSIDES is shown in Figure 8.4. A user (e.g., a domain expert) first starts with a problem statement to describe the design problem he/she is faced with, then searches PDSIDES for a DSP template to support the design. In PDSIDES, DSP template searching is a query-based process where a problem statement (a short text) is used as the input and a documented DSP template instance is the output. Both the problem statement and template instances are mathematically represented using the bag-of-word approach (Baeza-Yates and Ribeiro-Neto 2011) during the query process. The similarity between the problem statement and different template instances is measured by a cosine coefficient as shown in Equation 8.1. As this is not the key focus of this chapter, readers are referred to (Salton, Wong and coauthors 1975) for detail.

$$sim(\vec{A}, \vec{B}) = \frac{\vec{A} \times \vec{B}}{|\vec{A}| \cdot |\vec{B}|} \qquad \textbf{Equation 8.1}$$

$\vec{A}$ and $\vec{B}$ are two n-dimensional vectors that represents the word frequencies for the given problem statement and a specific template instance, respectively. It should be noted that the *bag-of-word* characterizing the template instance not only includes words from the textual slots such as "name" and "description", but also words from the structural slots such as "variables" and "constraints", etc. which will make the instance more comprehensive and easier to be matched. If no DSP template instance is matched then a new template needs to be created, execute and make the decision. If there exists some template(s), the designer needs to further determine how much modification needs to be made to the template. If only a change in the nature of a parameter is needed, then the designer just resets the parameter values, executes the template and makes a decision. If more adaption is needed, then the designer needs to do the editing before executing the template and make a decision.

8.3.3 Knowledge-Based Decision Support

The core of PDSIDES is the ontology that integrates the knowledge to support the three types of designers, namely, Template Creators, Template Editors and Template Implementers. In Figure 8.5 we represent how knowledge-based decision support is provided to the three types of designers in their associated working scenarios (taking the cDSP templates as an example).

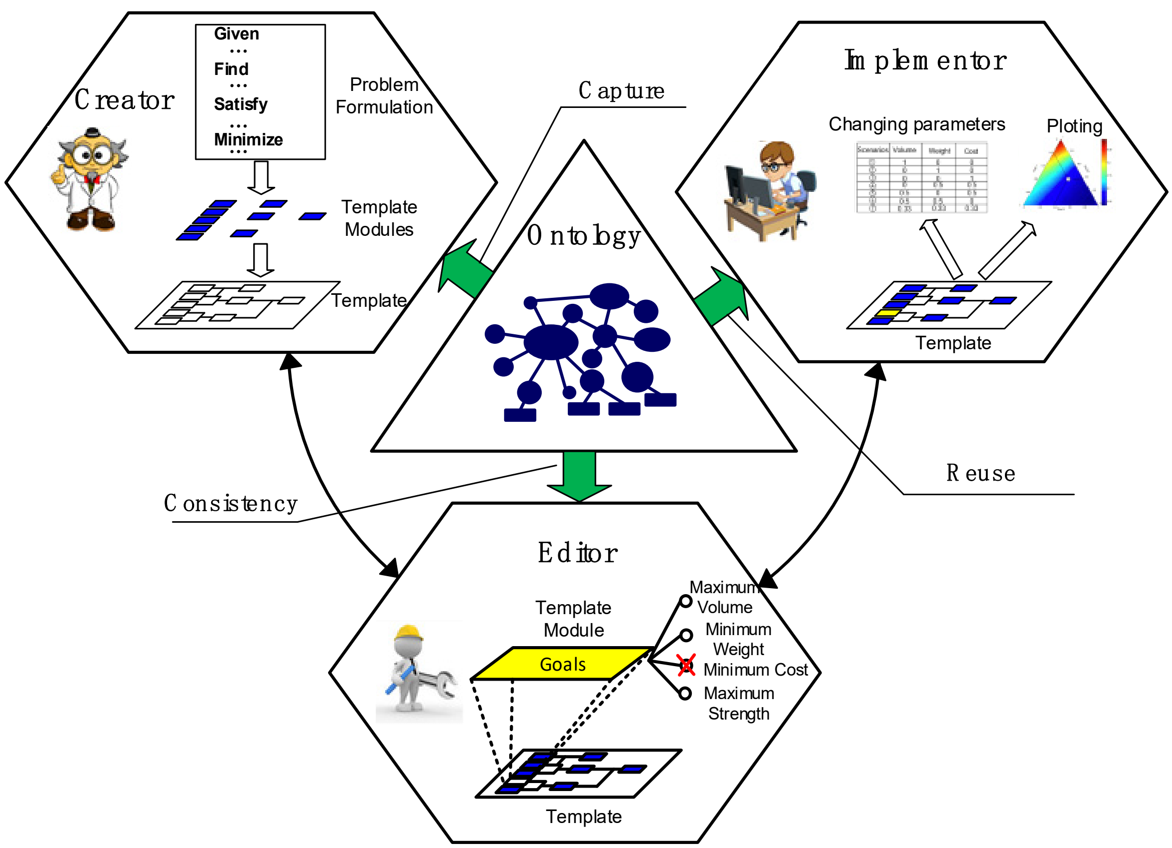


Figure 8.5: Knowledge-based decision support in PDSIDES

Template Creators – *provide the vocabulary to them for modeling decisions and capture knowledge from them*. Template Creators, need a formal language to help them describe and model the decisions for original design. The DSP ontologies in PDSIDES can provide them with the vocabulary to model their decisions. For example, the term *variable* is defined as a Class with several slots including *upper bound, lower bound, unit, value*, etc., which will help specify the module "*variables*" of the cDSP template. Using the classes and slots defined in the ontology, DSP templates can be quickly instantiated as instances, which are captured and stored in the database for reuse, as shown in the top-left picture of Figure 8.5.

Template Editors – *ensure consistency for editing*. As mentioned earlier, modification of existing DSP templates may incur inconsistency, especially when the template is highly complex (e.g., tens of *variables, constraints* or *goals*, etc.) and the editor who modifies the template is not the original creator and does not have the full knowledge about the template. Therefore, what they need is a consistency checking mechanism to identify the potential inconsistency. A rule-based reasoning mechanism is attached to the DSP ontologies in PDSIDES to provide consistency checking service to the Template Editors. The rules are extracted from the DSP constructs, such as the sum of the weights assigned to the *goals* must be equal to 1. An example that a Template Editor removes an existing goal (minimum cost) from the cDSP template is shown at the bottom of Figure 8.5; PDSIDES will check if this brought inconsistency and inform him.

Template Implementers – *reuse of the documented knowledge and perform post-solution analysis.* As we state in Section 8.3.2, Template Implementers are those who have little knowledge or interest in the analysis embodied in the templates, what they need is information that helps them exercise the template and make the decision. In PDSIDES; the knowledge provided to the Template Implementers includes both the declarative knowledge and procedural knowledge. The former is captured from Template Creators and Editors, and the latter is built in the platform such as design space exploration algorithms, plots, etc. which are hard-coded and can be invoked when needed. The picture on the top-right in Figure 8.5 represents a Template Implementer who is changing the weights assigned to different goals and using the ternary plot to identify the insensitive weight sets in order to make a robust decision, during which process the knowledge documented in the template is reused.

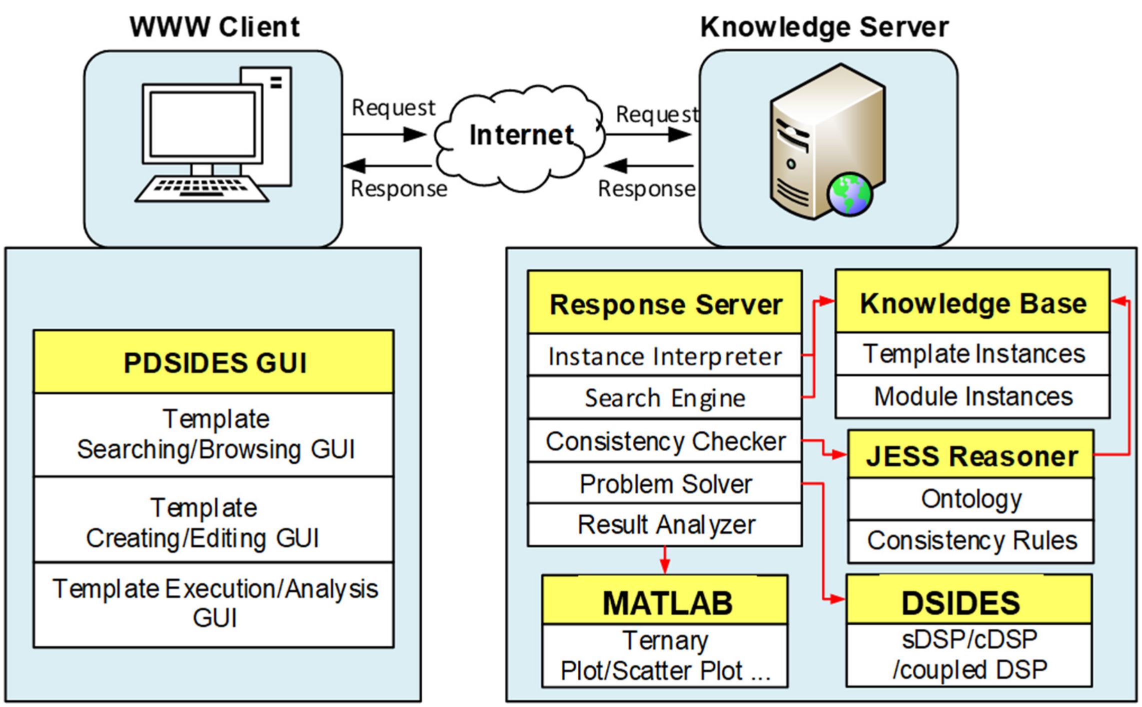


Figure 8.6: System architecture of PDSIDES

8.4 Implementation of Platform PDSIDES

PDSIDES is implemented as a two-tier client-server architecture to provide knowledge-based decision support with web browser-based graphical user interfaces (GUI) over the internet, as shown in Figure 8.6. In the client-server architecture, applications of PDSIDES are deployed to a web application server (marked as “Knowledge Server” in Figure 8.6) and provides remote user accesses using browsers such as Internet Explorer, Google Chrome, etc. Due to the easy access through web browsers, PDSIDES can reach out to a rich amount of users to get them involved in the decision template creating, editing and executing process for engineering system design, which is also a knowledge capturing, evolution, and reuse process over the internet. The maintenance and upgrades for PDSIDES in a client-server architecture are fairly convenient since the application package is deployed in one web server instead of distribution to a wide range of client computers. The client side of PDSIDES is the user interaction GUI including template searching and browsing GUI which are designed for locating the wanted DSP templates and presenting them, template creating and editing GUI which are designed based on the DSP template structures for the purpose of instantiation and modification of the DSP templates, the template execution and analysis GUI which are designed for executing DSP templates and performing post-solution analysis. The GUI is allowed to communicate with PDSIDES Knowledge Server by a request-response mode using the Hyper Text Transfer Protocol (HTTP). PDSIDES Knowledge Server includes five main parts, namely, Response Server, Knowledge Base, JESS Reasoner, DSIDES, and MATLAB. The Response Server is the central “brain” that integrates other four parts for responding to requests. The Response Sever itself has five components including a search engine, an instance Interpreter, a consistency checker, a problem solver. The instance interpreter is for interpreting the data collected from the Template Creators (or Editors) and formatting it into DSP Template instances according to the DSP ontologies, the generated template instances and module instances are stored in the Knowledge Base. The search engine is connected to the Knowledge Base to provide ontological semantic-based knowledge retrieval. Consistency checking is facilitated through a consistency checker together with the JESS Reasoner – the Rule Engine for the JavaTM Platform (Friedman-Hill 2015), which can provide rule-based intelligence inference. The problem solver is connected to DSIDES for solving the DSPs, it is invoked when a template executer executes a template. The Result analyzer is to help users especially Template Implementers analyze the results produced by the problem solver. MATLAB has a strong capability in providing data visualization tools such as ternary plots and scatter plots, therefore this feature is integrated to PDSIDES.

The front-end (i.e., the GUI) of PDSIDES is realized by JavaScript that can be embedded in the web pages. The development process is facilitated by the Sencha Inc.'s GXT (Sencha 2018). GXT is a comprehensive Java framework that uses the GWT (Google Web Toolkit) compiler (Google 2018), allowing developers to write applications in Java and compile their codes into highly optimized JavaScript that supports feature-rich web applications. Particularly, in order to enable graph-based interaction in terms of the operation of the DSP networks that may have multiple DSP templates and associated connections involved, Apache Flex (Adobe 2018) – a rich internet application developing framework is integrated to GXT to facilitate the creation of web-based diagrams. A DSP template such as a cDSP template may be very complex and have tens of *variables, parameters, constraints, goals,* etc., which usually makes data transmission overloaded between the front-end and the back-end. To address this issue, JSON (JSON 2018) - a lightweight data-interchange format, is used as the data transmission scheme together with the HTTP protocol.

The back-end (i.e., the sever side) of PDSIDES is written in Java to enable interoperability among different applications and cross-platform deployment. Many back-end applications such as the instance interpreter, search engine, consistency checker, and JESS reasoner, are heavily dependent on the DSP ontologies. As mentioned earlier, the DSP ontologies are formalized using the frame-based paradigm that contains Classes and Slots, the realization of this paradigm using the frame language is presented in this section, as shown in Figure 8.7.

The top box in the figure represents the definition of Class "*SystemGoal*" in the cDSP ontology, which includes definitions of slots such as *target, linearity, equality*, etc., and the associated facets such as *type, cardinality, allowed-values*, etc. The development of the DSP ontologies is facilitated using the protégé tool (Protégé 3.5), released by Stanford University which provides an environment for modeling the frame based ontologies and OWL ontologies. The frame-based ontology is actually an object-oriented mechanism based on which lots of instances can be populated. Two boxes at the bottom of Figure 8.7 represent two instances (i.e., *volume goal* and *weight goal*) of Class "*SystemGoal*" represented using frame language. The specific data in the slots of the instances are first collected using the template creating/editing GUI, then processed by the instance interpreter, and finally persisted in relational databases (in PDSIDES we use Oracle). Instances are treated as facts that are processed in the consistency checking process. In the JESS reasoner, all the facts are matched to the consistency rules and take certain actions if the corresponding rules are triggered. An example of the consistency rules is as follows:

```
(defrule MAIN::rule_5.1
  (object (is-a cDSPTemplate) (OBJECT ?a))
  =>
  (bind ?k (Sum (slot-get ?a preference) ONE))
  (if (and (<> ?k 1.0) (<> ?k 0.0)) then (printout t "MESSAGE: the sum of all the preferences is not
1.0!" crlf)))
```

The rule means that if the sum of the all preferences (i.e., the weights) in any instance of Class cDSPTemplate is not equal to 1, the reasoner will send a message about this inconsistency to the user who is operating the template instance.

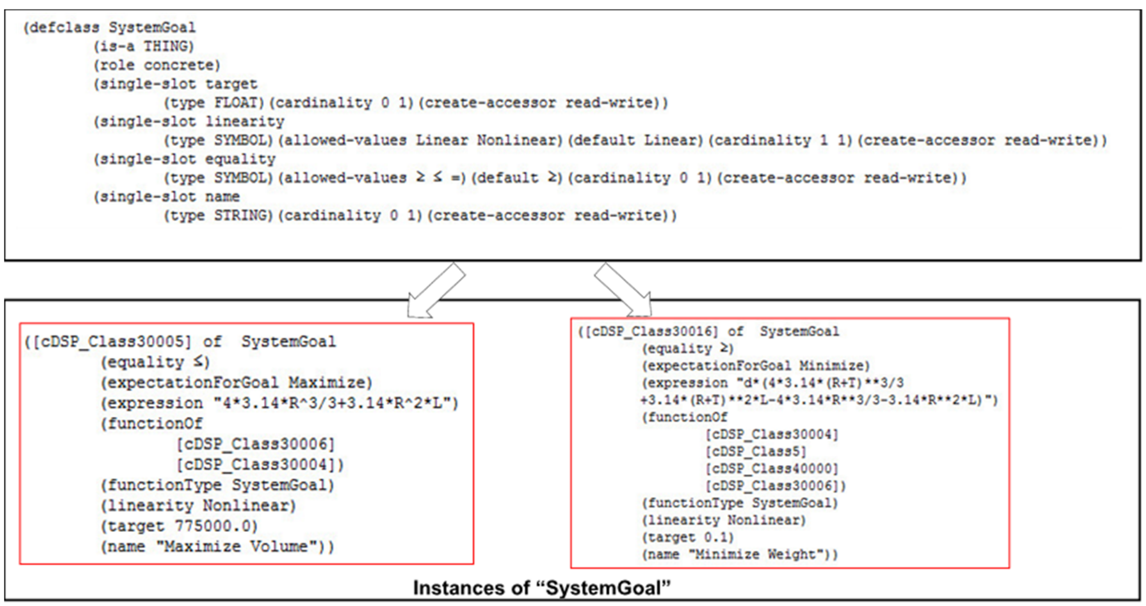


Figure 8.7: Frame based realization of the ontology and associate instances

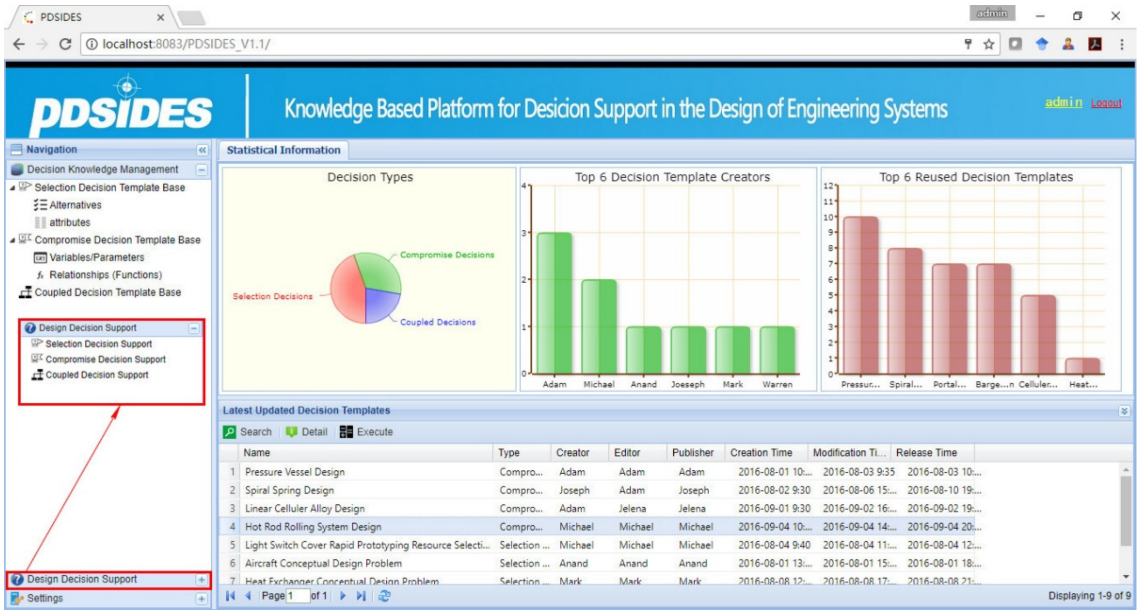


Figure 8.8: PDSIDES portal

The portal of PDSIDES is shown in Figure 8.8. A user can log in to PDSIDES through a web browser using a username and a password. Template Creators, Editors, and Implementers are three roles that are assigned to users of PDSIDES according to the knowledge they have in a specific domain. One designer can have more than one role. Each role has its particular view in the platform, the portal is the view shared by all three. The portal includes two main parts, the left-hand side is the navigation panel and the right-hand side is statistical information panel. The former represents the key functionalities of PDSIDES including the Decision Knowledge Management portion (managing knowledge about selection, compromise, and hierarchical decisions. Access is assigned to Creators and Editors), the Design Decision Support portion (providing DSP template executing and analysis service, access is assigned to Implementers), and the settings portion (purview management, access is assigned only to system administrators). The latter presents the charts and tables in terms of the decision-related knowledge and users. Users can see the number and the distribution of DSP templates in PDSIDES, the ranking of Creators who contribute their knowledge to PDSIDES, the ranking of templates that are reused frequently, and the latest updated DSP templates. They can also search, browser, and execute certain templates.

8.5 Testing the Platform PDSIDES

In this section, the performance of platform PDSIDES is tested via a gear manufacturing process design problem – a complex system design that calls for a series of decisions to be made. The foundational problem is contributed by our industrial partner – the Tata Consultancy Services in India (Allen, Mistree and coauthors). From the raw material to the final gear product, the material goes through multiple unit operations such as casting, rolling, cooling, forging, machining, etc., which are some of the processes in the steel manufacturing process chain. In order to obtain the desired end properties of the gear produced, proper decisions need to be made about the process control parameters (*set points*) at each of these processes. A large number of plant trials involving time and cost are needed to identify these operating set points. An alternative to this is to exploit the advancements in modeling tools and frameworks to carry out the design of the system to realize the end product. To couple the material processing-structure-property-performance spaces, we need to achieve the vertical and horizontal integration of models which further allows us to carry out the integrated decision-based design of the manufacturing processes to realize the end product (Nellippallil, Song and coauthors , Nellippallil, Song and coauthors 2016, Nellippallil, Allen and coauthors 2017). Decisions to be made at each manufacturing unit are formulated as cDSPs and linked as a decision network (mathematically modeled as coupled cDSPs) using a goal-oriented, inverse decision-based design method (Nellippallil, Allen and coauthors 2017). In this chapter, the hot rod rolling system design problem by Nellippallil and co-authors (Nellippallil, Allen and coauthors 2017, Nellippallil, Vignesh and coauthors 2017); addressed in Chapter 6 is modified and used as an example to test the performance of PDSIDES. As mentioned earlier, the problem includes multiple stages. We frame a boundary within the cooling stage and the end rod product requirements for the sake of simplicity.

8.5.1 Original Design

In original design, the template creator (domain expert) formulates in PDSIDES the cDSP for the problem boundary framed within the hot rod rolling process chain problem by taking into account the complete information flow across models thereby establishing relationships. The relationships established in the original design cDSP are the end mechanical properties of the product; YS (yield strength), TS (tensile strength), ITT (impact transition temperature) and HV (hardness) as a function of the system variables that are the output after rolling and input to cooling stage. The output parameters after cooling like FGS (ferrite grain size, D_α), X_f(phase fractions of ferrite), S_0 (pearlite interlamellar spacing) and composition variables that defines the end mechanical properties are defined as constraints in the cDSP formulated. The end product mechanical property goals, for example, maximizing YS, TS and minimizing ITT along with the goal for managing banding by maximizing ferrite fraction are captured in the cDSP. These goals are controlled by the independent system variables of this problem namely CR (cooling rate), AGS (grain size after rolling), C (carbon) and Mn (manganese). The upper and lower limits for the system variables and the maximum and minimum values for certain cooling stage parameters as well as for the mechanical properties are defined in the cDSP as bounds and constraints. The target values for the goals are defined as YS_{Target}= 400MPa, TS_{Target}= 780MPa, ITT_{Target}= -90°C, $X_{f\,Target}$= 0.8. The original design cDSP reads as follows:

Given

1) End requirements identified for the rod rolling process
   - Maximize Yield Strength (Goal)
   - Maximize Tensile Strength (Goal)
   - Minimize ITT (Goal)
   - Maximize Ferrite Fraction (Goal)
   - Maximize Hardness (Requirement)
2) Well established empirical and theoretical correlations, RSMs and complete information flow from the end of rolling to the end product mechanical properties (more description in reference (Nellippallil, Allen and coauthors 2017))
3) System variables and their ranges

Table 8.3: System Variables and Ranges for cDSP

Sr. No	System Variables	Ranges
1	X_1, Cooling Rate (CR)	11-100 K/min
2	X_2, Austenite Grain Size (AGS)	30-100 μm
3	X_3, the carbon concentration ($[C]$)	0.18-0.3%
4	X_4, the manganese concentration ($[Mn]$)	0.7-1.5%

Find

System Variables

X_1, Cooling Rate (CR)

X_2, Austenite Grain Size (AGS)

X_3, the carbon concentration ($[C]$)

X_4, the manganese concentration ($[Mn]$)

Deviation Variables

d_i^-, d_i^+, *i =1,2,3,4*

Satisfy

System Constraints

- Minimum ferrite grain size constraint
- Maximum ferrite grain size constraint
- Minimum pearlite interlamellar spacing constraint
- Maximum interlamellar spacing constraint
- Minimum ferrite phase fraction constraint (manage banding)
- Maximum ferrite phase fraction constraint (manage banding)
- Minimum manganese concentration constraint (manage banding)
- Maximum manganese concentration constraint (manage banding)
- Maximum carbon equivalent constraint (manage banding)
- Minimum yield strength constraint
- Maximum yield strength constraint
- Minimum tensile strength constraint
- Maximum tensile strength constraint
- Minimum hardness constraint

- Maximum hardness constraint
- Minimum ITT constraint
- Maximum ITT constraint

System Goals

Goal 1:

- Maximize Yield Strength

$$\frac{YS(X_i)}{YS_{Target}} + d_1^- - d_1^+ = 1$$

Goal 2:

- Maximize Tensile Strength

$$\frac{TS(X_i)}{TS_{Target}} + d_2^- - d_2^+ = 1$$

Goal 3:

- Minimize ITT

$$\frac{ITT_{Target}}{ITT(X_i)} - d_3^- + d_3^+ = 1$$

Goal 4:

- Maximize Ferrite Fraction

$$\frac{X_f(X_i)}{X_{f\,Target}} + d_4^- - d_4^+ = 1$$

Variable Bounds

Defined in Table 8.3

Bounds on deviation variables

$$d_i^-, d_i^+ \geq 0 \text{ and } d_i^- * d_i^+ = 0, \text{i} = 1,2,3$$

Minimize

We minimize the deviation function

$$Z = \sum_{i=1}^{4} W_i(d_i^- + d_i^+);\ \sum_{i=1}^{4} W_i = 1$$

By the formulation of cDSP, knowledge associated with the following inverse problem is captured: *Given the end product mechanical properties of a new steel product mix, what should be the microstructure after rolling and design set points for cooling stage that satisfies the requirements identified?* To facilitate knowledge capturing process in the computational environment, PDSIDES provides the GUI for the template creator to create DSP templates, as shown in Figure 8.9

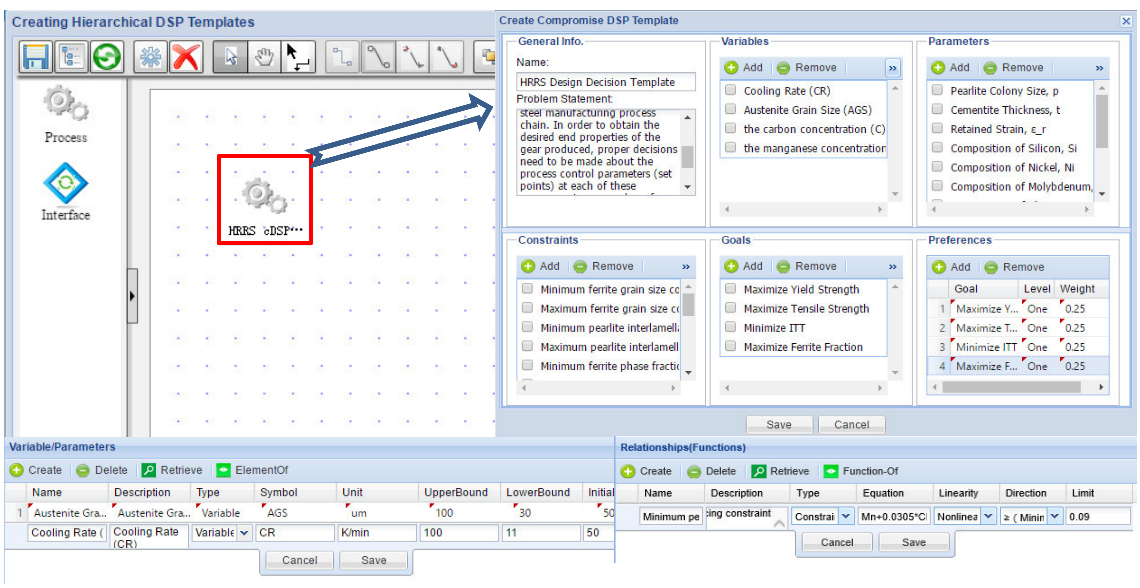


Figure 8.9: Creating the HRRS design decision template in PDSIDES

On the left-hand side of the canvas are the building blocks, including *Process* and *Interface*, which are formally defined in the ontology for the purpose of creating decision network templates (Hierarchical DSP templates). Since there is only one cDSP formulated for the original design of HRRS, the template creator can simply instantiate a *process* on the canvas and embody it with a cDSP template. The cDSP template is created in the "Compromise Decision Template Base" portion of PDSIDES. As shown in the window on the top-right of Figure 8.9, the template creator can instantiate the HRRS cDSP template by specifying the slots including *name, problem statement, variables, parameters, constraints, goals, and preferences* using data such as Cooling Rate, Austenite Grain Size, Carbon Concentration, etc. of the HRRS cDSP. Facet information of the slots, such as *symbol, unit* of a *variable* and *equation*, *limit* of a *constraint*, are further specified using the GUI designed for the instantiation of template modules, as shown in the two panels on the bottom. When the HRRS cDSP template is populated with specific information, it is sent to the knowledge server for consistency checking, calculation of results, persistence in the knowledge base, and is ready for future reuse in adaptive and variant designs.

8.5.2 Adaptive Design

In adaptive design, the template editor (senior designer) modifies the existing original design cDSP template according to new requirements. In the hot rod rolling problem addressed, the cDSP template of the original design relates the end product mechanical properties as a function of microstructure factors after rolling and the cooling stage operating parameters. The intermediate factors, for example, the ferrite grain size after cooling and the pearlite interlamellar spacing, which directly influence mechanical properties, are defined as constraints. Suppose, a situation arises that the designer is interested in knowing the range of microstructure factors after cooling that will satisfy a given end mechanical property requirements. In such a situation, new decision models need to be created by considering the microstructure factors after cooling as independent variables to define the end mechanical properties. This requirement can be easily satisfied by editing the existing formulated original design cDSP template in PDSIDES. The editing involves two major steps: Step 1, decompose the original cDSP template into two separate cDSP templates, and Step 2, link the two separate cDSP templates using an *Interface*.

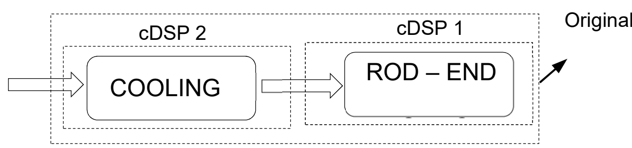


Figure 8.10: Decomposition of the original design cDSP

The process of the first step is shown in Figure 8.10. The original cDSP is decomposed into two cDSPs, namely, *cDSP 1* and *cDSP 2*. *cDSP 1* relates the end mechanical properties as a function of microstructure factors (D_α, X_f, S_0, Mn, Si, N) after cooling. The combination of microstructure factors after cooling that best satisfies the end requirements are identified by exercising this sub-cDSP. While, *cDSP 2* has the best combination of microstructure factor values after cooling identified from *cDSP 1* as goals. Using *cDSP 2*, the relationship between the microstructure factors after cooling with the microstructure after rolling and the cooling stage operating parameters (AGS, CR, C, Mn) is established. To realize the decomposition, modification of the original cDSP is as follows.

- For *cDSP 1*:

- Set ferrite grain size (D_α), phase fraction of ferrite (X_f), pearlite interlamellar spacing (S_0), manganese concentration ($[Mn]$), the composition of Si ($[Si]$), and the composition of N ([*N*]) which are system constraints of the original cDSP, to be system variables.
- Keep the rest constraints and goals the same as the original cDSP.

■ For *cDSP 2*:

- Keep the system variables, namely, Cooling Rate (CR), Austenite Grain Size (AGS), the carbon concentration ($[C]$), and the manganese concentration ($[Mn]$), the same as they are in the original cDSP.
- Set ferrite grain size (D_α), phase fraction of ferrite (X_f), and pearlite interlamellar spacing (S_0), which are system variables of *cDSP 1*, to be system goals.
- Set the final values of D_α, X_f, and S_0 obtained from *cDSP 1*, to be the targets of the system goals of *cDSP 2*.

The connection between *cDSP 1* and *cDSP 2* is that the output (i.e., the final values of the system variables) of *cDSP 1* comprises the input (i.e., the targets of the system goals) of *cDSP 2*. This connection represents the information workflow that links two cDSPs, which maps to Step 2 mentioned earlier for editing the original cDSP template. On the platform, the editing and the associated consistency checking process is shown in Figure 8.11. The template editor can instantiate two new cDSP templates on the canvas, as highlighted by two red rectangles marked as "End Product cDSP" and "Cooling cDSP" that represent *cDSP 1* and *cDSP 2* respectively. The instantiation of these two cDSP templates is the same as that is shown in Figure 8.11. It is noted that many modules of the original cDSP template are reused due to the modularization during the instantiation process of the two new cDSP templates. The link between two cDSP templates is captured by the instantiation of an *Interface* marked as "Exchange" that is highlighted in the circle. Configuration of the Interface is performed in the right window, where information in terms of interface type, strength, information flow, etc. is specified. According to the interaction between the two cDSP templates, the information flow is weak (one-way), sequential and flows from *cDSP 1* to *cDSP 2*. The content of the flow are the values of the five system variables of *cDSP 1*. Before executing the edited decision templates, the editor needs to check if there is any inconsistency due to the editing. The consistency checking process is shown in the panel on the bottom of Figure 8.11. Consistency rules can be dynamically defined and added into the reasoner for reasoning. If no rule is violated, the newly edited cDSP templates would be ready for execution, storage and reuse.

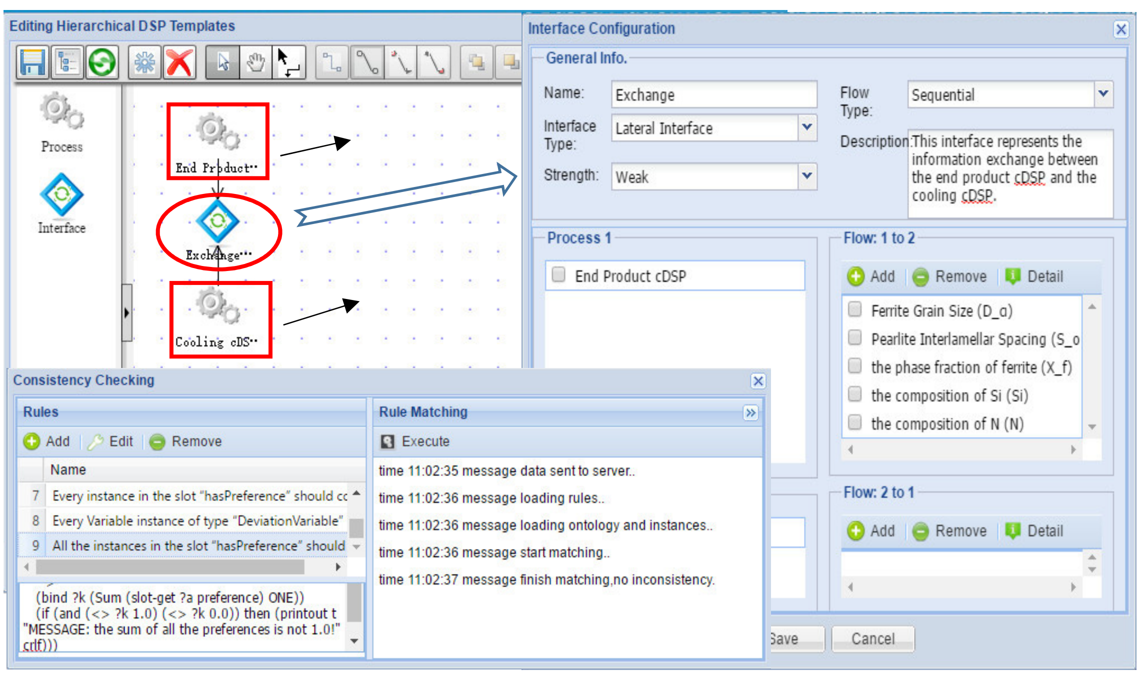


Figure 8.11: Editing the HRRS design decision template in PDSIDES

The results are obtained after exercising the *cDSP 1* and *cDSP 2* are provided in reference (Nellippallil, Allen and coauthors 2017) and are not repeated here.

8.5.3 Variant Design

In variant design, the Template Implementer makes parametric modifications to the already developed decision templates and executes the templates for different scenarios. In this chapter, we showcase variant design by executing the cDSP template of the original design for different scenarios identified by assigning weights to the deviations associated with each goal. We also illustrate the efficacy of ternary plots in PDSIDES to support the Template Implementer in exploring the solution space of variant designs to make appropriate design decisions. For the problem formulated in original cDSP, the Template Implementer is interested in accomplishing the following goals: maximizing ferrite fraction (to manage banding), maximizing tensile strength, maximizing yield strength and minimizing impact transition temperature. To visualize the goals in ternary space, it needs the Template Editor to first edit the original cDSP template to remove the goal on impact transition temperature and assign it as a constraint with minimum and maximum value. This is carried out because it is known that the impact transition temperature is directly influenced by changes in weights to other goals and hence need not be considered as a direct goal. Thus, the variant design cDSP has three goals – maximizing ferrite fraction, maximizing tensile strength and maximizing yield strength. Having developed the variant design cDSP, the next step for the template implementer is to identify design scenarios for execution.

On the platform, the identification of design scenarios is facilitated by the panel shown in Figure 8.12. The template implementer can specify several weight combinations (each combination stands for one scenario) for goal deviations using the table on the top, PDSIDES will calculate the result with respect to each of the weight combination. In this example, 19 different scenarios are identified, for more information on identifying scenarios see (Nellippallil, Song and coauthors). The template implementer exercises the original cDSP template in variant design scenarios and the results obtained are sent to MATLAB (at the back-end of PDSIDES) to plot as ternary plots shown in the bottom panel of Figure 8.12. The template implementer identifies regions (weight combinations) that satisfy the requirements from the ternary plots. More information on the creation of ternary plots and the evaluation of the same is available in reference (Nellippallil, Song and coauthors).

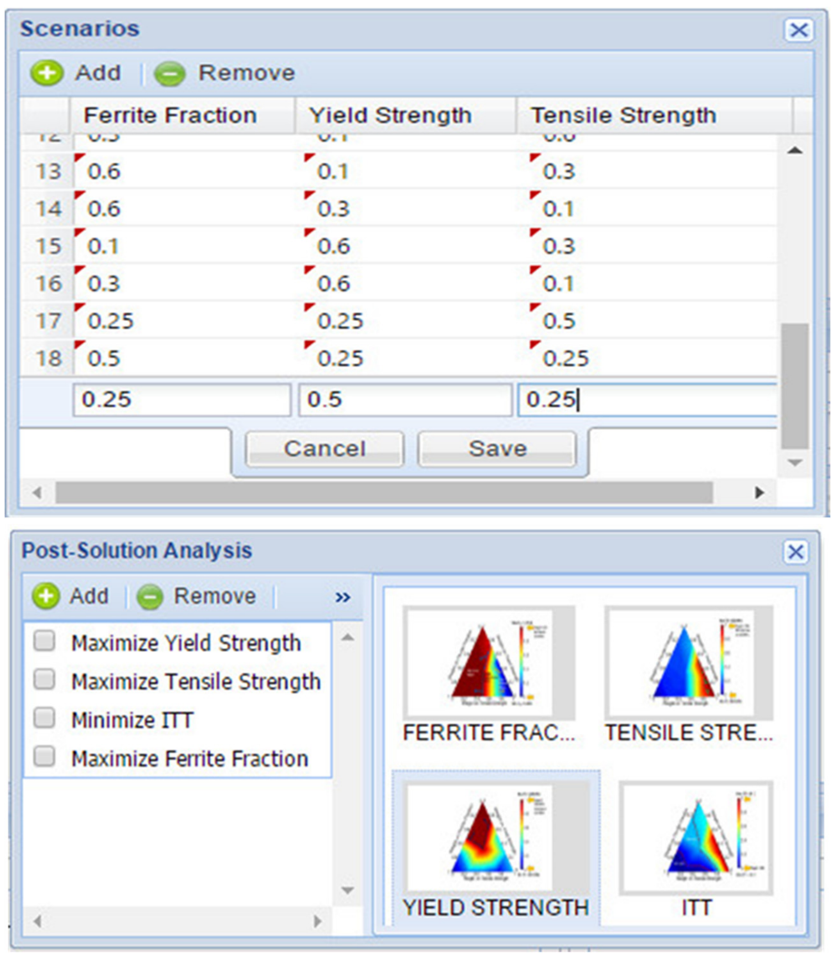


Figure 8.12: Exercising the HRRS design decision template in PDSIDES

The ternary plot for ferrite fraction is shown in Figure 8.13. The requirement for the template implementer is to maximize ferrite fraction to a value of 0.8 and the maximum value achieved on exercising the cDSP is 0.7116 identified by the light blue dashed line in the red contour region of Figure 8.13. Any weight combination of goals in this region achieves high ferrite fraction. Similarly, the high pearlite fraction region is identified by the blue region in Figure 8.13. The highly banded ferrite-pearlite microstructure region is identified in the boundary between these two regions. The same method is extended to identify the regions that satisfy the requirements of tensile strength, yield strength, and impact transition temperature.

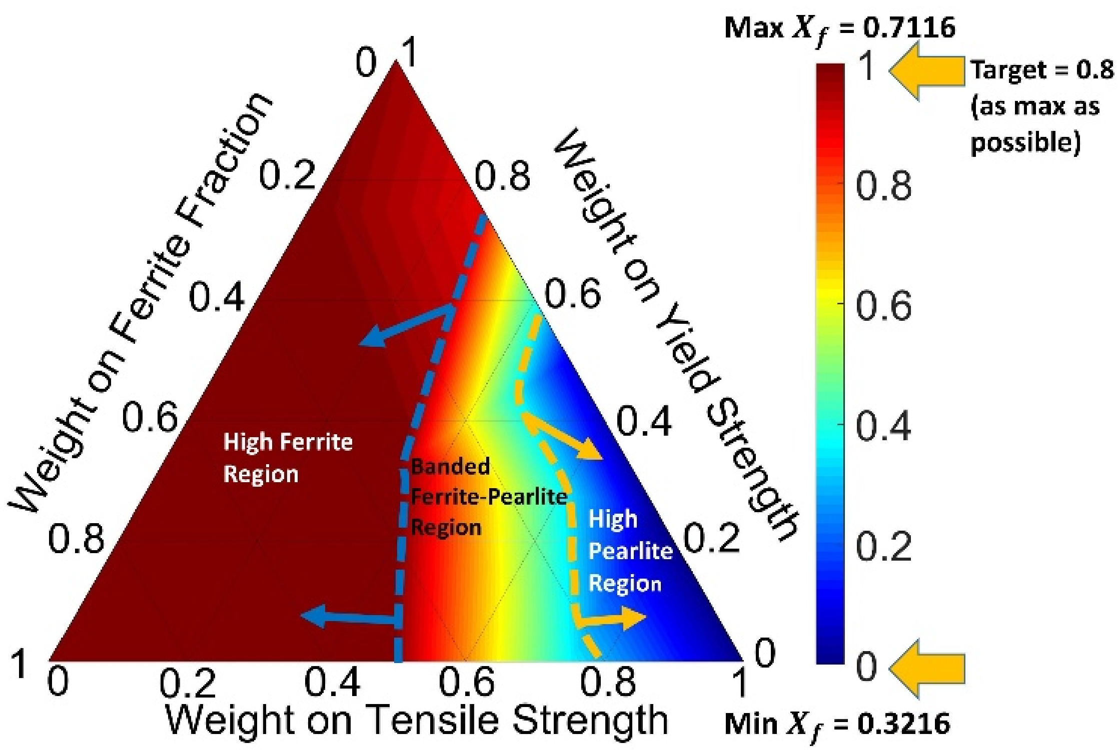


Figure 8.13: Ternary plot for ferrite fraction

Since the template implementer's interest is to identify a common region that satisfies all the goals, a superimposed ternary plot having all the goals is generated as showcased in Figure 8.14. From the superimposed ternary plot several solution weight points (A, B, C, D, E, F, G) are identified and analyzed. The results associated with these solution weight points are summarized in Table 8.4.

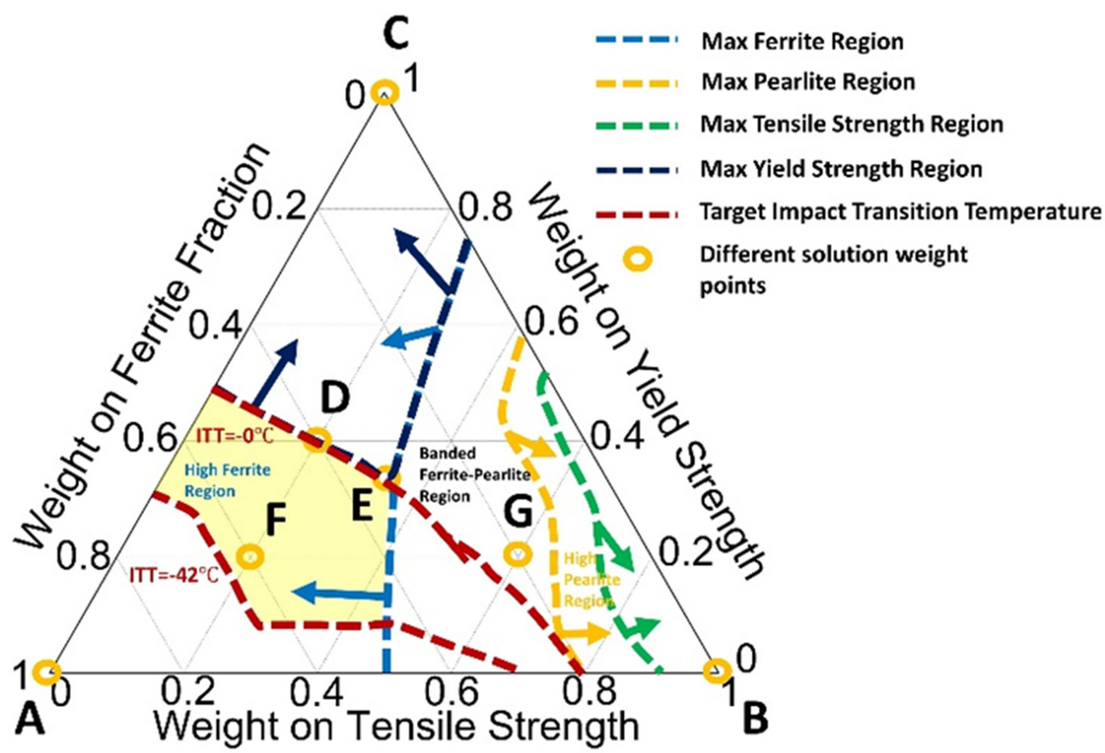


Figure 8.14: Superimposed ternary plot

On analyzing Figure 8.14 and Table 8.4, it is seen that the light yellow region satisfies all the requirements for managing banding (high ferrite), maximizing yield strength, maximizing tensile strength and minimizing ITT in the best possible manner. However, the requirements for high tensile strength and high yield strength are compromised to satisfy requirements like managing banding and minimizing ITT. It is also observed that a high ferrite region supports the maximization of yield strength and minimization of ITT. The maximization of tensile strength however is supported by high pearlite fraction. Point F out of these multiple solutions listed in Table 8.4 is picked as F satisfies all the requirements in the best possible manner.

Table 8.4: Identified solution points after exploration

Sol. Pt	CR K/min	AGS (μm)	C (%)	Mn (%)	X_f	YS MPa	TS MPa	ITT ℃
A	16.5	99.9	0.18	0.7	0.71	232	487.7	-26
B	99.9	30	0.29	1.5	0.32	248	662	99
C	22.8	30	0.18	1.5	0.7	284	526	3.5
D	11	30	0.18	1.5	0.71	283	519	0
E	11	30	0.18	1.5	0.71	283	519	0
F	11	30	0.18	0.7	0.7	244	513	-42
G	62	30	0.19	1.5	0.65	281	547	15

By reusing the knowledge archived in the original HRRS design cDSP template for execution and utilizing the ternary plot for post-solution analysis, the template implementer explores the solution space of variant designs and makes appropriate design decisions.

8.6 On Verification and Validation

Theoretical Structural Validation

Theoretical structural validation refers to accepting the validity of individual constructs of PDSIDES and accepting the internal consistency of the way the constructs are put together for PDSIDES. Theoretical structural validation involves systematically identifying the scope of the platform's application, reviewing relevant literature and identifying the research gaps that is existing, identifying the strengths and limitations of the constructs used based on literature review, determining the constructs and approaches that can be leveraged for developing the platform, reviewing literature on the advantages, disadvantages and accepted domains of application, and checking the internal consistency of the constructs both individually and when integrated into the platform. The internal consistency of the individual constructs is checked by a critical review of the literature. The verification and validation of Research Hypothesis 4 is carried out in detail in Section 10.2.4. The readers are referred to this section for more details.

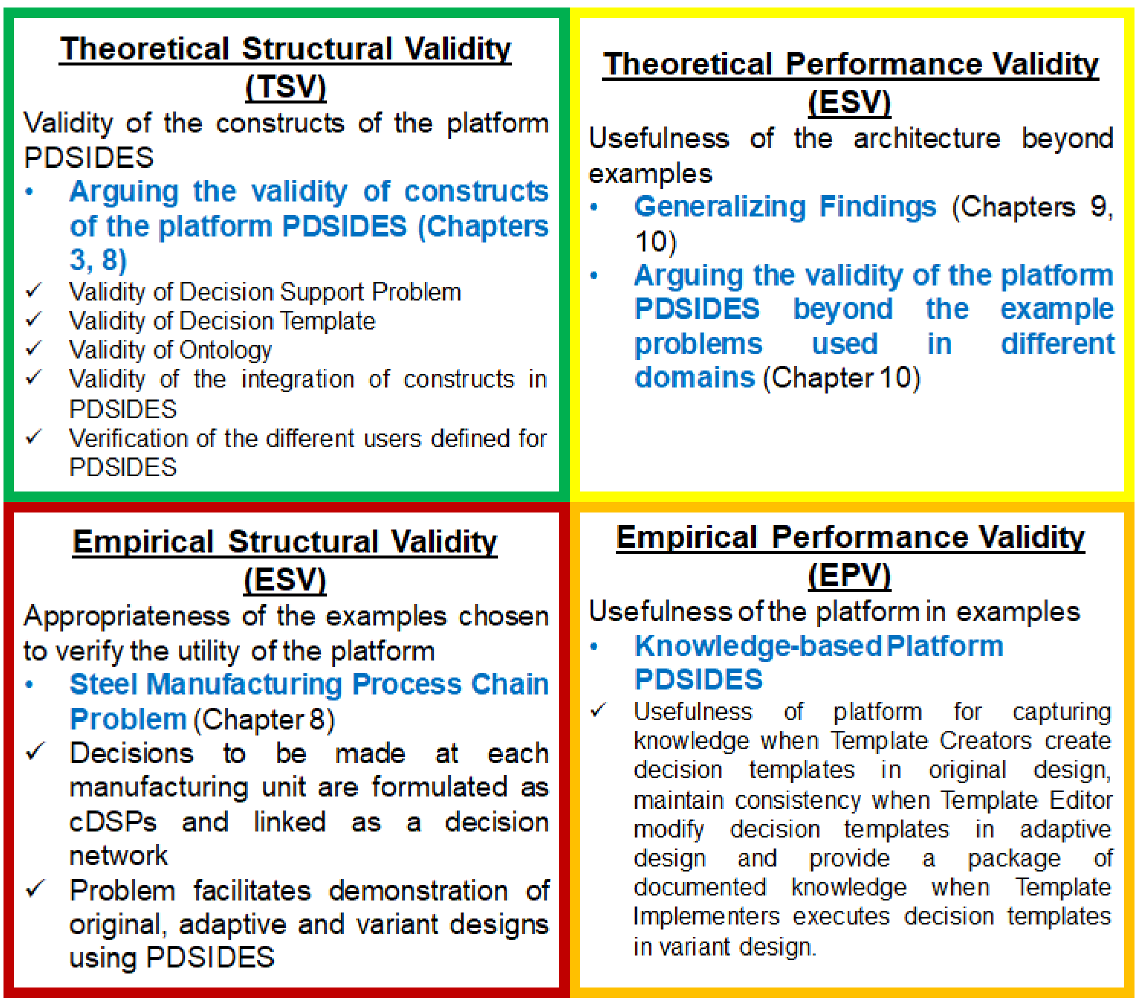


Figure 8.15: Verification and validation aspects addressed in Chapter 8

The verification and validation aspects addressed in Chapter 8 is shown in Figure 8.15. In Chapter 8, the foundations are briefly revisited and the PDSIDES platform is presented. The constructs used in the platform are discussed in Section 8.2. The ontology for capturing the decision-related knowledge is introduced in Section 8.2.3. The design of the platform PDSIDES is introduced in Section 8.3. Three types of users of the platform – creators, editors and implementors are introduced and their associated working scenarios are described in detail in Section 8.3.2. In Section 8.3.3, the knowledge-based decision support in PDSIDES is presented and the roles played by each of the users of PDSIDES is established. The internal information flow in the platform is checked to ensure sufficient information availability to execute next steps. Through critical evaluation of each step in the design of the platform and the way individual constructs are put together, internal consistency of the platform PDSIDES is verified and accepted.

The theoretical structural validity of PDSIDES is accepted by the logical procedure of literature review, gap analysis and development and evaluation individual and integrated constructs within the platform. Empirical studies are further carried out to establish the usefulness and effectiveness of the platform.

Empirical Structural Validation

Empirical structural validation involves accepting the appropriateness of the example problem used to verify the performance of the PDSIDES for original, adaptive and variant designs. In Chapter 8, Section 8.5, the gear manufacturing process design problem focused on rod rolling – a complex system design that calls for a series of decisions to be made – is introduced. Decisions to be made at each manufacturing unit are formulated as cDSPs and linked as a decision network. In original design addressed in Section 8.5.1, the template creator (domain expert) formulates in PDSIDES, the cDSP for the problem boundary framed within the hot rod rolling process chain problem by taking into account the complete information flow across models thereby establishing relationships. Using the cDSP formulated the ability of the PDSIDES platform to carry out original design is demonstrated. In adaptive design addressed in Section 8.5.2, the template editor (senior designer) modifies the existing original design cDSP template according to new requirements. The requirement can be easily satisfied by editing the existing formulated original design cDSP template in PDSIDES. The editing involves two major steps: Step 1, decompose the original cDSP template into two separate cDSP templates, and Step 2, link the two separate cDSP templates using an *Interface*. Two cDSPs are formulated from the original design cDSP to demonstrate adaptive design. The cDSPs are interlinked via an interface of design variables that are shared. Using the cDSPs formulated, the ability of the PDSIDES platform to carry out adaptive design is demonstrated.

Empirical Performance Validity

Empirical performance validation consists of accepting the usefulness of the outcome with respect to the initial purpose and accepting that the achieved usefulness is related to using PDSIDES for original, adaptive and variant designs; addressed in Chapter 8. In PDSIDES, decision-related knowledge is modeled as modular, computational templates based on the DSP constructs using ontology to facilitate execution and reuse. The advantages of PDSIDES is that it provides the functionality to capture knowledge when Template Creators create decision templates in original design, maintain consistency when Template Editor modify decision templates in adaptive design and provide a package of documented knowledge when Template Implementers executes decision templates in variant design.

8.7 Role of Chapter 8 and Remarks on the Knowledge-based Platform PDSIDES

Engineering system design is fundamentally a decision-making process and knowledge plays a critical role in facilitating decision making. In this chapter, we present a Knowledge-Based Platform for Decision Support in the Design of Engineering Systems. In PDSIDES, decision-related knowledge is modeled as modular, computational templates based on the DSP constructs using ontology to facilitate execution and reuse. In order to provide users of different knowledge levels with a proper decision support, we define three types of users, namely, Template Creators, Template Editor, and Template Implementers, who perform original design, adaptive design, and variant design respectively. The unique advantage of PDSIDES is that it provides the functionality to capture knowledge when Template Creators create decision templates in original design, maintain consistency when Template Editor modify decision templates in adaptive design and provide a package of documented knowledge when Template Implementers executes decision templates in variant design.

Distributed information control is not yet considered in the current version of PDSIDES. Future research opportunities lie in enabling the negotiation of collaborative decisions that are controlled by different stakeholders. For example, in the HRRS design example process designers at different stages such as rolling, and cooling may not be willing to sharing the full information in their own decision-making process, and then the negotiation of a collaborative decision is needed. Providing the functionality for negotiating collaborative decisions would be of great potential for the application of

PDSIDES in a supply chain environment, where the decision makers are distributed. All these can be addressed by enabling the PDSIDES platform with the cloud (Cloud-based PDSIDES). The cloud-based features of PDSIDES is addressed in Chapter 10.

Chapter 9: Template-based Ontological Method for Systematic Design Space Exploration – Generalizing the Exploration Process

The realization of complex engineered systems using models that are typically incomplete, inaccurate and not of equal fidelity requires the understanding and prediction of process behavior in design. This necessitates the need for extending designer's abilities in making design decisions that are robust, flexible and modifiable particularly in the early stages of design. To address this requirement, an ontology for design space exploration and a template-based ontological method that supports systematic design space exploration ensuring the determination of the right combination of design information that meets the different goals and requirements set for a process chain is proposed in this chapter. Using the proposed method, a designer is able to (1) systematically adjust the design space in due time to manage the risks of errors accumulating and propagating during the design of different stages of the process chain, (2) improve the ability to communicate and understand the interactions between design information in the process chain. The said is achieved through: 1) a procedure for design space exploration is identified to determine the sequence of activities needed for the systematic exploration of design space under uncertainty; 2) the decision-based design information flow is archived using the design space exploration process template and represented by utilizing frame-based ontology to facilitate the management of re-usable information. In this chapter, the efficacy of this template-based ontological method for design space exploration is demonstrated by carrying out the design of a multi-stage hot rod rolling system in steel manufacturing process chain.

9.1 Frame of Reference – Answering Research Question 4

Due to the limited information in the early stages of design, the designer has to deal with different types of uncertainty. The presence of incomplete, inaccurate and infidel models for complex engineering systems also adds to this uncertainty. Several challenges are involved in managing the uncertainty associated with the model-based realization of complex engineered systems (Allen, Panchal and coauthors 2015). Two major challenges are: 1) the challenge of creating knowledge about the complex engineered systems and; 2) the challenge of capturing and reusing tacit knowledge, building the ability to learn from data and cases, and developing knowledge-based methods for guided assistance in decision-making. Design productivity can be enhanced by both increasing design knowledge in the early stages of designs and maintaining design freedom throughout the design process (Chen, Allen and coauthors 1997). Therefore, in response to the first challenge, some research results are put forward from the decision-based design perspective. These include cDSP-centric robust design methods (RCEM, IDEM) (Chen, Allen and coauthors 1996), exploration of solution space utilizing cDSP (Sabeghi, Smith and coauthors 2015), etc., which have a wide application in the civil transport aircraft development, multiscale materials design, etc. There is an only limited research focus on the second challenge and addressing it is crucial for providing decision support in the design of complex engineering systems.

To provide decision support and design complex engineered systems requires various types of design information to be assembled to form a representation of the context (Cook, Augusto and coauthors 2009). Semantic technologies are widely accepted for context modeling due to the functionalities offered to communicate and understand the information interaction. They also play a crucial role in the management of things, devices, and services in Industry 4.0 (Wu, Rosen and coauthors 2016). The ontology-based approach is an active area of research in semantic integration, which effectively facilitates the share and reuse of knowledge as well as interoperability between different systems. Thus, in order to achieve an intelligent environment for designing complex engineering systems, a good understanding of predicting process behavior is paramount. Achieving this using decision-based design necessitates a systematic, flexible, dynamic, and adaptive designing of the decision workflows involved. The decision-based design results associated with these workflows should be robust i.e. relatively insensitive to the uncertainties involved. The design results should also be flexible enough to accommodate any risk of errors that may accumulate along the decision workflows. To address above demands, an ontology for design space exploration and a template-based ontological method that supports systematic design space exploration in the model-based realization of complex engineered systems is proposed in this chapter. Using this proposed method, a designer is able to determine the right combinations of design information that meets the different goals set thereby satisfying the end requirements for each stage of the process, and also adjust the design space to achieve solutions that are robust and flexible enough to manage any risk of error propagation in continuous multi-stage design.

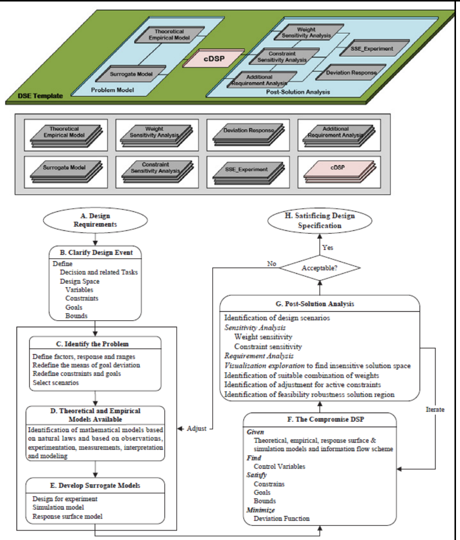
The remainder of this chapter is organized as follows. In Section 9.2, we describe the foundation for this work – the Decision Support Problem (DSP) and its applicability in providing insight to designers for managing complexity and uncertainty. We also address the utility of ontology-based knowledge modeling in facilitating efficiency and effectiveness in the applications of DSPs. In Section 9.3, we propose a template-based method for computationally modeling the processes of Design Space Exploration (DSE) in response to the defined requirements for DSE, which includes a systematic procedure for DSE, design space adjustment, and a DSE template scheme. In Section 9.4, we develop an ontology that represents the underlying knowledge related to the DSE process template, as well as the instantiation approach in keeping with the DSE process template model. The efficacy of this method is illustrated by using an example associated with the design of a multi-stage hot rod rolling system in Section 9.5, and we end with the closing remarks in Section 9.6.

A portion of Table 1.6 that is relevant to this chapter is reproduced in Table 9.1. We revisit the research question and research hypotheses in Table 9.2.

Table 9.1: Research Question and Research Hypotheses 4 addressed in Chapter 9

Secondary Research Question 4	Research Hypothesis 4
RQ4. What are the foundations needed for maintaining ***structural consistency*** of the decision-based design workflow for the manufacturing process chain involving the material and product, ensuring ***robust, flexible and modifiable*** decisions while incorporating newer ***data, information and knowledge*** associated with the system?	***H4.3.*** Developing an ontology for design space exploration and a template-based ontological method that supports systematic design space exploration ensuring the determination of the right combination of design information that meets the different goals and requirements set for a process chain (To address **G8**).

Table 9.2: Requirements, constructs of PDSIDES, and associated hypothesis validated in Chapter 9

Requirements	Constructs of the Systems-based Design Architecture developed in this Dissertation	Research Hypotheses	Validation Examples
3. Facilitation of systematic design exploration through decisions that are robust, flexible and modifiable particularly in the early stages of design. .	 **Ontology and template-based method for Design Space Exploration**	**RH4.3.** Ontology for design space exploration and a template-based ontological method that supports systematic design space exploration	1. Integrated design of steel (material), manufacturing processes (rolling and cooling) and hot rolled rods (product) for automotive gears

9.2 Brief Review of Foundational Constructs

9.2.1 The Decision Support Problem Construct

Due to the complexity and uncertainty associated with complex systems with emergent behavior, the model-based realization of complex engineering systems are characterized by models that are typically incomplete, inaccurate and not of equal fidelity especially in the early stages of design (Allen, Panchal and coauthors 2015). From the perspective of decision-based design, the primary role of a designer is to make robust design decisions given the uncertainties associated with the system and models (Mistree, Bras and coauthors 1995). Mistree and co-authors (Mistree, Hughes and coauthors 1993) present the compromise Decision Support Problem (cDSP) as a decision construct to aid designers in carrying out trade-offs among multiple conflicting goals.

Using the cDSP *satisficing* solutions for the desired system performance are sought rather than optimum solutions that are valid only in the narrow range of conditions. The generic mathematical formulation of the cDSP construct is shown in Figure 9.1. Robustness, in engineering design refers to mitigating the consequences of variability to variations, which means the ability to tolerate perturbations from some noise source. Many researchers have focused on the methods and application for robust design in engineering design, Taguchi being the first to provide initial insight into the robust design and its principles which are widely advocated by both industry and academia. In spite of this, there are some limitations to the Taguchi approach, the details of which are available in (Allen, Seepersad and coauthors 2006).

Given

An alternative to be improved, domain dependent assumptions

n	number of system variables
q	inequality constraints
p + q	number of system constraints
m	number of system goals
$g_i(X)$	system constraint function
$f_k(d_i)$	function of deviation variables to be minimized

Find

X_i System variables i = 1, …, n

d_i^+, d_i^- Deviation Variables i = 1, …, m

Satisfy

System constraints (linear, nonlinear)

$g_i(X) = 0$ i = 1, …, p

$g_i(X) \geq 0$ i = p+1, …, p+q

System goals (linear, nonlinear)

$A_i(X) + d_i^- - d_i^+ = G_i$ i = 1, …, m

Bounds

$X_i^{min} \leq X_i \leq X_i^{max}$ i = 1, …, n

$d_i^+, d_i^- \geq 0;\ d_i^+ \cdot d_i^- = 0$

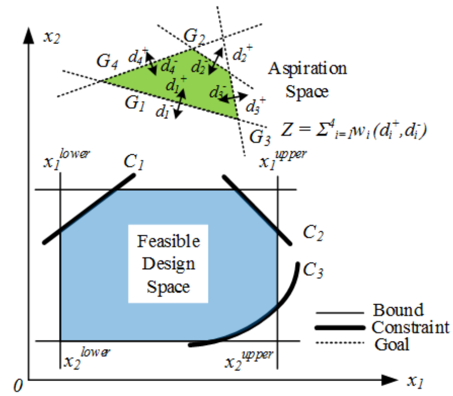
Minimize

Deviation Function:

Archimedean: $Z = \Sigma_{i=1}^{m} w_i(d_i^-, d_i^+)$

Preemptive: $Z = [f_i(d_i^-, d_i^+), \ldots, f_k(d_i^-, d_i^+)]$ i = 1, …, m

(a)



(b)

Figure 9.1: Mathematical Formulation of the cDSP Construct (Mistree, Hughes and coauthors 1993)

The design decisions in the earlier stages of design have a profound impact on the performance and quality of the final product. Chen and co-authors formulate a robust design problem as a decision model using the cDSP (Chen, Allen and coauthors 1996). Building on this work, they present the Robust Concept Exploration Method (RCEM) and its applications (Chen, Allen and coauthors 1997). These work are foundational in addressing the incorporation of robustness in the early stages of design. Based on these foundational work, several integrated computational methods are proposed to explore the design space by utilizing the cDSP, see Nellippallil and co-authors (Nellippallil, Song and coauthors) and Shukla and co-authors (Shukla, Goyal and coauthors 2015). Nellippallil and co-authors (Nellippallil, Allen and coauthors 2017) present a goal-oriented, inverse decision-based design method to achieve the vertical and horizontal integration of models for a multi-stage hot rod rolling system using well-established empirical models, response surface models generated from simulation experiments as well as the cDSP construct supported by the Concept Exploration Framework (CEF). We will be addressing this work in the following sections.

9.2.2 Ontology based Knowledge Modeling

Ontology is defined as a specification of a conceptualization, which can provide a common vocabulary for the representation of domain-specific knowledge (Noy and McGuinness 2001). Ontology has a great potential impact on the designing of engineering system (Wang, De and coauthors 2012). The expected benefits of using ontologies are the following (Chun and Atluri 2003, Lin, Harding* and coauthors 2004, Preuveneers, Van den Bergh and coauthors 2004):

- Flexibility - knowledge is defined in terms of an ontology instead of “hardcoding” within the platform;
- Intelligent behavior - knowledge can be derived from the factual knowledge explicitly represented in the ontologies;
- Semantic interoperability - semantics of the (possibly several) languages used by the platform’s external parties can be defined by a set of interrelated ontologies;
- Expressiveness - context information is represented using a formal representation language, which enables to check the consistency of the models automatically.

In past work, to facilitate efficiency and effectiveness in design, ontologies to represent the knowledge in cDSP template (Ming, Yan and coauthors 2016), a selection DSP (sDSP) template (Ming, Wang and coauthors 2016), and a hierarchy DSP template (Ming, Yan and coauthors 2016) are presented, respectively. A PEI-X ontology for meta-design process hierarchies (Wang, Wang and coauthors 2017) is proposed, which can support a designer to capture, represent and document the knowledge for supporting the re-usability of information in the decision workflows.

9.3 Modeling the Processes of Design Space Exploration

In this section, according to the requirements for DSE defined for the model-based realization of engineered systems, a templated-based method for computationally modeling the processes of exploration is proposed, which includes a systematic procedure for DSE, design space adjustment, and a DSE template scheme.

9.3.1 Requirements for Design Space Exploration

Design Space Exploration (DSE) refers to the activities of exploring (discovering and evaluating) design alternatives or space of potential design candidates before implementation during the system development phase. The management of complexity and uncertainty during the processes of DSE are required to be considered in the model-based realization of engineered systems. Kang and co-authors (Kang, Jackson and coauthors 2010) suggest that an effective DSE framework needs to consist of the following ingredients: 1) a suitable representation of the design space, 2) an effective exploration method, 3) machine-assisted techniques for analyzing the solutions. To further ensure the validity of design, we identify the following requirements for DSE:

- **Support Decision-Centric Robust Design**

Decision-Based Design (DBD) helps bridge the gap between a physical world and model world (Smith, Milisavljevic and coauthors 2015) and emphasizes the core role of human designers as decision makers in the computer design environment. It is widely accepted that design is viewed as decision-making processes, which involves making rational decisions based on the available alternatives that satisfy one's preference (Bloebaum and McGowan 2010, Tribus 2016). Robust decision-making involves a particular set of methods aimed to help human designers identify potential robust strategies under conditions of complexity and uncertainty. As one embodiment of DBD, DSPs provide domain-specific mathematical models built as structured templates, which can be used to formulate a suitable representation of the design space.

- **Support Understanding and Predicting of Process Behavior**

To support different decision-making needs, the exploration process of design space need to aggregate several functions. It should allow for analysis, evaluation, and synthesis, as well as define the tasks to be performed at different levels of detail. This is done using methods that guide a sequence of tasks from one level of abstraction to the next lower level. Computer Aided Engineering (CAE) tools, can enhance the efficiency and facilitate the accomplishment of the tasks. Thus, from the perspective of model-based realization of engineered systems (Estefan 2007, Micouin 2014), the application of methods, and tools in the exploration of design space necessitates an environment that can integrate the associated information and provide improved communications to support human designers in understanding and predicting the process behavior in DSE.

- **Support Interaction and Visualization**

In a computer environment, the model-based realization of engineered systems cannot be carried out without the information flows that facilitate the ability to interact with models. Due to the complex characteristics of the engineered systems, the hierarchy of design processes needs to organize and manage the information flows to support vertical and horizontal integration. Therefore, a method for supporting integrated information flows across different dimensions and stages of design process is essential. Meanwhile, visualization is also indispensable to support an effective decision-making in the design space exploration process.

9.3.2 Procedure for Design Space Exploration – Generalizing the CEF

In this chapter, a systematic design space exploration process that support decision-centric robust design is proposed to identify design alternatives and generate *satisficing* solutions for the specific design problem. The exploration is inspired from RCEM (Chen, Allen and coauthors 1996) and CEF (Nellippallil, Allen and coauthors 2017) – proposed in Chapter 4. The frame of DSE is a logical sequence of activities performed to achieve a particular objective, as shown in Figure 9.2.

Step 0: Data Input/Output - ***Input A and Output H in Figure 9.2***

The DSE procedure begins with the designer identifying design requirements for the current design event that provides data-entry from a static problem statement or dynamic data (e.g., sensors data of operation) for DSE. It ends with the identification of design solution regions or points that satisfy the requirements identified for supporting the designer to make comprehensive decisions. Design requirements necessitate taking account of the possibly conflicting wants of the various stakeholders because an effective product attribute deployment incorporates the needs of both the consumers and producers in decision-making. This facilitates the conceptualization of design alternatives and constraints (Hoyle and Chen 2009).

Step 1: Pre-Process - *Processor B in Figure 9.2*

The DSPs are generic discipline-independent modeling technique that supports partitioning of a problem and planning the decision processes. This is namely meta-design (Mistree, Bras and coauthors 1995).

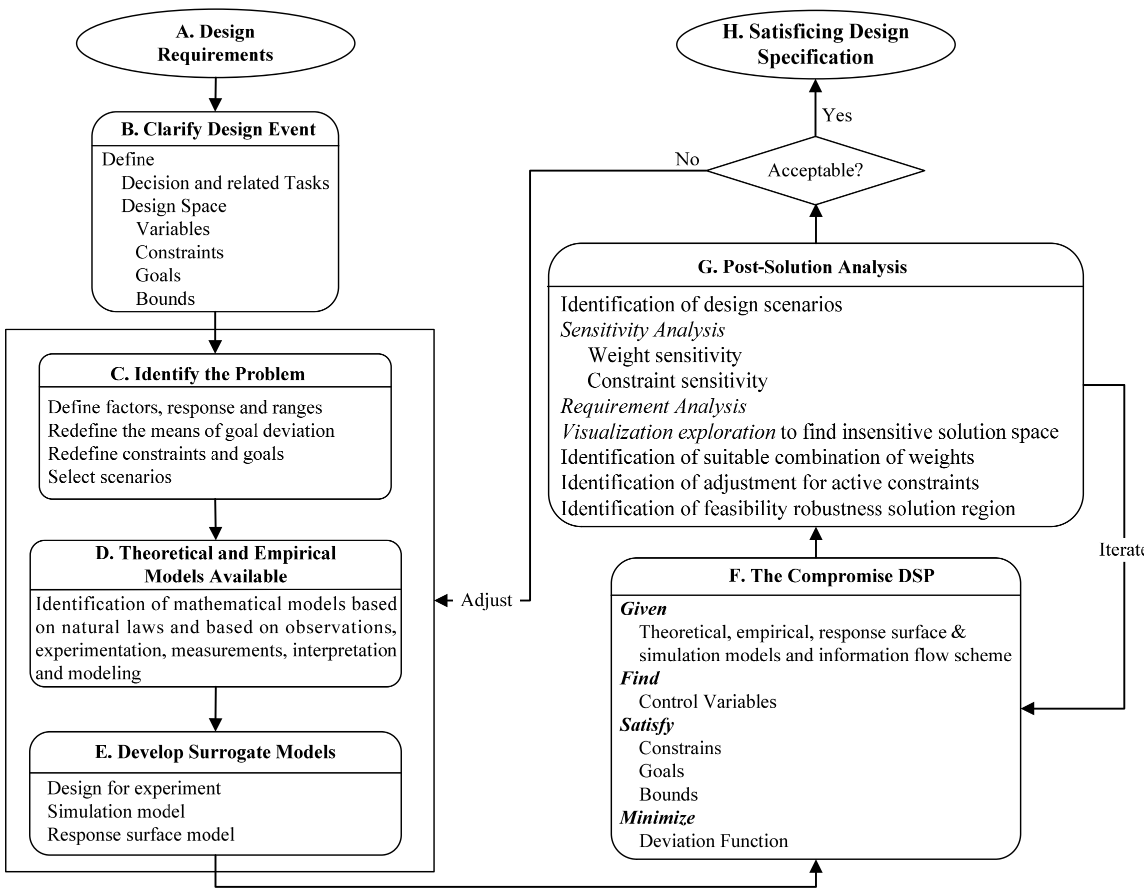


Figure 9.2: Procedure for Design Space Exploration – Generalizing the steps of CEF

PEI-X (Phase-Event-Information - X) diagram is used to model the design processes from a perspective of event-based time. To ensure the applicability of the *Support Problems* to solve and carry out computer-based design and analysis of the design space, there is a need to refine the complexity of the identified problem. This is by clarifying the design event by defining the decisions and related tasks. The information associated with design space (i.e., variables, constraints, goals, and bounds) is gathered from various sources to start the problem formulation.

Step 2: Problem Modeling - ***Processor C, D, and E in Figure 9.2***

To determine the initial design space and provide a combination of design information as the inputs for the cDSP construct, the designer needs to use three processors shown in Figure 9.2 (*Processor C, D,* and *E*). These processors are used to model the specified problem in terms of the mathematical formulations. In the first processor, significant design parameters and variables in the specific design problem is identified. They are classified as control factors (**x**, design variables that designers can control), noise factors (**z**, design variables that designers cannot control) and responses (**y**, performance measures identified as goals). The associated ranges for these parameters and variables are also identified. Next, the designer defines the functional relationship (*f*) between factors and responses, namely $\mathbf{y}=f(\mathbf{x})$. In *Processor C,* some available theoretical and empirical mathematical models based on the existing knowledge from natural laws or experiments/modeling in literature are identified and reused. In case the functional relationships are not available or if there is a need to develop reduced order models to reduce the size of the problem, then the designer is required to develop surrogate/reduced order models for the problem formulated. Statistical techniques (e.g., statistical design of experiments and response surface method) are widely used in engineering design to address these concerns (Simpson, Poplinski and coauthors 2001). A model of the model (meta-model) is developed by building approximations of the computer analysis codes to yield insight into the functional relationship between **x** and **y**. As shown in Figure 9.3, a generic procedure of response surface modeling is summarized and provided to generate prediction function $g(x)$ by approximating the true response surface function $f(x)$ via integration of Base Steps and Support Tools.

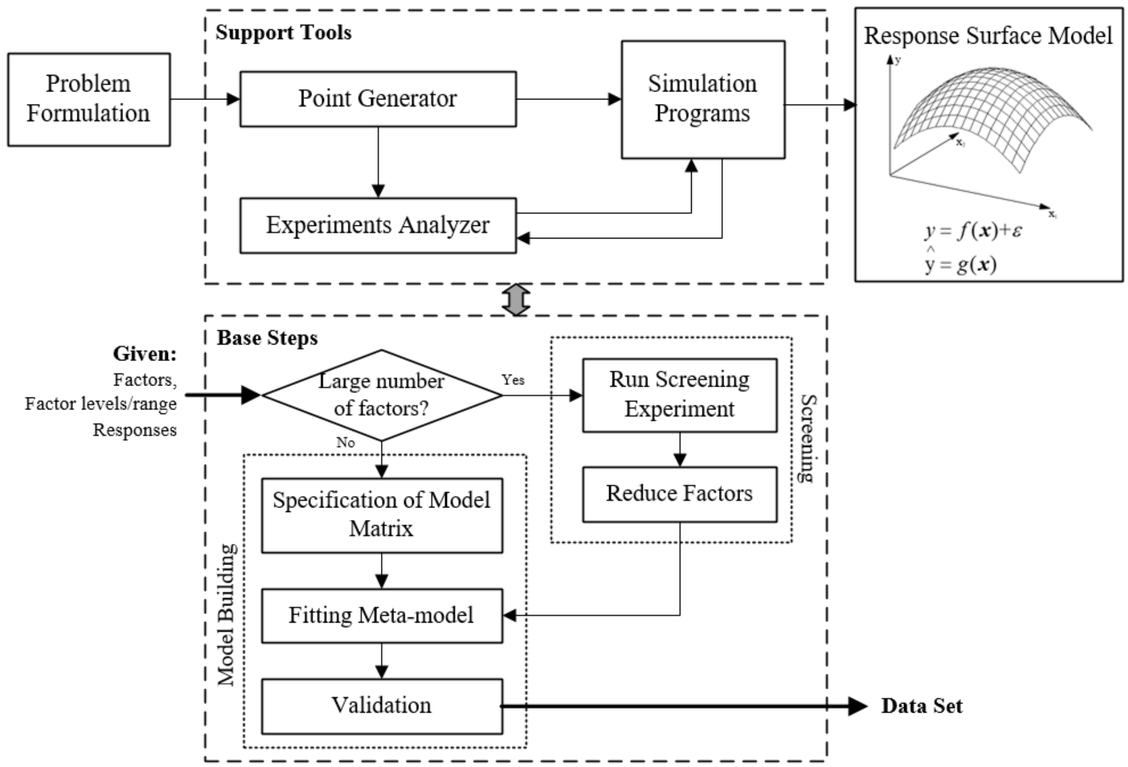


Figure 9.3: Generic procedure for Response Surface Modeling

In the development process of surrogate models, some candidate factors are selected and their ranges are defined based on existing knowledge to carry out Design of Experiments (DoE). The *Simulation Program* is used to run the experiments. This is defined as a "slot" for inserting Finite Element Analysis (FEA) programs or other simulation programs depending on the requirements of the problem. To generate data set for creating response surface models, two stages of sequential experimentation is involved. They include base steps for building approximations of computer analyses, namely screening, and model building. More detailed study of response surfaces modeling is provided in (Montgomery and Myers 1995). *Point Generator* and *Experiments Analyzer* are used to design and evaluate the essential experiments and their results (Chen, Allen and coauthors 1996).

Step 3: Compromise DSP - *Processor F in Figure 9.2*

The core step of DSE is the *compromise Decision Support Problem* (cDSP), which is a means to synthesize information for designing with multiple goals under uncertainty (Bras and Mistree 1993). The design information generated using the problem models identified/developed are communicated to the *Processor F*, namely cDSP, which is capable of handling constraints, bounds, and multiple objectives. The cDSP is used to minimize a deviation function and ultimately find the design variable values to satisfy a set of conflicting goals. The selection of two types of deviation function (Z = $[f_1(d_i^-, d_i^+), \ldots, f_k(d_i^-, d_i^+)]$), Preemptive Formulation; Z = $\sum W_i(d_i^- + d_i^+)$, Archimedean Formulation) depends on whether the designer has sufficient information and knowledge to indicate the priority of the different objectives. Various design preference P_i associated with weights W_i for the corresponding design goals G_i are defined as different design scenarios to explore the solution space. To solve the cDSP formulated, a tailored computational infrastructure known as DSIDES has been developed. The DSIDES incorporates Adaptive Linear Programming (ALP) algorithm (Mistree, Hughes and coauthors 1993), and requires a user-specified input file consisting of data defining the size of the design space, and a user supplied FORTRAN file having routines (for monitoring of the solution process) to create, formulate and execute the problem.

Step 4: Post-Solution Analysis - *Processor G in Figure 9.2*

The notion of a multi-objective approach based on the cDSP formulation originates from an understanding of the problem defined by looking at different performance criteria. Instead of finding the best single-point solution (optimization philosophy), the cDSP is used to identify satisficing solutions. Using the deviation function, the designer during post-solution analysis explores the design space by assigning different combination of weights to identify satisficing range of solutions by carrying out trade-off among the conflicting goals.

In Figure 9.4, the desired solution space is identified by exploring the design preferences and analyzing the sensitivity of design weights on the system goals. Different design scenarios are created and grouped in 'Scenarios Experiments' according to the designer's interests. These scenarios are exercised to explore the design space. The generated results of the solution space are visualized and analyzed via the comparison charts and/or ternary plots so as to develop insight for decision makers. In the comparison chart, the changing trend of goal deviations in different design scenarios is shown as a graphic display. In the ternary plot, the values inside the color contours of the plot are the deviation associated with each system goal or the actual attained values of goals for each scenario. The color bar next to the triangles indicates the range of the color values inside the plot. Based on the sensitivity analysis, satisficing solution regions are identified and recommended as that meeting the multiple design goals.

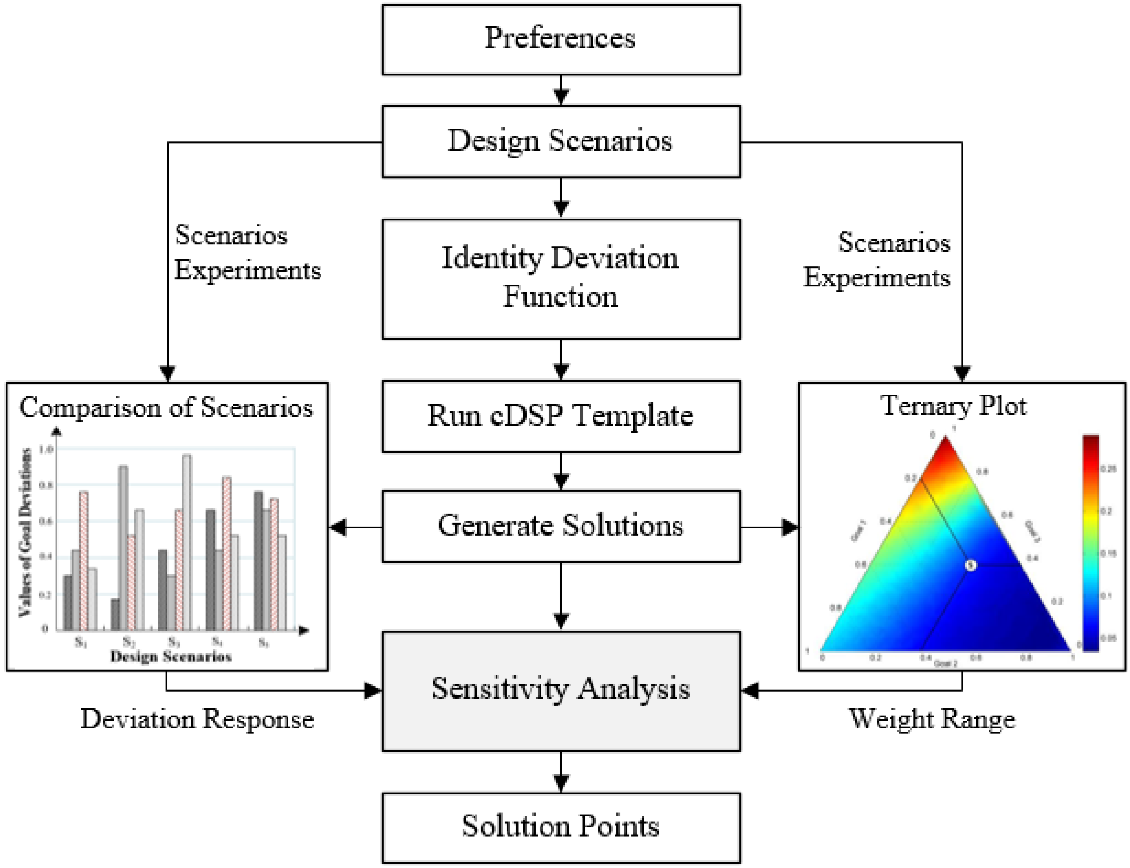


Figure 9.4: Generic procedure of design preference exploration

After the exploration process, the designer identifies a satisficing region for all the different goals by plotting a superposed plot. In the case that there exists a common region for all the goals, the designer can select weight range that satisfies all the goals from the superposed common region and identify values of the solution space. This includes values of achieved goals and system variables. Another case is when such a common regions does not exist (Nellippallil, Song and coauthors). In such a situation there is a need to modify the target value of system goals assigned in the cDSP to lower the deviations and thereby enhance the overlap possible, or even reformulate the constraints/goals to adjust the feasible design space. Both of those two cases will be discussed in the following sections. After the weight sensitivity analysis, some solution points selected in the satisficing range are recommended to the designers. The designers then have to make trade-offs among the conflicting goals and make a decision to choose one solution point as input to the next stage according to their knowledge and preference.

9.3.3 Design Space Adjustment

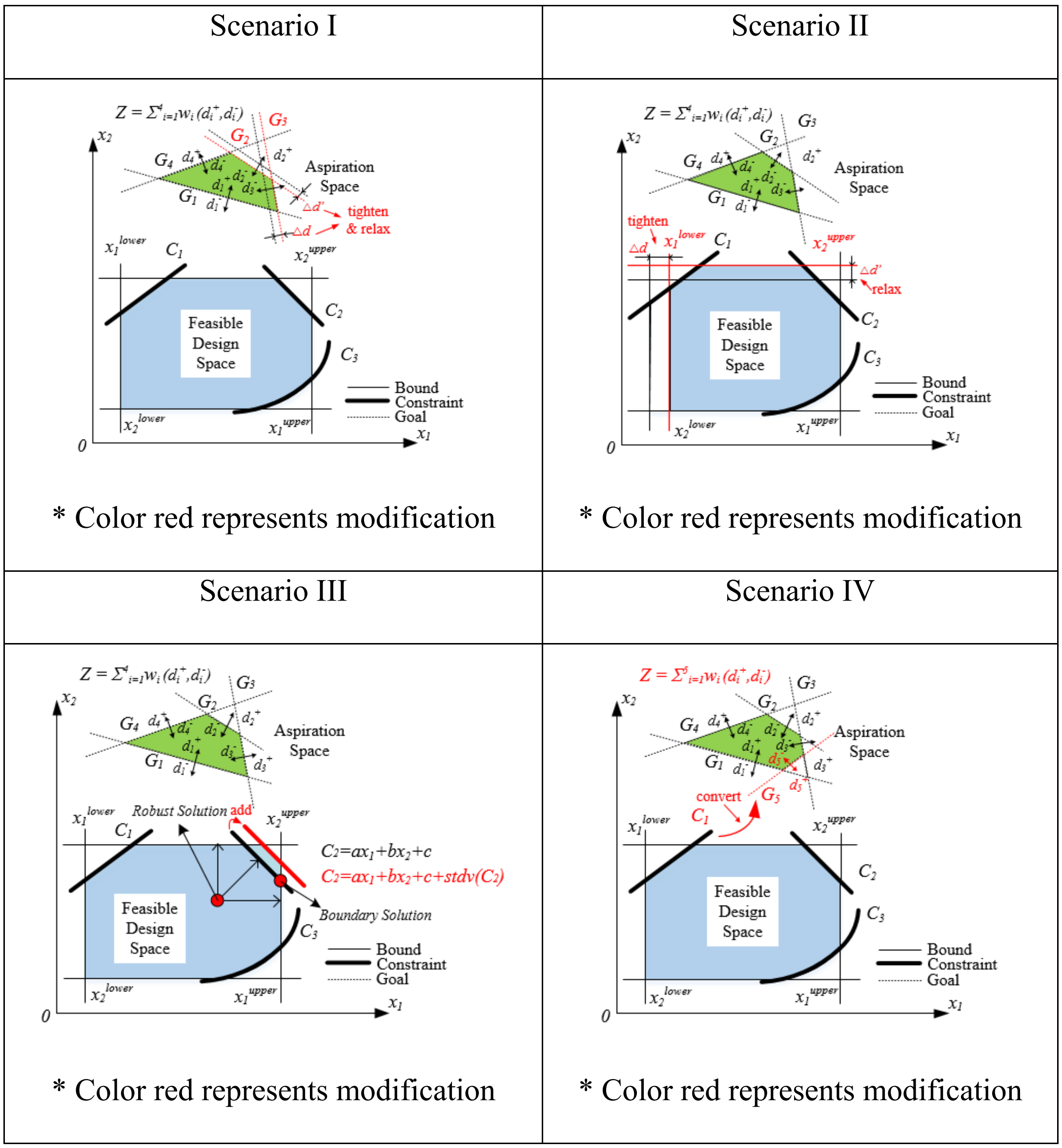


Figure 9.5: Four Possible Scenarios for the Design Space Adjustment

Taking into account the interdependencies between different design events in design process, the design space exploration process should be modifiable and robust to manage the risk of design errors caused by other design stage issues (e.g., processing error propagating to next stage). In the cDSP formulation, the system constraints/goals are the functions of system variables, namely, $f(x_i)$ and $g(x_i)$, and hence the designer can get a response value for these functions according to the minimization of deviation variables under different design scenarios. The other influential factors in a design space, namely the design constraints/goals/variables, also need to be further analyzed to check for feasibility robustness. We consider four possible scenarios that happen in the design space changes, as shown in Figure 9.5. These four scenarios can be explored by the designer for identifying a common satisficing region depending on the requirements of the design space for the problem under consideration.

In Figure 9.5, the Scenario I, II, and III involves adjusting target values associated with goals, variables, and constraints in the initial design space, respectively. Generally, in practice, the modifications are based on the designer's empirical knowledge and corresponding comparison of the initial design results. Therefore, a detailed response analysis will increase the confidence of the designer in decision-making. For Scenario III, the extra capacity of design space depending on the constraints is determined by the identification of adjustments needed after analyzing the active constraints (Sabeghi, Smith and coauthors 2015). This reduces the risk of boundary solutions with zero tolerances becoming infeasible in the face of variations. Thus, it is necessary to analyze the constraint sensitivity for determining those constraints that need to be modified by adding an extra capacity. For Scenario IV, the designer considers the newer requirements from the side of constraints or system variables in addition to the system goals to make a decision. These "additional requirements" when incorporated would change the design space thereby allowing the designer to make a confident design decision. Scenario IV is illustrated in the designing of the multi-stage steel manufacturing process (Nellippallil, Allen and coauthors 2017) addressed in Chapter 6 and is further discussed in detail in this chapter in Section 9.5.3. The application of those four scenarios depends on the specific design problem and the settings of the initial design space.

9.3.4 Modular Process Template for DSE

In the computational environment, modular-based design methods will enhance design flexibility and help improve the design efficiency. So, a modular-based process template model for design space exploration is developed to achieve the capabilities of reusability and executability. The main contents of DSE process template includes the three sub-templates: *Problem Model* (PM), *compromise Decision Support Problem* (cDSP), and *Post-Solution Analysis* (PSA). The PM sub-template has two modules: *Theoretical and Empirical Model* and *Surrogate Model*. The PSA sub-template has five modules: *Weight Sensitivity Analysis* (WSA), *Constraint Sensitivity Analysis* (CSA), *Additional Requirement Analysis* (ARA), *SSE_Experiment* (Solution Space Exploration Experiment), and *Deviation Response*. The detailed modules of the cDSP template are explained in (Ming, Yan and coauthors 2016). The functions of each module are described in detail in Section 9.4.

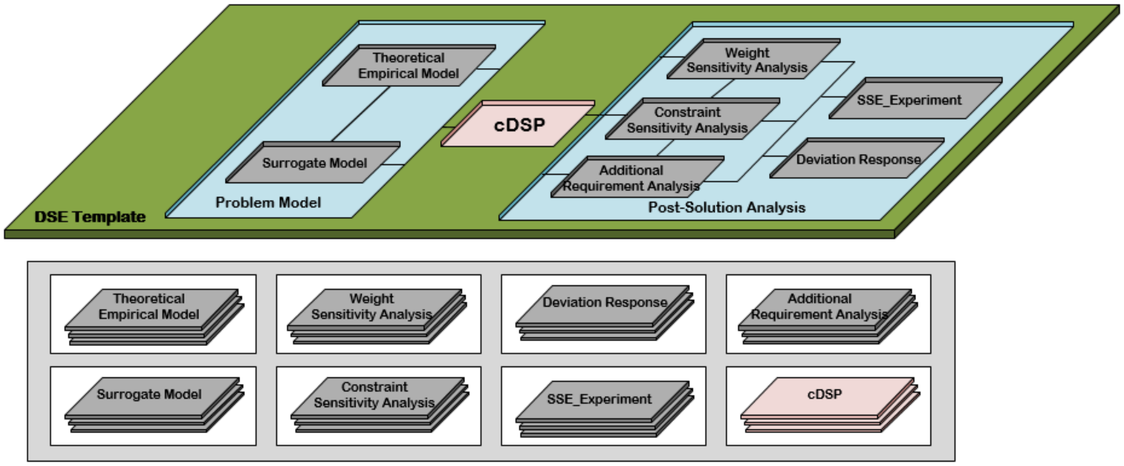


Figure 9.6: The DSE Process Template

In Figure 9.6, the DSE process template is expressed as a structure similar to a printed board assembly having some electronic components. The elements (modules), like *the theoretical and empirical model*, *deviation response*, etc., are represented as "chips" and the procedure introduced in Section 9.3.2, is represented by the "breadboard." Due to the modular structure, the DSE process template includes three reuse scenarios:

1) Reuse the "breadboard." The procedure for design space exploration corresponding to the "breadboard" is reused in the instantiation of any problem by populating specific information on the board.

2) Reuse the "chips." Specific information (e.g., *Surrogate Model*) corresponding to the "chips" is reused in any different instantiation of a problem for the exploration process template.

3) Reuse the assembly. An instantiated DSE process template with specific information corresponding to the "chips" is reused, where some "chips" (e.g., *SEE_Experiment*) are modified whereas others remain unchanged.

The modular DSE process template provides the ability to capture and reuse the information and knowledge associated with DSE, which increases the confidence of designer in decision-making and provide the designer with insights to make comprehensive decisions, particularly in the early stages of design.

9.4 Ontology Development for Design Space Exploration Process Template

To further satisfy the requirements of DSE presented in Section 9.3.1, a frame-based ontology for DSE process template is developed to support the management of reusable information and enhance the designer's understanding of process behavior. In this section, the classes and slots that constitute a frame-based ontology are formally defined, as well as the instantiation of exploration processes using the ontology is presented in keeping with the DSE process template model.

9.4.1 Definition of Class and Slot

In the DSE process template, the "chips" embedded in the "breadboard" constitute the main structure of the ontology. The concepts in the DSE process template are explicitly defined as `Classes`, like *DSE_Template*, *PM_Template*, *PSA_Template*, etc. Some additional associated `Classes`, like *ResponseSurface, Response, Factor*, etc., are identified to capture the re-usable information of DSE; which also increases the semantic richness and integrity of the DSE process template ontology. The detailed definitions of the `Classes` are shown in Table 9.3.

Meanwhile, the semantic relationships between `Classes` are captured using `Slots`. There are two types of `Slots` - data slots and object slots. Data slots are used to link classes to end data (e.g., *weightRange* links the *WS_Analysis* to capture a value of weight range), while object slots are used to link classes to other classes (e.g., *hasWSA* links

PSA_Template to *WS_Analysis*) or to themselves. Based on the exploration processes and the DSE process template structure, the data slots and object slots of the ontology are defined as shown in Table 9.4 and Table 9.5, respectively. Some slots that reuse other ontologies will not be described here, like *name, value, image*, etc.

Table 9.3: Classes of DSE Process Template Ontology

Class	Definition
DSE_Template	A formulation that integrates all the associated template modules and represents the information structure of DSE processes
PM_Template	A sub-template that integrates all the associated modules and represents the information structure for a specific problem
PSA_Template	A sub-template that integrates all the associated modules and represents the information structure of solution space exploration
TheoreticalEmpiricalModel	A module that integrates all the related information of mathematical model for initial design space
SurrogateModel	A module that integrates all the related information of surrogate model and experimental design
WS_Analysis	A module that integrates all the related information of weight analysis to define a satisficing range solution to all the system goals
CS_Analysis	A module that integrates all the related information of constraint analysis to define an extra capacity of design space

AR_Analysis	A module that integrates all the related information of additional requirement analysis to define a common range solution
SSE_Experiment	A module that represents a set of design scenarios corresponding to the associated goal weight
DeviationResponse	A module that represents a set of goal deviation corresponding to the associated design scenario
ResponseSurface	A module that integrates all the related information of surrogate model using response surface methodology
Response	A class represents a mathematical model for performance measures
Factor	A class represents input variables corresponds to a specific process
GoalWeight	A class represents the designers' interest in the associated system goal
GoalDesponse	A class represents the achieved value of the associated system goal in a specific design scenario
ConstraintResponse	A class represents the achieved value of the associated constraint in a specific design scenario, including "*Active Constraint*" and "Inactivate Constraint"
VariableResponse	A class that represents the achieved value of the associated system variable in a specific design scenario

DesignScenario	A class that represents a set of preference value corresponds to the associated design weight
FactorValue	A class that represents the value of a specific factor corresponds to the associated factor level
FactorLevel	A class that represents the value of a factor level identified by the designers
Preference	A class that represents the value of preference corresponds to the associated system goal in a specific design scenario
SolutionPoint	A class that represents the value of a point in the specific satisficing range solution
TernaryPlot	A class that represents the visualizing information of desired and sensitive regions of solution space

Table 9.4: Data Slots of DSE Process Template Ontology

Class	**Definition**	**Type**
lowest_SSE	The value of the lowest sum of squares error (highest R^2) used to be fitting the regression model of response	Float
factorVaule	The value of a specific factor corresponds to the associated factor level, and it is used in simulations of DoE	Float
dataPoint	A set of goal deviation values associated a specific system goal, and it used to generate the ternary plot	Float

resluts_of_SSE	A set of values (system variables and goals) for solution points that satisfy all the design requirements and goals	Float
extraCapactiy	A value of standard deviation that is added to the active constraints with zero or limited capacity	Float
achievedValue	A value that can be achieved in response to the result of minimizing the deviation function	Float
preferenceValue	A set of preference values for a specific design scenario and experiment of solution space exploration	Float
acceptableValue	A value of the minimum target for requirements that can be accepted or approved	Float
deviationValue	A set of response values that is normalized treatment to generate the ternary plot	Float
weightRange	The range value of weight for an associated goal which satisfies all the system goals	Interval
simulationPrograms	The (path of) code execution that is used to run the simulation programs of designed experiments	String
modelMatrix	The (path of) model matrix that represents the treatment combinations corresponding to the type of DoE	String
typesOfFittingModel	The types of fitting model that represents a regression meta-model	Symbol

validationRSM	The verification results of response surface model	String

Table 9.5: Object Slots of DSE Process Template Ontology

Class	**Definition**	**Type**
hasPM	Specifies the *PM_Template* instance of *DSE_Template*	Instance
hasPSA	Specifies the *PSA_Template* instance of *DSE_Template*	Instance
is_Solved	Specifies the *cDSP_Template* instance of *DSE_Template*	Instance
hasSM	Specifies the *SurrogateModel* instance of *PM_Template*	Instance
hasTEM	Specifies the *TheoreticalEmpiricalModel* instance of *PM_Template*	Instance
hasFactor	Specifies the *Factor* instance of *ResponseSurface*	Instance
hasResponse	Specifies the *Response* instance of *ResponseSurface*	Instance
functionOf	Specifies the *Factor* instance of *Response*	Instance
associatedFactor	Specifies the *Factor* instance of *FactorValue*	Instance
toFactorLevel	Specifies the *FactorLevel* instance of *FactorValue*	Instance
hasWSA	Specifies the *WS_Analysis* instance of *PSA_Template*	Instance
hasCSA	Specifies the *CS_Analysis* instance of *PSA_Template*	Instance

hasARA	Specifies the *AR_Analysis* instance of *PSA_Template*	Instance
constraintResponse	Specifies the *ConstraintResponse* instance of *CS_Analysis*	Instance
associatedVariable	Specifies the *Variable* instance of *AR_Analysis* and *SolutionPoint*	Instance
associatedGoal	Specifies the *Goal* instance of *TernaryPlot, GoalDeviation, GoalWeight,* and *SolutionPoint*	Instance
associatedConstraint	Specifies the *Constraint* instance of *AR_Analysis* and *ConstraintResponse*	Instance
associatedWeight	Specifies the *GoalWeight* instance of *Preference*	Instance
toScenario	Specifies the *DesignScenario* instance	Instance
preferenceValue	Specifies the *Preference* instance of *DesignScenario*	Instance

9.4.2 Instantiation of Exploration Using DSE Process Template Ontology

According to the procedure for DSE defined in Section 9.3.2, the DSE process template is assembled using three sub-templates: PM template, cDSP template, and PSA template, as shown in Figure 9.7. Before instantiating the DSE process template, the designer needs to clarify the corresponding design event defined in the PEI-X diagram. This is useful for the designer to determine the relevant design information and knowledge involved in the design problem that is addressed. In this chapter, we focus on creating and populating the PM template and the PSA template. The instantiation procedures for these are listed below.

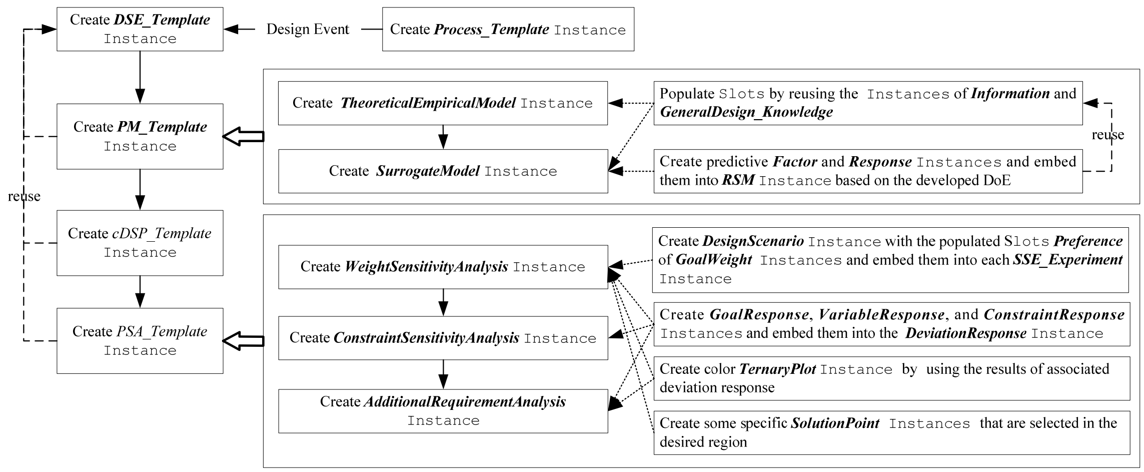


Figure 9.7: Instantiation Procedure of the DSE Process Template

(1) **Create *PM_Template* `Instance`**. Based on the input instances of `Classes` *Information* and *GeneralDesign_ Knowledge* that are defined in the design event, create and populate the *TheoreticalEmpiricalModel* `Instance`. When TEM instances are not directly available from literature, there is a need to create *SurrogateModel* `Instance`. This involves creating predictive *Factor* and *Response* `Instances` and embedding them into *RSM* (Response Surface Model) `Instance` based on the developed DoE. The newly created template instance for the surrogate model will be stored as new knowledge to achieve subsequent reuse.

(2) **Create *PSA_Template* `Instance`**. The PSA template can be equipped with three modules, i.e., weight sensitivity analysis, constraint sensitivity analysis, and additional requirement analysis, which are combined based on the needs of the specific problem and populated into the `Slots` of PSA template instance. The `Instance` of WSA is a basic module used to support the designer to determine the desired solution regions. The input `Slot` of WSA module is the experiment of solution space exploration (*SSE_Experiment*), and the output `Slots` are *TernaryPlot* and *DeviationResponse* sub-

modules used to provide insight for the designer in decision-making. At the beginning of post-solution analysis, the *DesignScenario* `Instance` with the populated `slots` *Preference* of *GoalWeight* `Instances` is created and embedded into each *SSE_Experiment* `Instance`. The results of the cDSP template are captured by the instances of `Classes` *GoalResponse*, *VariableResponse*, and *ConstraintResponse*. Meanwhile, these various types of response instances are populated into the *DeviationResponse* `Instance`. The `Instance` of color *TernaryPlot* for each system goal is created by using the results of associated goal deviation response for the scenarios considered in WSA module. Based on the analysis of ternary plots, a common region that satisfies all the system goals is generated by the formation of the superposed ternary plot.

In some special problem cases when no common region in the initial design solution space exists, the designer needs to carry out a detailed post-solution analysis to explore and identify regions that satisfy requirements. This increases the understanding of the design response and the designer's confidence in the prediction. Therefore, the `Instances` of CSA module and ARA module are created to capture the reusable information for design space adjustment so as to identify satisficing range. In the CSA module, the extra capacity of design space is identified by analyzing the active constraints. While, in the ARA module, the variables/constraints are further analyzed as an additional requirement along with the system goals, and the *TernaryPlot* `Instance` for the variables/constraints are created by using the results (variable/constraint response) for each design scenario. All the information from WSA, CSA, and ARA modules that are embedded into PSA template instance contributes to the determination of the desired solution region. From the solution space generated, specific *SolutionPoint* `Instances` are selected that best satisfices the designer's interests.

According to the scenarios defined in Section 3.3, the modified information based on the deviation response can be documented by the different instance versions. Such as, the target for requirements that can be accepted or approved, the acceptable value is modified based on the designer's experience knowledge or preference to get a satisficing common region. The adjusted acceptable value is captured by the different versions of the *TernaryPlot* `Instance`, which is embedded into the corresponding WSA, CSA, and ARA modules.

9.5 Testing the DSE Process Template Ontology using the Hot Rod Rolling Example Problem

In this section, the utility of DSE template ontology is illustrated via an automotive gear manufacturing process design problem - a complex system design that calls for a series of decisions to be made. A key transmission element of vehicles, gears are made of various grades of carburized steels. Due to the increasing demand for light weight in the automotive sector, steel manufacturers urgently require the rapid development of newer grades of advanced high strength steels in response to the competition from other materials, especially some emerging materials with performance (Nellippallil, Vignesh and coauthors 2017). The manufacturing process of automotive gear involve several different stages, in this example, we primarily focus on the hot rod rolling process. The details of the example are available in Chapter 6.

9.5.1 Designing of Hot Rod Rolling (HRR) Process Chain

The products of steel manufacturing processes include rod, bar, sheet, etc. The process chain involves a series of unit operations like continuous casting, reheating, rolling, cooling, forging, machining and finishing. Nellippallil and co-authors (Nellippallil, Allen and coauthors 2017) define vertical and horizontal integration for hot rod rolling process chain problem and showcase the information flow using Figure 9.8. More details available in Chapter 6.

Horizontal integration means the integration of different unit operations having sequential information flows (material) to produce the final product. To achieve horizontal integration there needs to be information in detail regarding the individual processes happening at different length scales for each unit operation. This is achieved by carrying out modeling of material behaviors at different scales within a unit operation and integrating the information generated. This is defined as vertical integration of models within a unit process/operation. Vertical integration allows the designer identify the information to be communicated from one unit operations to next thereby allowing to achieve the horizontal integration of the entire manufacturing process chain The vertical and horizontal integration of models further allows the designer to carry out the integrated decision-based design exploration of the manufacturing process chain to realize the end product.

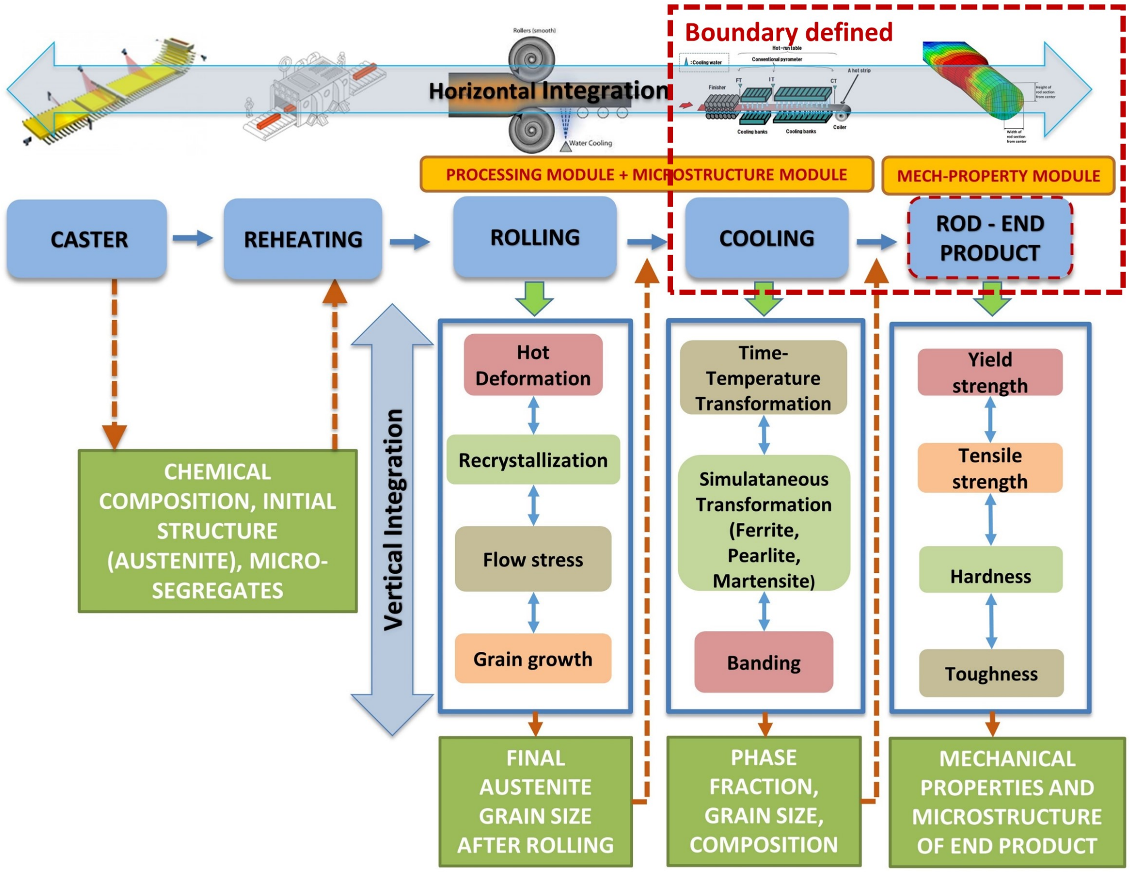


Figure 9.8: Integration of models with information flow in hot rod rolling process chain (Nellippallil, Allen and coauthors 2017). See Chapter 6 for details.

In the hot rod rolling process, the designer has to deal with large amount information (e.g., process parameters, constraints, bounds, etc) that raises the complexity of designing. Hence the requirement of defining a boundary and framing the right problem is critical. The designer has to precisely control the process variables to obtain the desired mechanical properties and microstructure for the rod and to achieve this model coupling at different scales is required. To illustrate the reusability of information during the design space exploration process using the DSE process template, we are framing a boundary within the problem defined in Chapter 6 (Nellippallil, Allen and coauthors 2017). Our focus in this chapter is to demonstrate how a designer can capture, represent, and document reusable information using the hot rod rolling problem and thereby support the process designers to make decisions by considering robustness in design.

9.5.2 Populating a Basic DSE Process Template Instance

According to the procedure for DSE mentioned in Section 9.3.2 and the instantiation approach for DSE process template mentioned in Section 9.4.4, a basic DSE process template instance is created. The populated sub-templates for problem model and post-solution analysis are illustrated by using the cooling module process stage of hot rod rolling problem.

Create and Populate Process Template for Problem Model

The purpose of the problem model template is to allow the designer to determine the initial design space and then provide/use this design information to formulate a cDSP. In other words, the process designer needs to initially determine the basic elements of the design space before carrying out the exploration processes. We showcase the same using Figure 9.9. For the hot rod rolling process chain problem addressed in this chapter, see the embedded `Instance` "ProblemModel-1" presented in the window "① " of Figure 9.9. The input to the problem module are the chemical composition (e.g., the carbon concentration [C], the manganese concentration after rolling [Mn]), final austenite grain size after rolling (D), the cooling conditions, i.e., cooling rate (CR). The output includes the mechanical properties of end product, i.e., yield strength (YS), tensile strength (TS), and hardness (HV) for the rod, which are dependent on the final microstructure after cooling like the ferrite grain size after cooling (FGS, D_α), the phase fractions of ferrite (X_f) and pearlite ($1 - X_f$), the pearlite interlamellar spacing (S_0) and the composition variables like silicon ([Si]), nitrogen ([N]), phosphorous (P), manganese ([Mn]).

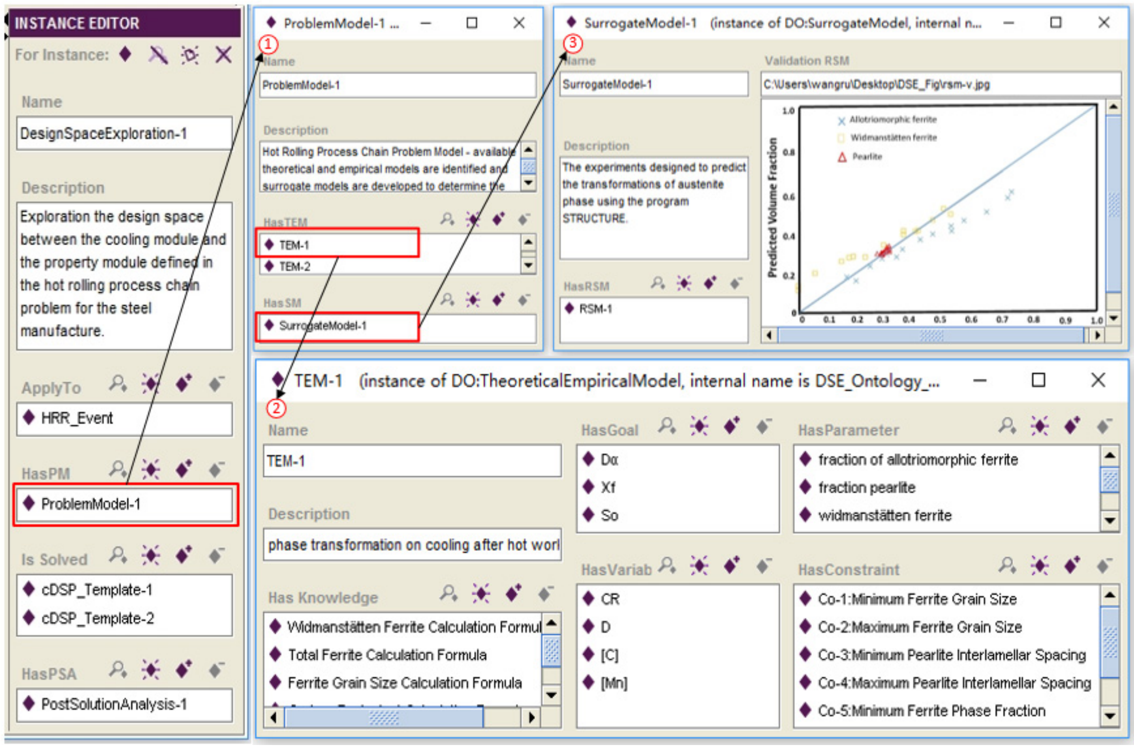


Figure 9.9: Instances of the PM Template embedded in DSE Process Template

According to the boundary defined within the problem described in Section 5.1, the problem formulation for cooling module and property module in HRR is addressed via two compromise Decision Support Problem (cDSP) mathematical constructs with information flow between the two cDSPs. Therefore, the process designer populates two theoretical and empirical model (TEM) modules for providing a combination of design information as the inputs for the cDSP models, i.e., "TEM-1" and "TEM-2". As shown in Figure 9.9, the design information that constitutes the module includes: "system goal," "constraint," "system variable," "design parameter," and "existing knowledge" about the available functional relationships. The details of these information instances are given in (Nellippallil, Allen and coauthors 2017). For example, the "TSM-1" embedded in the `Instance` "ProblemModel-1" is presented in the window "②" of Figure 9.9.

In the hot rod rolling problem addressed, there is a need to design an experiment for predicting the transformations of the austenite phase. Depending on the cooling criteria, the phase transformations that happens during cooling after hot working converts the austenite phase to different steel phases like Allotriomorphic ferrite, pearlite, Widmanstätten ferrite, bainite, and martensite, etc. (Jones and Bhadeshia 1997). In this problem, there is a requirement to predict these transformed phases to manage the banding phenomena that happens in the microstructure. A meta-modeling approach is used to develop surrogate models for the different phases of steel that is transformed, as shown the window "③" in Figure 9.9. In this case, we assume that the transformations of austenite only happen to ferrite and pearlite phases. In the window "①" of Figure 9.10, a three-level fractional factorial design is carried out to develop response surface models for the transformation of austenite to ferrite and pearlite via the embedded `Instance` of "RSM-1". Four factors are identified for the design of experiments to develop the responses for the phases and they are selected due to their huge influence on austenite transformations and the formation of banded microstructures (Robson and Bhadeshia 1997). The factor values corresponding to the relevant factor levels for the simulations are identified, see the window "②" of Figure 9.10. The simulation runs are performed using simulation programs to obtain the input-output correlations so that the cDSP for the problem can be formulated. For example, in the problem addressed in (Nellippallil, Song and coauthors), the simulation program used is the finite element software ABAQUS in which a finite element model for hot rod rolling is developed to predict the oval to round geometry conversion during rolling. Here, we carry out the experimental runs to predict the steel phases using the 'STRUCTURE' program based on the data and tools available in (Jones and Bhadeshia 1997). The input and output data sets are used to estimate the parameter values of the meta-model using least squares. Typically, a regression meta-model belongs to one of the three classes: 1) main effects model (a first-order polynomial), 2) main effects + interaction effects (a first-order polynomial augmented with two-factor interactions), 3) quadratic model with quantitative factors (a second order polynomial including purely quadratic).

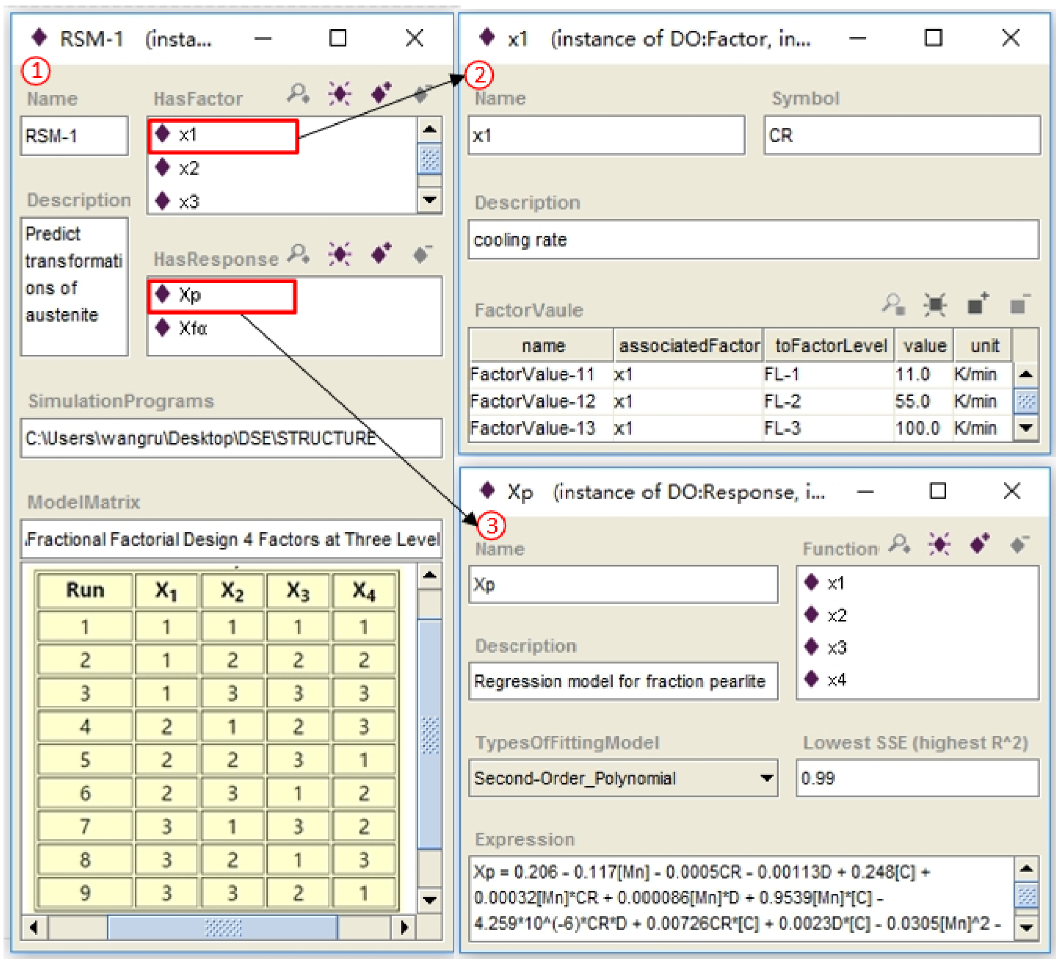


Figure 9.10: Instance of the RSM Model

In the window "③" of Figure 9.10, the regression model developed for fraction pearlite X_p a R^2 value of 0.99 is given. The model is generated by fitting a second order polynomial type function to the simulation results after DoE.

Create and Populate Template for Post Solution Analysis

Based on the given combination of design information that is generated from the specific problem model shown in Figure 9.9, two cDSP templates are formulated. The cDSPs are used to find the values of the design variables that satisfy a set of conflicting goals, such as, minimizing D_α, S_0 for the microstructure space after cooling, and maximizing YS, TS for the end mechanical properties of rod. The detailed information of the cDSP formulations are available in (Nellippallil, Allen and coauthors 2017), and the description on creating and populating the cDSP template is illustrated in (Ming, Yan and coauthors 2016). In this chapter, we focus on the achieving flexibility in identifying design solutions under uncertainty thereby allowing designers to rapidly explore the solution space and identify solutions that meets conflicting goals. The information on sensitivity analysis and deviation response in the exploration process is captured via the `Slots` of *PSA_Template*.

As shown in Figure 9.11, design scenarios 1-4 in "Experiment-1" is a situation where the designer's interest is to achieve the target of one of the system goals (S1, S2, and S3) or give equal preference to all the goals considered (S4). The design scenarios 5-7 are in "Experiment-2" where two goals are given equal preference, while the third goal is not given any preference. The design scenarios 8-13 are in "Experiment-3" where the designer gives greater preference to one goal, a lesser preference to the second goal and zero preference to the third goal. Design scenarios 14-19 are in "Experiment-4" where all the goals are given preferences with two of them being the same preference. The preferred value for each goal weight in the design scenarios identified is captured, see the window "②" in Figure 9.12.

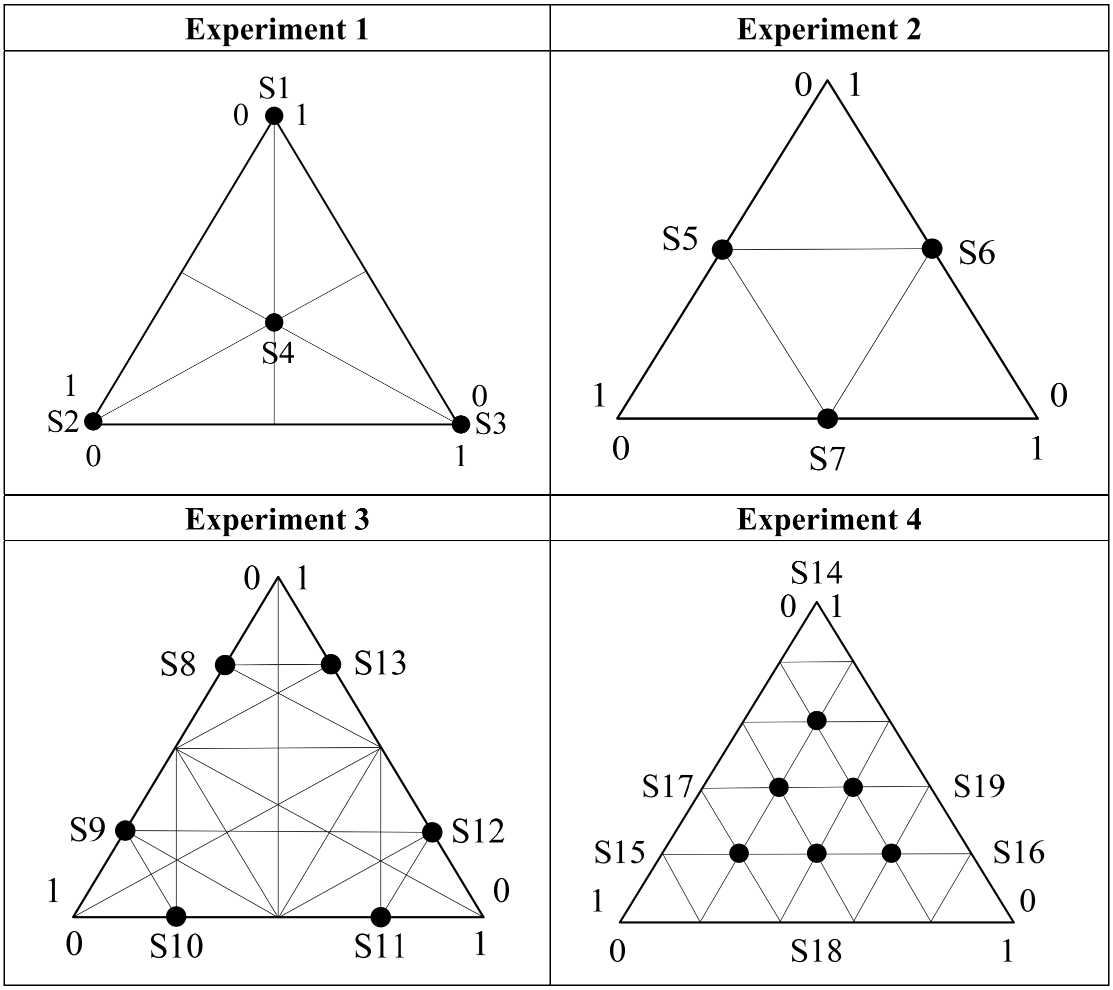


Figure 9.11: Experiment Scenarios for Solution Space Exploration

In Figure 9.12, the weight sensitivity analysis is carried out first to obtain the desired solutions that satisfy high priority goals. Here, the deviation function is identified as *Archimedean* formulation so that the process designer can explore as many scenarios as possible by assigning various combinations of weights to the associated system goals. In this case, the process designer creates four types of exploration experiments that are captured by the `Slots` "Input" in "WeightSensitivityAnalysis-1" (see the window

"①" in Figure 9.12) for the "cDSP_Template-1". It is used to determine the microstructure factors after rolling and operating set points for cooling that satisfies the requirements identified (i.e., system goals D_α, X_f, and S_0 are defined by system variables CR, D, [C], and [Mn]). The cDSP template formulated is exercised for different design scenarios by running the computational infrastructure DSIDES. Using DSIDES the cDSPs are executed to minimize the deviation function and identify the corresponding values of system variables. Then, the deviation variables of system goals which represent the degree by which achieved value is off the target are captured; shown in the window "③" of Figure 9.12. Ternary plots for each goal are generated to visualize and explore the solution space based on those sets of deviation variables. For example, the solution space for "G1" (minimizing ferrite grain size D_α) is shown in Figure 9.12. The process designer can find the minimum achieved value of D_α using the current configuration information of cDSP template as 10.06 μm, which satisfies the acceptable value from the existing empirical knowledge 15 μm. We can see the contour region identified by the red dashed lines satisfy the design requirements for "G1". Similar ternary plots for all the system goals are populated in the `Slots` "Output" of `Instance` "WeightSensitivityAnalysis-1". Based on the analysis of individual ternary plots for each goal, the process designer then creates a superposed plot including all the goals to identify a common region that satisfies all the goals and thereby identify solutions. This process adds confidence to the designer's decision-making. The superposed region is seen as the pink area in window "①" of Figure 9.12.

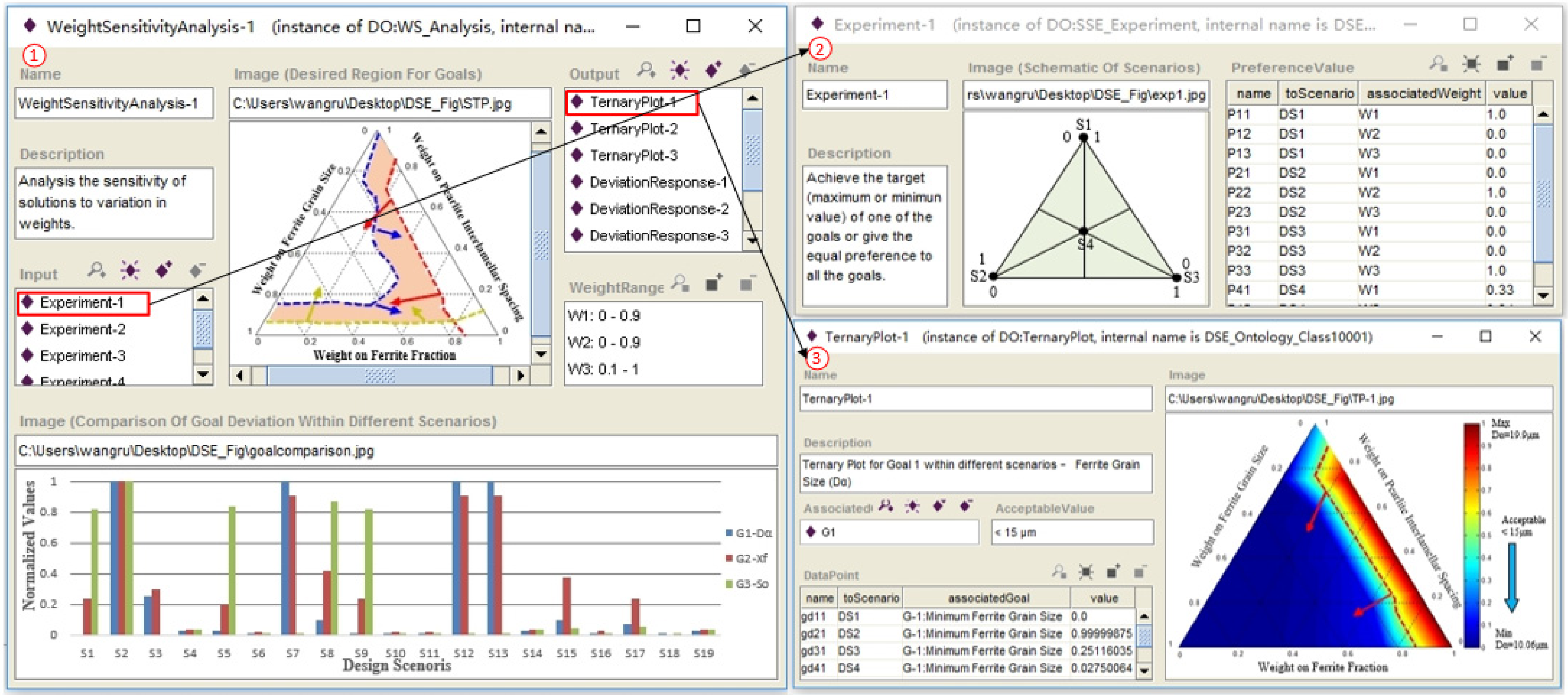


Figure 9.12: Instance of Weight Sensitivity Analysis for Cooling Module

To increase the designer's understanding of the solution space, a bar chart that represents the comparison of goal deviation for different design scenarios are created. In this bar chart, the shorter bar indicates a better design point/solution as the solution's deviation from the target defined is less in that situation. By observing and analyzing the superimposed region for the problem discussed, we are able to predict that some satisfactory solution points may occur in the following design scenarios: S6, S10, S11, S16, and S18. The process designer only needs to carry out design trade-offs based on the specific requirements and select the final design among those satisfactory solution points.

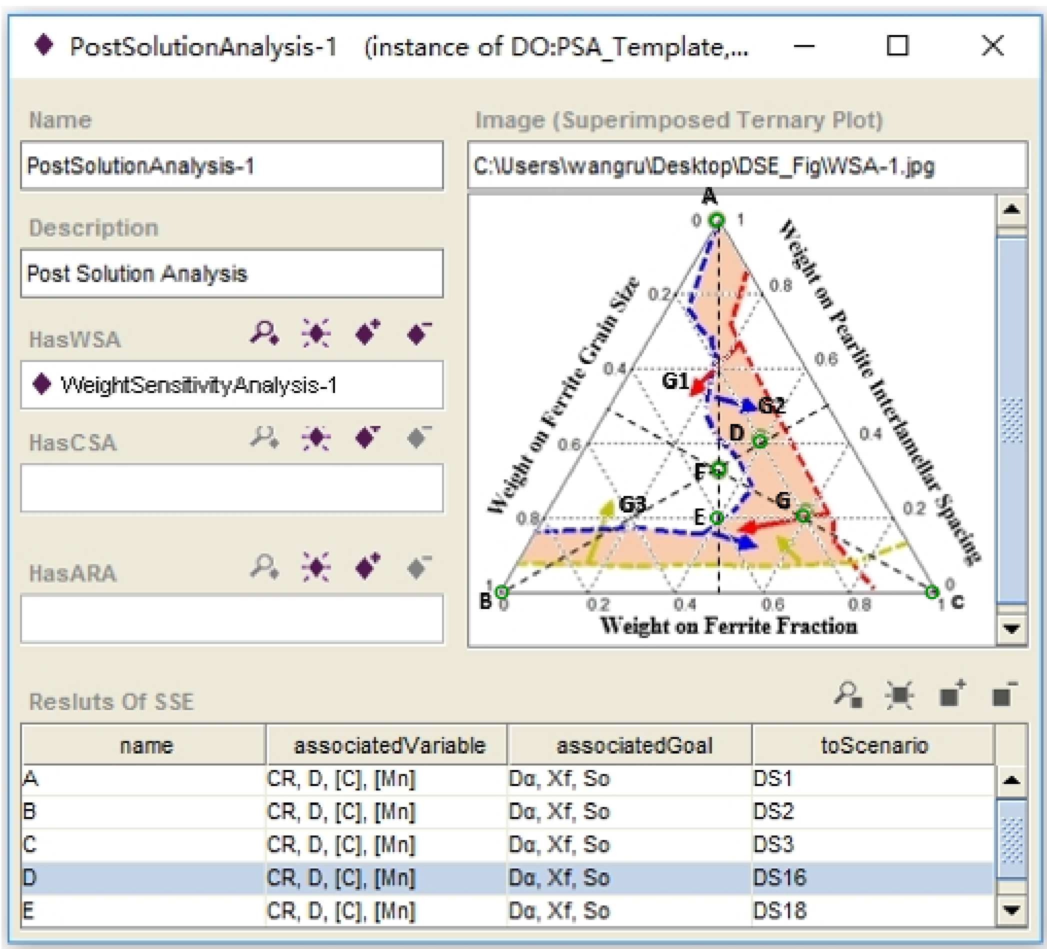


Figure 9.13: Instance of PSA Template for Cooling Module

To further explain this process, we pick seven points to fully compare the good and bad of solutions within the different scenarios both from the common region identified, boundary, and outside, as shown in Figure 9.13. The information of design points is populated in the `Slots` "Results_SSE" (results of solution space exploration) of `Instance` "PostSolutionAnalysis-1". The detailed results of the selected points are listed in Table 9.6.

Table 9.6: Comparison Results for the Selected Points

Sol. Pt	$\boldsymbol{D_\alpha}$	$\boldsymbol{X_f}$	$\boldsymbol{S_0}$ μm	***CR*** K/min	***D*** μm	**[C]** %	**[Mn]** %
A	12.5	0.684	0.149	11	30	0.19	1.02
B	10.06	0.681	0.176	99.9	30	0.18	0.7
C	19.9	0.714	0.182	11	74.2	0.18	0.7
D	10.74	0.681	0.151	44.4	30	0.18	0.94
E	10.33	0.673	0.151	70.3	30	0.18	0.93
F	10.33	0.673	0.151	70.1	30	0.18	0.93
G	11.05	0.687	0.151	33.06	30	0.18	0.95

In Table 9.6, we observe that solution points A, B, and C satisfy the associated goals respectively, i.e., minimum ferrite grain size (D_α), maximum ferrite fractions (X_f), and minimum pearlite interlamellar spacing (S_0). Compared to other design points E, F, and G, the point D that lies in the common region identified and corresponds to design scenarios S16 satisfies all the conflicting goals in the best possible manner. Thus, the point D is selected as the recommended solution to the subsequent process stage. This information will be passed to next cDSPs formulated for subsequent manufacturing operations thereby achieving the horizontal integration of manufacturing process chain.

9.5.3 Populating a Special DSE Process Template Instance

In Section 9.5.2, a basic DSE process template instance is created by instantiating the PM template and the PSA template, and the reusable information of design space exploration for the cooling module in HRR is populated. In that case, there exists a common region that satisfies all the goals simultaneously in the processes of post-solution analysis. The process designer has sufficient confidence to identify the design set points from the desired solutions identified for cooling that meet the target microstructure requirements defined. In this section, another case where there doesn't exist a common region is discussed via instantiating a special DSE process template.

In the HRR problem defined in Section 9.5.1, the subsequent process stage after microstructure correlation calculation (cooling module) is the property module for predicting the mechanical properties. Here the mechanical property system goals for the rod (end product) are identified as yield strength (YS), tensile strength (TS), and hardness (HV). The theoretical and empirical models of property module (TEM-2 `Instance`) are populated into the PM template instance as shown in Figure 9.9. This allows the designer/user to determine the design elements (e.g., goal, constraint, variable, etc.) and the mathematical models involved in the cDSP formulation (cDSP_Template-2 `Instance`) that is used to solve the property module. Similar to the exploration processes explained in previous section, the basic module of PSA template "WeightSensitivityAnalysis-2" `Instance` is created and its output `Slots` are populated based on the results of cDSP_Template-2 `Instance` by carrying out the experiment scenarios for solution space exploration (see Table 9.6).). As per the ternary plots developed for each system goal (mechanical properties of rod) using the results associated with the goal deviation response, a superposed ternary plot is generated to support the designer to determine a desired solution region that satisfies the requirements, as shown in Figure 9.14.

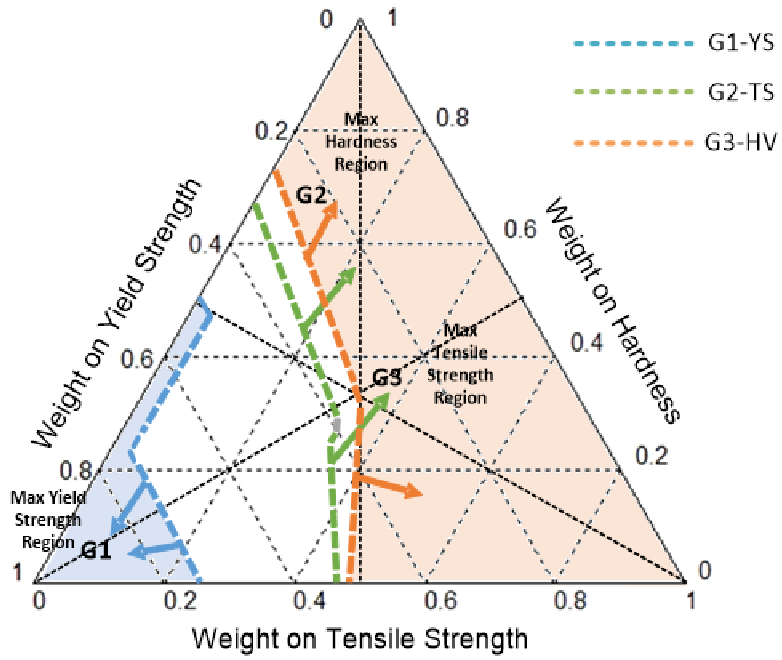


Figure 9.14: Superimposed Ternary Plot

In the superposed ternary plot, the blue contour region identified by the blue dashed lines satisfies the system goal - 1 of maximizing yield strength and the maximum yield strength achieved is 320.6 MPa when the weight assigned to yield strength goal is 1.0. The pink contour region identified by the orange and green dashed lines simultaneously satisfy the system goals of maximizing tensile strength and hardness. The target values of tensile strength and hardness are achieved when the weight of their associated goals tends to 1. The maximum value achieved for tensile strength is 750 MPa and for hardness is 170. In Figure 9.14, we observe that there does not exist a common region that satisfies all the system goals even if the designer adjusts the acceptable value of the target. In this situation, the process designer has to consider some additional requirements for adjusting the initial design space and use the information associated to make a design decision. The information associated with system variables and constraints associated with the problem under study, when incorporated into the solution space exploration scheme along with the system goals will/could provide the designer with information that can then be used to make a design decision in such situations. We explain the same for the HRR problem in the following section.

In the HRR problem, there are other important design requirements that affect the mechanical properties of the product, such as the material's impact toughness and the banded microstructure after cooling. The impact transition temperature (ITT) denotes the boundary between brittle and ductile failure when subjected to impact loads and is used to define the toughness of a material. In this problem, it is identified as a constraint in the initial design space. Meanwhile, the management of banded microstructure after cooling is studied by considering the ferrite fraction (X_f) and pearlite fraction ($1 - X_f$) obtained after cooling. The ferrite fraction (X_f) is identified as a system variables in the "TEM-2" instance and was a system goal in the previous process stage (i.e., cooling module). In the post-solution analysis for mechanical properties module, the `Slot` of additional requirement analysis needs to be populated after the instantiation of "WeightSensitivityAnalysis-2". As shown in Figure 9.15, the "AdditionalRequirementAnalysis-2" `Instance` is created based on the deviation responses for the system variable (ferrite fraction) and the constraint (impact transition temperature) identified for this problem.

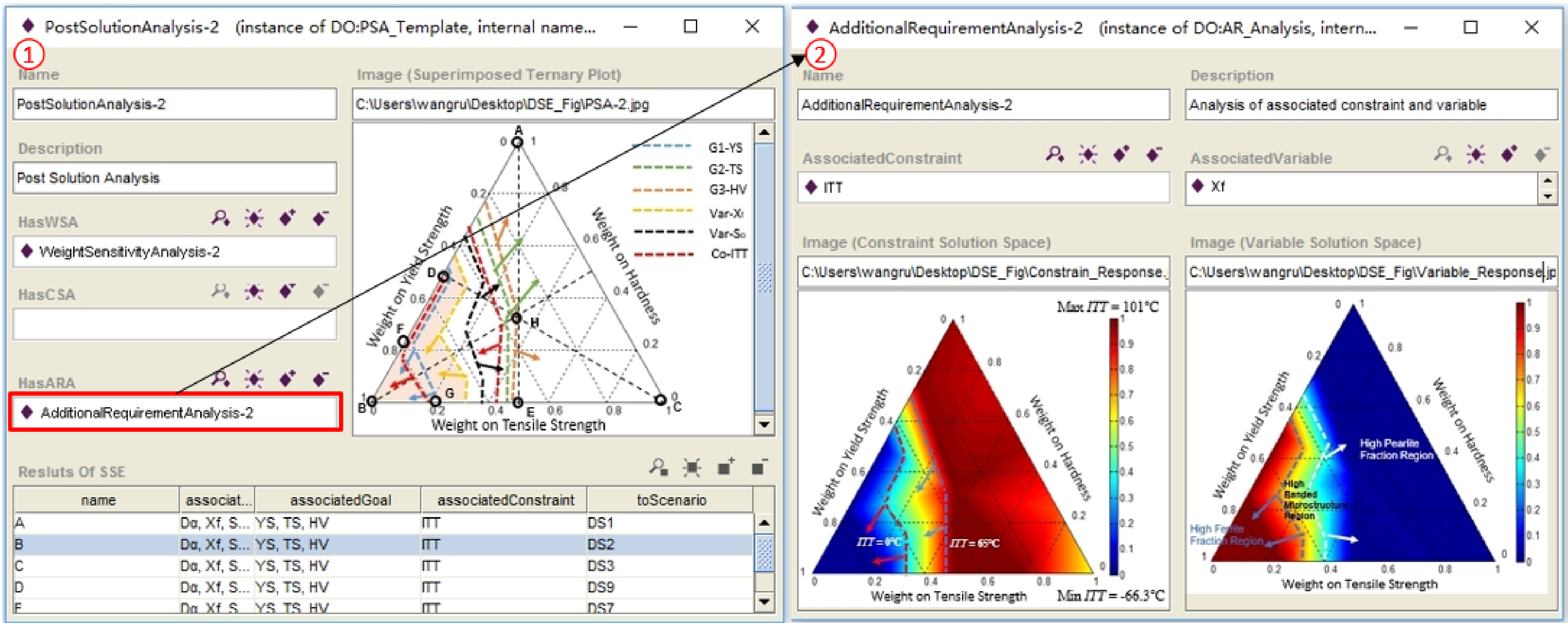


Figure 9.15: Instance of PSA Template for Mechanical Properties Module

The ternary plots for the achieved solution space for the constraint (impact transition temperature (ITT)) and the system variable (ferrite fraction (X_f)) with respect to the change in weights assigned to the system goals defined by yield strength (YS), tensile strength (TS), and hardness (HV) are shown in window "②" in Figure 9.15.

In the constraint solution space, the contour region identified by the red dashed lines are where the impact transition temperature is minimum. The red dashed line corresponds to an ITT of 0 °C. In the variable solution space, the gray and white dashed lines define the contour regions of high ferrite fractions and high pearlite fractions respectively and the intermediate region is the highely banded microstructure having both ferrite and pearlite. Comparing both the plots we observe that the achieved value of ITT increases (0-100 ℃) as the pearlite fraction increases which is not at all acceptable in practice design. Our wish here is to achieve a minimum value of ITT and a maximum value of ferritr fraction thereby managing the banding of microstructure. All these additional requirements and system goals are identified in the superimposed ternary plot (shown in window "①" in Figure 9.15) to support the process designer in carrying out trade-off and thus make a decision. The pink contour region with high ferrite fraction is identified in a compromised manner. In this region, both yield strength and impact transition temperature requirements are met while compromising on the requirements on tensile strength and hardness. Again, some special design points are selected to further illustrate this process, see the window "①" in Figure 9.15. Finally, the solution point B having the highest ferrite fraction and maximum yield strength is recommended as the solution of interest.

9.5.4 *Discussion on the demonstration carried out using example problem*

Using the cooling module and the mechanical properties module identified in HRR process chain, we instantiate a DSE process template to demonstrate the reusability of information in the design space exploration process. As per the proposed DSE process template construct, the PM template for HRR problem is created first and a combination of design information is provided as the input for the cDSP template. The goal here is to minimize the deviation function for satisfying a set of conflicting goals. The PSA template is also created and populated via the DSE process by considering the design preference embedded in different design scenarios. As a basic module of PSA template, the WSA instance is populated and this supports the designer to determine the desired solution region. Meanwhile, to increase the designer's confidence, the modules CSA and ARA also needs to be created based on the specific problem requirements identified.

9.6 On Verification and Validation

The verification and validation of Research Hypothesis 4 is carried out in detail in Section 10.2.4. The readers are referred to this section for more details.

9.7 Role of Chapter 9 in this Dissertation and Remarks on the Template based Ontological Method for DSE

Model-based realization of complex engineered systems involves managing information associated with models that are typically incomplete, inaccurate and not of equal fidelity. Designing such systems therefore demands the designers to carry out rapid and systematic exploration of design space to identify solutions that are relatively insensitive to the uncertainties associated. To address this requirement, the ontology for design space exploration and a template-based ontological method that supports systematic design space exploration in the model-based realization of complex engineered systems is proposed in the chapter.

Using the proposed method, we demonstrate the computational formulation and execution of the procedures in Design Space Exploration (DSE). The systematic exploration of design space involves a procedure for DSE, design space adjustment, and a DSE template scheme. The DSE process template and the method proposed helps a designer in determining the right combination of design information that meets the different goals and requirements set for a process chain. Using the ontology developed and the proposed method, a designer is able to (1) systematically adjust the design space in due time to manage the risks of errors accumulating and propagating during the design of different stages of a process chain, (2) improve the ability to communicate and understand the interactions between design information in the process chain.

We demonstrate the efficacy of DSE process template ontology by carrying out the decision-based design of a multi-stage hot rod rolling system in a steel manufacturing process chain. Using this industry-inspired example problem, we illustrate the utility of ternary plot feature in Post-Solution Analysis (PSA) template to explore the design space. The microstructure space solutions that satisfies the conflicting mechanical property goals in the best possible manner for the rod produced are identified by carrying out design trade-offs. The template-based ontological method for design space exploration facilitates the understanding and prediction of process behavior in design via extending designer's abilities and supporting them to make decisions with the features of robustness, flexibility and modifiability, particularly in the early stages of design.

Chapter 10: Advancing the Vision for the Systems-based Design Architecture via a Cloud-based Platform for Decision Support in the Design of Engineered Systems (CB-PDSIDES)

In this chapter, a summary of this dissertation is given at first. Then, research questions are revisited as well as verification and validation of the research hypotheses is addressed in Section 10.2. Achievements and contributions are summarized in Section 10.3, along with limitations and opportunities for future work in Section 10.4. Finally, the author's vision for research in systems-based design architecture is addressed in Section 10.5.

10.1 Summary of Dissertation

Problem: A materials design revolution is underway in the recent past where the focus is to design (not select) the material microstructure and processing paths to achieve multiple property or performance requirements that are often in conflict. The advancements in computer simulations have resulted in the speeding up of the process of discovering new materials and has paved way for rapid assessment of process-structure-property-performance relationships of materials, products, and processes. This has led to the simulation-based design of material microstructure (microstructure-mediated design) to satisfy multiple property or performance goals of the product/process/system thereby replacing the classical material design and selection approaches. The foundational premise for this dissertation is that systems-based materials design techniques offer the potential for tailoring materials, their processing paths and the end products that employ these materials in an integrated fashion for challenging applications to satisfy conflicting product and process level property and performance requirements. The primary goal in this dissertation is to establish some of the scientific foundations and tools that are needed for the integrated realization of materials, products and manufacturing processes using simulation models that are typically incomplete, inaccurate and not of equal fidelity by managing the uncertainty associated. Accordingly, the interest in this dissertation lies in establishing a ***systems-based design architecture*** that includes system-level synthesis methods and tools that are required for the integrated design of complex materials, products and associated manufacturing processes starting from the end requirements. Hence the primary research question: ***What are the theoretical, mathematical and computational foundations needed for establishing a comprehensive systems-based design architecture to realize the integrated design of the product, its environment, manufacturing processes and material as a system?*** Major challenges to be addressed here are: a) integration of models (material, process and product) to establish processing-structure-property-performance relationships, b) goal-oriented inverse design of material microstructures and processing paths to meet multiple conflicting performance/property requirements, c) robust concept exploration by managing uncertainty across process chains and d) systematic, domain-independent, modular, reconfigurable, reusable, computer interpretable, archivable, and multi-objective decision support in the early stages of design to different users.

Approach: In order to address these challenges, the primary hypothesis in this dissertation is to establish the theoretical, mathematical and computational foundations for: 1) forward material, product and process workflows through systematic identification and integration of models to define the processing-structure-property-performance relationships; 2) a concept exploration framework supporting systematic formulation of design problems facilitating robust design exploration by bringing together robust design principles and multi-objective decision making protocols;

3) a generic, goal-oriented, inverse decision-based design method that uses 1) and 2) to facilitate the systems-based inverse design of material microstructures and processing paths to meet multiple product level performance/property requirements, thereby generating the problem-specific inverse decision workflow; and 4) integrating the workflows with a knowledge-based platform anchored in modeling decision-related knowledge facilitating capture, execution and reuse of the knowledge associated with 1), 2) and 3). This establishes a comprehensive systems-based design architecture to realize the integrated design of the product, its environment, manufacturing processes and material as a system.

Validation: The systems-based design architecture for the integrated realization of materials, products and associated manufacturing processes is validated using the validation-square approach that consists of theoretical and empirical validation. Empirical validation of the design architecture is carried out using an industry driven problem namely the '**Integrated Design of Steel (Material), Manufacturing Processes (Rolling and Cooling) and Hot Rolled Rods (Product) for Automotive Gears'**. Specific sub-problems are formulated within this problem domain to address various research questions identified in this dissertation.

Contributions: The contributions from the dissertation are categorized into new knowledge in four research domains: a) systematic model integration (vertical and horizontal) for integrated material and product workflows, b) goal-oriented, inverse decision support, c) robust concept exploration of process chains with multiple conflicting goals and d) knowledge-based decision support for rapid and robust design exploration in simulation-based integrated material, product and process design.

The creation of new knowledge in this dissertation is associated with the development of a systems-based design architecture involving systematic function-based approach of formulating forward material workflows, a concept exploration framework for systematic design exploration, an inverse decision-based design method, and robust design metrics, all integrated with a knowledge-based platform for decision support. The theoretical, mathematical and computational foundations for the design architecture are proposed in this dissertation to facilitate rapid and robust exploration of the design and solution spaces to identify material microstructures and processing paths that satisfy conflicting property and performance for complex materials, products and processes by managing uncertainty.

The details of specific achievements and contributions from this dissertation are discussed in Section 11.3. The validation of research hypotheses is addressed next in Section 11.2.

10.2 Answering the Research Questions and Validating the Hypotheses

Specific tasks to verify and validate the hypotheses proposed in this research are summarized in Figure 10.1 and described in the following. A summary of arguments made throughout the dissertation regarding theoretical structural and empirical validation for each of the hypotheses are provided in Sections 10.2.1, 10.2.2, 10.2.3, and 10.2.4. In Section 10.2.4, focus is on theoretical performance validation, which involves building confidence in the systematic approach presented for scenarios beyond the specific examples chosen for validation.

Theoretical Structural Validity (TSV) Validity of the constructs of the systems-based architecture • Literature review (Chapters 2, 3, 7, 8, 9) • Gap analysis (Chapters 1, 2, 3, 7, 8, 9) • Checking internal consistency • Reasoning on applicability of constructs (Chapters 2, 3, 4, 7, 8, 9)	**Theoretical Performance Validity (ESV)** Usefulness of the architecture beyond examples • Generalizing Findings (Chapters 9, 10) • Arguing the validity of the systems-based design architecture developed beyond the example problems used in different domains (Chapter 10)
Empirical Structural Validity (ESV) Appropriateness of the examples chosen to verify the architecture • Horizontal Integration of Hot Rod Rolling Process Chain (Chapter 5) • Exploration of Microstructure Space for End Mechanical Properties of Rod (Chapter 5) • Vertical and Horizontal Integration of Hot Rod Rolling Process Chain (Chapters 6, 7, 8, 9)	**Empirical Performance Validity (EPV)** Usefulness of the architecture in examples • Systematic model integration (Chapter 6) • Inverse Design (Chapters 5, 6) • Robust Concept Exploration (Chapter 7) • Knowledge Capture, Reuse and Systematic Design Exploration (Chapters 8, 9)

Figure 10.1: Overview of validation tasks in this dissertation

10.2.1 Research Area 1 - Systematic Model Integration and Information Flow

The first secondary research question addressed in this dissertation is regarding systematic model integration and establishment of information workflow. The research question formulated is as follows,

> ***RQ1***. *What are the foundations needed for* ***systematically identifying*** *and* ***integrating*** *material models with models of the rest of the system (product, manufacturing processes, and environment), so as to define the* ***processing-structure-property-***

performance *relationships and associated* ***information workflow*** *at early stages of design?*

The hypotheses used to answer this research question is,

RH1.1. *Through a systematic approach from a systems perspective, consisting of concept generation which includes*

a) functional decomposition to generate multilevel function structures across the process chain for the end performance requirements, followed by

b) identifying material and process phenomenon associated with function structures and systematically mapping them to solution principles (models identified from literature or developed through experiments),

and framing the system structure for problem via,

c) vertical integration of identified/developed material models and horizontal integration of identified/developed process models to systematically map material processing to material microstructure phenomena and next to macrolevel properties and performances,

the design of product, process and material concepts are integrated, and conceptual materials design is rendered more systematic (To address **G1** and **G2**).

The hypothesis is embodied in a systematic function-based approach to integrate the design of materials and products. The systematic function-based approach is leveraged from the work of Mathias Messer in his PhD. The approach is introduced in Chapter 4 and its application is demonstrated in Chapter 6 for the comprehensive example problem. The function-based systematic approach supports concept flexibility as early stages of design and enables designers establish material structure-property relations on multiple scales by leveraging underlying phenomena and solution principles and through the use of design catalogs. The design catalogs are open ended maps that supports dynamic updates based on the changing markets and technological updates.

Theoretical Structural Validation

As discussed in Chapter 4, Section 4,9, theoretical structural validation refers to accepting the validity of individual constructs used in the systematic function-based approach and accepting the internal consistency of the way the constructs are put together. Theoretical structural validation involves systematically identifying the scope of the proposed approach's application, reviewing relevant literature and identifying the research gaps that is existing, identifying the strengths and limitations of the constructs uses based on literature review, determining the constructs and approaches that can be leveraged for the systematic function-based approach while reviewing literature on the advantages, disadvantages and accepted domains of application, and checking the internal consistency of the constructs both individually and when integrated.

In Chapter 4, we establish the generic nature of the systematic approach and why the approach is appropriate for concept generation during early stages of design for the integrated design materials, products and associated manufacturing processes. By carrying out literature search, it is shown that the systematic function-based approach and the associated constructs have been previously applied for problems in various domains in a successful manner and are verified and validated. The use of these generic systematic approach for the integrated design exploration of materials, products and associated manufacturing processes so as to establish systematic model integration and establishment of information workflow is not addressed in past literature.

Based on the critical review of literature in Chapter 4, it is inferred that the application of function-based systematic method is mostly on areas related to mechanical, control, software and process engineering and is mostly applied for selection of materials for different applications from existing classes of solutions. The focus is also more on product design by developing concepts at early stages of design. Our focus by using function-based design is in establishing model integration and information flow chain so as to facilitate systematic problem-oriented conceptual design via functional decomposition and representation of the problem in solution-neutral natural language taking into account the input and output flows. This allows to establish the integrated conceptual design of materials and products in a more systematic and domain-independent manner which helps in increasing the designer's flexibility and easy establishment of the information workflow for material/product system.

Once the phenomena and associated solution principles (models in our case) are identified, design catalogs are used to facilitate function-based systematic material and product design. Based on literature review in Chapter 4, it is established that design catalogs are previously used and validated for facilitating function-based systematic design in different domains successfully. However, the use of design catalogs for identifying and capturing material and product models to facilitate integrated materials and product design is not addressed in literature. The determination of phenomena and associated solution principles on multiple system levels is crucial and this allows for developing a wide range of principal solution alternatives and increase a designer's concept flexibility.

The use of design catalogs in past literature has been confined mechanical components like gearboxes, bearings, connections etc. The use of design catalogs for defining processing-structure-property-performance relationships via material models at multiple levels/scales using information generated through integration of such models is not addressed till now.

In this dissertation, the past efforts on function-based design and identification of phenomena and associated solution principles is leveraged to achieve the integrated design of materials, products and manufacturing processes. The focus in this dissertation is to establish processing-structure-property relations from a systems perspective by addressing phenomena and associate solution principles thereby integrating conceptual design of materials and products in a systematic and domain independent manner. To facilitate function-based systematic design at the level of phenomena and solution principles, the functionalities associated with design catalogs are leveraged to support a designer in designing material and product concepts in an integrated fashion.

The systematic approach followed is shown as a flow chart in Figure 1.7. The details are provided with description of each task in step by step manner in Chapter 4. The input needed, and the output generated is clarified, the internal information flow is checked to ensure sufficient information availability to execute next steps. Through critical evaluation of each step and the way individual constructs are put together, internal consistency of the systematic approach is verified and accepted.

The theoretical structural validity of the function-based systematic approach for conceptual materials and product design to achieve systematic model integration and information workflow is accepted by the logical procedure of literature review, gap analysis and development and evaluation individual and integrated constructs. Next, empirical studies need to be carried out to establish the usefulness and effectiveness of the approach.

Empirical Structural Validation

Empirical structural validation involves accepting the appropriateness of the example problems used to verify the performance of the method. The integrated design of material (steel), product (rod) and associated manufacturing processes (hot rod rolling and cooling) is an industry-inspired complex multilevel and multiscale design problem. Three example problems are discussed in this dissertation that ties to the design problem domain. The comprehensive design problem discussed in Chapter 4 is used to test the function-based systematic approach for exercising systematic conceptual design not only on various system levels down to the component level, but, also on the multiscale materials level. Moreover, the problem is suitable for demonstrating the different aspects of integrated materials, product and manufacturing process design. Hence, the integrated design of material (steel), product (rod) and associated manufacturing processes (hot rod rolling and cooling) example consists of decisions related to product and materials design. Decisions on product and materials design depend on each other and ultimately affect the final system performance.

Empirical Performance Validation

Empirical performance validation consists of accepting the usefulness of the outcome with respect to the initial purpose and accepting that the achieved usefulness is related to applying the method. The function-based systematic approach involving functional decomposition via analysis, abstraction and synthesis, and design catalogs for phenomena and associated solution principles establishes systematic conceptual design of the system and the different components including the multiscale material levels. Identification of solution principles – models in our case, helps in integrating models and establishing the information workflow that further supports concept exploration and coming up with promising concepts that increases system performances. The advantages associated with the whole approach includes:

- Domain-independent representation and solution exploration schemes;
- Generation of a broader solution filed;
- Abstraction of essential problem characteristics;
- Allows for defining a problem boundary and problem formulation;
- Designers are more likely to explore new solutions than known solutions;
- Easy to identify non-intuitive solutions;
- Supports systematic problem formulation, design space generation and expansion, and exploration of design and solution space;
- A foundation for modular and reconfigurable design
- Generation of rough idea of uncertainty and its propagation across process flow chain;
- Facilitation of planning and managing of design;
- Practical and easy to use for designers in any domain and can be interfaced with systems-based design exploration methods; and
- Emergence of innovative solutions and the logic underpinning the solutions can be clearly understood.

10.2.2 Research Area 2 - Concept Exploration and Inverse Design Exploration

The second secondary research question addressed in this dissertation is regarding concept exploration and inverse design exploration. The research question formulated is as follows,

> ***RQ2.*** *What are the computational foundations needed for performing the* ***systematic*** *and* ***rapid concept exploration*** *of complex engineered systems involving the material, product and manufacturing processes* ***satisfying certain end performance requirements****, when simulation models are typically* ***incomplete, inaccurate and not of equal fidelity****?*

The hypotheses used to answer this research question is,

> ***RH2.1.*** *Developing a concept exploration framework anchored in decision-based design construct – the cDSP can support the designer in formulating the design problem systematically and exploring the solution space to generate satisficing design specifications* **(To address G3).**
>
> ***RH2.2.*** *Developing a goal-oriented inverse design method that uses the concept exploration framework to facilitate the systems-based inverse design exploration of material microstructures and processing paths to meet multiple product level performance/property requirements* **(To address G4).**

The hypothesis is embodied in a Concept Exploration Framework that supports systematic problem formulation and solution space exploration thereby supporting the human designer make design decisions by considering the different alternatives that are available to come up with satisficing design specifications; and a goal-oriented inverse design method that that uses the concept exploration framework to facilitate the systems-based inverse design exploration of material microstructures and processing paths to meet multiple product level performance/property requirements. The CEF is introduced in this dissertation as a general framework that includes systematic steps to identify design alternatives and generate *satisficing* design solutions. The CEF is inspired from the RCEM (Chen, Allen and coauthors 1997) with addition of features (processors) to consider different material and product models and options to explore the solution space for different design scenarios. Core to the CEF is the foundational mathematical construct – the compromise Decision Support Problem (cDSP) (Mistree, Hughes and coauthors 1993). The cDSP construct used here is anchored in the robust design paradigm first proposed by Taguchi. The fundamental assumption is that the models are not complete, accurate and of equal fidelity (Taguchi , Bras and Mistree 1993).

Theoretical Structural Validation

Theoretical structural validation refers to accepting the validity of individual constructs used in the concept exploration framework and the goal-oriented inverse design method and accepting the internal consistency of the way the constructs are put together. Theoretical structural validation involves systematically identifying the scope of the proposed framework's and design method's application, reviewing relevant literature and identifying the research gaps that is existing, identifying the strengths and limitations of the constructs used based on literature review, determining the constructs and approaches that can be leveraged for the concept exploration framework and inverse design method while reviewing literature on the advantages, disadvantages and accepted domains of application, and checking the internal consistency of the constructs both individually and when integrated.

In Chapter 1, the need for a concept exploration framework for the systematic concept exploration of materials and products is established. The CEF is inspired from the RCEM. The RCEM is critically reviewed in Chapter 3 and the functionalities and limitations associated with the method is established. The limitations of RCEM in terms of the following is discussed: i) RCEM does not take into account already available material and product models and relationships and focuses on establishing reduced order meta models/surrogate models, ii) RCEM has limitations in terms of exploration of solution space and does not have processors for establishing design scenarios for exercising the cDSP, iii) RCEM also lacks visualization tools and constructs for solutions space exploration and carry out design trade-offs, iv) RCEM cannot be individually used to support design exploration of process chains and thus needs support from a design method to achieve the same, v) RCEM in terms of EMI and DCI does not address robust design of a system having multiple conflicting goals that require different types of robust design across process chains. Based on these limitations, the requirements for an improved framework and a design method that facilitate the integrated design exploration of materials, products and associated manufacturing processes is established. To address the need for the inverse design method, the current research efforts focusing on inverse design exploration of material hierarchies are reviewed in detail in Chapter 1 and 2. The existing challenges and limitations are addressed and the need for a systems-based, top-down design exploration method is established in Chapters 1 and 2. In Chapter 4, the goal-oriented inverse design method is proposed. Several challenges associated with similar inverse design exploration methods like the IDEM is highlighted in Chapter 3 and some these challenges are addressed by the inverse design exploration method proposed in this dissertation. A detailed analysis of the functionalities offered compared to methods like IDEM is provided in Chapter 6. The basic idea of the method proposed in Chapter 4 for finding satisficing solutions in a multi-level, multi-stage process chain that involves the Processing-Structure (PS), Structure-Property (SP) relations is passing down the satisficing solution ranges in an inverse manner, from given final performance range to the design space of the previous space (defined by model input and output) with designer having the flexibility to choose solution of preference. The method is goal-oriented because the designer starts with the end goals that need to be realized for the product as well as process and then design the preceding stages to satisfy these end goals as closely as possible by exploring the design space. Then the design decisions that are made for the end requirements of the product/process after exploration are communicated to the stages that precede them to make logical decisions at those stages to satisfy the requirements identified thereby carrying out a design space exploration process in an inverse manner.

The proposed concept exploration framework is shown in Figure 4.8 and the goal-oriented inverse design method along with the associated steps is shown in Figure 4.9. The details of the framework and the design method with description of each steps to be performed to formulate, exercise and explore a complex systems design problem are provided in Chapter 4. The input needed, and the output generated is clarified, the internal information flow is checked to ensure sufficient information availability to execute next steps. Through critical evaluation of each step and the way individual constructs are put together, internal consistency of the concept exploration framework and the inverse design method is verified and accepted.

The theoretical structural validity of the concept exploration framework and the goal-oriented inverse design method to achieve inverse decision-based design exploration of process chains from a systems perspective is accepted by the logical procedure of literature review, gap analysis and development and evaluation individual and integrated constructs like the cDSP, surrogate modeling techniques, ternary analysis and plots, the inverse design method, etc. Empirical studies need to be carried out to establish the usefulness and effectiveness of the framework and the method.

Empirical Structural Validation

Empirical structural validation involves accepting the appropriateness of the example problems used to verify the performance of the framework and the method. The CEF and the inverse design method is first tested using two example problems in Chapter 5. In the first example problem, the horizontal integration of rod rolling is considered. Using the framework and method, the integrated design of rolling passes and the final rod product is carried out in an inverse manner starting from the end goals. The example thus is appropriate to demonstrate the utility of the framework and method as it involves complex information flow across manufacturing stages that needs systematic problem formulation and exploration across stages to design the entire system. In this example, only macrostructural effects associated with hot rod rolling is considered. In the second example, we want to illustrate the utility of the method and framework in supporting the design of the material microstructure for given end mechanical properties of the product. To illustrate the same, a rather simple problem is formulated to design the microstructure after cooling process to satisfy certain end mechanical properties like yield strength, tensile strength, hardness and toughness of the rod produced. The example is appropriate as the example supports in demonstrating the utility of method and framework in carrying out microstructure-mediated design. The example is further improved and expanded to the comprehensive problem on vertical and horizontal integration of hot rolling process chain in Chapter 6. Using the comprehensive example problem in Chapter 6, the utility of the framework and the method is tested for the integrated design exploration of materials, products and manufacturing processes.

Empirical Performance Validation

Empirical performance validation consists of accepting the usefulness of the outcome with respect to the initial purpose and accepting that the achieved usefulness is related to applying the framework and method. The utility of the proposed method is demonstrated by carrying out the integrated solution space exploration of the processing and microstructure spaces of the rolling and cooling processes to identify *satisficing solutions* that realizes the end mechanical properties of the rod product in Chapter 6. The primary advantage of the proposed method is in empowering a process designer to rapidly explore the design space for manufacturing processes using simulation models by managing the uncertainty associated with models. The ability to predict the design and operating set points using models reduces the need for expensive plant trials resulting in reduced time and cost involved in the production of a new grade of steel product mix with improved properties using a new class of material. The proposed method is generic and supports the integrated decision-based design of other manufacturing stages that are connected and having a sequential flow of information by identifying the design and operating set points that best satisfies the requirements identified. Through the proposed method and demonstration carried out in this chapter using an industry-driven problem, we propose an approach for *microstructure-mediated design* by *integrating the design of the material, product and associated manufacturing processes* involved.

The functionalities offered by the method supported by CEF as illustrated using the comprehensive example problem includes (Selected from Chapter 4 and proved based on the testing done using the comprehensive example problem in Chapter 6, see Chapters 4 and 6 for details):

- Requirements driven, "top-down" design of system and associated subsystems by taking a goal-oriented approach which is different to the standard practice of bottom-up modeling and design of material and product systems,
- Human perception of a satisficing design space across process chains,
- augmenting the human ability to make design decisions - visualizing a solution space and making logical judgements through trade-offs to identify satisficing solution regions of interest,
- Capability to handling 'n' number of design variables – this is an advantage over other design exploration methods like IDEM where there is a limitation on the number of design variables,
- Propagation of end goal requirements (product performance or properties) across a process chain with the designer having the capability to check whether the end goals are actually achievable at previous spaces in their current configuration or not – designer can recommend adjustments in the design space if needed,

- Offers flexibility in design: The capability to define new goals and requirements at each level as the method uses individual cDSPs to facilitate information flow allowing to formulate a design space at each level - advantage over other design exploration methods like IDEM and pyDEM where the design space is defined by mapping from previous spaces (Choi, McDowell and coauthors 2008, Kern, Priddy and coauthors 2017),
- The capability to carry out rapid, integrated design exploration of material and products using simulation models that we accept are typically incomplete and inaccurate,
- The capability to coordinate information and human decision making,
- The CEF offers the capability to prioritize models, input factors, output responses and computational tools in terms of their value in design, and
- ensuring feasible design solutions that allows to invest on new complex material systems with confidence.

The proposed method and the concept exploration framework are generic and supports the integrated decision-based design of similar manufacturing processes involving the material and product. Given any complex systems problem that involve sequential flow of information across processes/levels, the proposed method has the potential to be applied to support information flow and human decision making across the processes/levels in order to realize an end goal.

10.2.3 Research Area 3 – Robust Concept Exploration

The third secondary research question addressed in this dissertation is regarding robust concept exploration. The research question formulated is as follows,

RQ3. *What are the requirements for an* ***inverse, goal-oriented design approach*** *for realizing the* ***robust design exploration*** *of the material, product and process as a system by managing the associated uncertainties?*

The hypothesis used to answer this research question is,

RH3.1. *Introduction of specific robust design goals and constraints anchored in the mathematical constructs of* ***error margin indices*** *and* ***design capability indices*** *to determine ''****satisficing robust design****'' specifications for given performance requirement ranges using the goal-oriented, inverse design method can bring in robustness for multiple conflicting goals across process chains.*

The hypothesis is embodied in specific robust design goals, constraints and metrices to determine ''satisficing robust design'' specifications for given performance requirement ranges using the goal-oriented, inverse design method proposed in Chapter 6. The primary mathematical construct used in the enhanced inverse method is the compromise Decision Support Problem with the constructs of Error Margin Index and Design Capability Index (cDSP with EMI-DCI) supported by the Concept Exploration Framework (CEF) to generate satisficing Type I, II and III robust design solutions across process chains.

Theoretical Structural Validation

Theoretical structural validation refers to accepting the validity of individual constructs of error margin index and design capability index and accepting the internal consistency of the way the constructs are put together with the concept exploration framework and the goal-oriented inverse design method. Theoretical structural validation involves systematically identifying the scope of the two construct's application, reviewing relevant literature and identifying the research gaps that is existing, identifying the strengths and limitations of the constructs used based on literature review, determining the constructs and approaches that can be leveraged for robust concept exploration, reviewing literature on the advantages, disadvantages and accepted domains of application, and checking the internal consistency of the constructs both individually and when integrated.

In Chapter 3, robust design is reviewed in detail. Robust design from the perspective of materials and products is reviewed first in Section 3.4. This is followed by reviewing the different classification of uncertainty – from the perspective ICME, multiscale modeling and engineering systems design. A detailed review of robust design is then carried out starting with the work of Taguchi in Section 3.4.2. The significance of Taguchi's work is emphasized, and the associated criticisms and limitations are highlighted. Work carried out by other researcher's on addressing the limitations of Taguchi's approach is reviewed further. A review of Suh's axiomatic design and how the axioms by Suh tie to robust design is addressed next in Section 3.4.3. In this review, the association of robust design to Suh's information axiom is explored and the connection to Shannon's information theory is established. Further review is carried out on Robust Design Type II proposed by Wei Chen in Section 3.4.4. The Design Capability Index (DCI) is introduced and reviewed in detail along with the Robust Concept Exploration Method (RCEM). The utility of the index in Robust Design Type II for a single goal is addressed. This is followed by the review of Robust Design Type III in Section 3.4.5. The Error Margin Index (EMI) is reviewed further, along with RCEM-EMI for robust design type III of systems with a single goal. The capabilities of EMI for type III robust design is reviewed and the limitations associated are discussed. In Section 3.4.6, robust design across process chains is discussed. The Inductive Design Exploration Method is reviewed in this section as a method that facilitates robust design during propagation of uncertainty. The limitations associated with IDEM is reviewed here and the need for an approach for robust design across process chains is established. In Chapter 7, robust concept exploration of materials, products and manufacturing processes is proposed. The proposed robust concept exploration approach is shown in Figure 7.5. The modified concept exploration Framework and the goal-oriented inverse design method that supports robust concept exploration is shown in Figure 7.1 and 7.4 respectively. The details of the framework and the design method with description of each steps to be performed to formulate, exercise and explore a complex systems design problem in a robust manner using the metrices of EMI and DCI are provided in Chapter 7. The input needed, and the output generated is clarified, the internal information flow is checked to ensure sufficient information availability to execute next steps. Through critical evaluation of each step and the way individual constructs are put together, internal consistency of the concept exploration framework and the inverse design method is verified and accepted.

The theoretical structural validity of the robust concept exploration of process chains is accepted by the logical procedure of literature review, gap analysis and development and evaluation individual and integrated constructs like the DCI, EMI and modified CEF. Empirical studies need to be carried out to establish the usefulness and effectiveness of the framework and the method.

Empirical Structural Validation

Empirical structural validation involves accepting the appropriateness of the example problems used to verify the performance of the framework and the method. In Chapter 7, the robust concept exploration of process chains using the cDSP-EMI-DCI constructs and GoID method is illustrated using the comprehensive example problem discussed in Chapter 6. The example problem is reformulated using robustness metrics of EMI and DCI. Specific robust design constraints and goals are defined to achieve Type I, II, and III robust across process chains for multiple conflicting goals.

Empirical Performance Validation

Empirical performance validation consists of accepting the usefulness of the outcome with respect to the initial purpose and accepting that the achieved usefulness is related to applying the robust design metrics, goals and constraints. Functionalities of the cDSP with EMI-DCI combination metrics and corresponding robust design goals and constraints include:

- Supporting a human designer under complex material system's random variability and/or model parameter uncertainty and/or model structure uncertainty in making decisions that satisfies multiple conflicting goals,
- Managing uncertainty in the system without removing the source and supporting in identifying robust design solutions across process chains, and
- Ensuring the identification of robust solution space using robust solution constraints. The designer can explore this space to further identify satisficing robust design specifications.

10.2.4 Research Area 4 - Knowledge-based Platform for Decision Support

The third secondary research question addressed in this dissertation is regarding robust concept exploration. The research question formulated is as follows, *RQ4.* ***RQ4.*** *What are the foundations needed for maintaining* ***structural consistency*** *of the decision-based design workflow for the manufacturing process chain involving the material and product, ensuring* ***robust, flexible and modifiable*** *decisions while incorporating newer* ***data, information and knowledge*** *associated with the system?*

The hypothesis used to answer this research question is,

R.H4.1. *Using ontology to represent decision-related knowledge that is modeled as Decision Support Problem (DSP) templates can capture, analyze, archive and update the decision-based design workflow as per the needs of the individual decision-maker. Separation of declarative (problem specific) knowledge and procedural (process specific) knowledge in the information flow scheme can help in generalizing the decision models in the design workflow* (To address **G6**).

R.H4.2. *Defining three types of users, namely Template Creators, Template Editors, and Template Implementers, and providing customized decision support to these users during the design of engineering systems can help perform original design, adaptive design, and variant design respectively* (To address **G7**).

R.H4.3. *Developing an ontology for design space exploration and a template-based ontological method that supports systematic design space exploration ensuring the determination of the right combination of design information that meets the different goals and requirements set for a process chain* (To address **G8**).

The hypothesis is embodied in an Ontology for decision-based design and design space exploration, the Decision Support Problem and the DSP Templates. The primary mathematical constructs used in the knowledge-based platform for decision support are the Decision Support Problem (DSP), the Decision Support Problem Templates and an Ontology to represent decision-related knowledge.

Theoretical Structural Validation

Theoretical structural validation refers to accepting the validity of individual constructs of PDSIDES and accepting the internal consistency of the way the constructs are put together for PDSIDES. Theoretical structural validation involves systematically identifying the scope of the platform's application, reviewing relevant literature and identifying the research gaps that is existing, identifying the strengths and limitations of the constructs used based on literature review, determining the constructs and approaches that can be leveraged for developing the platform, reviewing literature on the advantages, disadvantages and accepted domains of application, and checking the internal consistency of the constructs both individually and when integrated into the platform.

In Chapter 1, the research gaps associated with providing decision support in decision workflows is addressed in the context of designing complex systems. This includes lack of both reusable and executable decision knowledge schemes and lack of classification of users in terms of decision support. To address the aforementioned needs, a Knowledge-Based Platform for Decision Support in the Design of Engineering Systems is proposed. Thus, in Chapter 1 the need for the platform is established with identification of the research gaps that exists. In Chapter 3, a literature review on the status of design foundations used in this dissertation to address the needs of the platform is carried out. A discussion about the advantages, limitations of current design tools, methods, approaches, and constructs is carried out followed by establishing the need for research area 4 in this dissertation. The foundations for the platform for decision support from a template-based decision centric perspective is reviewed in Chapter 4. This includes hierarchical systems view of design processes as decision workflows in Section 3.5.1. The concept of modeling design processes using domain-independent decision templates is reviewed in detail in this section. The importance of the separation of declarative and procedural information and knowledge while developing decision templates is discussed in Section 3.5.2. The foundational philosophy in this dissertation of design as a decision centric activity from the context of the platform is discussed in Section 3.5.3, thus establishing the logical soundness of constructs used – individually and integrated for the platform-PDSIDES. In Chapter 8, the foundations are briefly revisited and the PDSIDES platform is presented. The constructs used in the platform are discussed in Section 8.2. The ontology for capturing the decision-related knowledge is introduced in Section 8.2.3. The design of the platform PDSIDES is introduced in Section 8.3. Three types of users of the platform – creators, editors and implementors are introduced and their associated working scenarios are described in detail in Section 8.3.2. In Section 8.3.3, the knowledge-based decision support in PDSIDES is presented and the roles played by each of the users of PDSIDES is established. The internal information flow in the platform is checked to ensure sufficient information availability to execute next steps. Through critical evaluation of each step in the design of the platform and the way individual constructs are put together, internal consistency of the platform PDSIDES is verified and accepted.

The theoretical structural validity of PDSIDES is accepted by the logical procedure of literature review, gap analysis and development and evaluation individual and integrated constructs within the platform. Empirical studies are further carried out to establish the usefulness and effectiveness of the platform.

Empirical Structural Validity

Empirical structural validity involves building confidence in the appropriateness of the test example problem chosen for illustrating and verifying the performance of the platform PDSIDES. Empirical structural validation involves accepting the appropriateness of the example problem on hot rolling used to verify the performance of the PDSIDES for original, adaptive and variant designs. It also involves accepting the platform and the constructs involved. In Chapter 8, Section 8.5, the gear manufacturing process design problem focused on rod rolling – a complex system design that calls for a series of decisions to be made – is introduced. Decisions to be made at each manufacturing unit are formulated as cDSPs and linked as a decision network. In original design addressed in Section 8.5.1, the template creator (domain expert) formulates in PDSIDES, the cDSP for the problem boundary framed within the hot rod rolling process chain problem by taking into account the complete information flow across models thereby establishing relationships. Using the cDSP formulated the ability of the PDSIDES platform to carry out original design is demonstrated. In adaptive design addressed in Section 8.5.2, the template editor (senior designer) modifies the existing original design cDSP template according to new requirements. The requirement can be easily satisfied by editing the existing formulated original design cDSP template in PDSIDES. The editing involves two major steps: Step 1, decompose the original cDSP template into two separate cDSP templates, and Step 2, link the two separate cDSP templates using an *Interface*. Two cDSPs are formulated from the original design cDSP to demonstrate adaptive design. The cDSPs are interlinked via an interface of design variables that are shared. Using the cDSPs formulated, the ability of the PDSIDES platform to carry out adaptive design is demonstrated.

Empirical Performance Validity

Empirical performance validation consists of accepting the usefulness of the outcome with respect to the initial purpose and accepting that the achieved usefulness is related to using PDSIDES for original, adaptive and variant designs; addressed in Chapter 8. In PDSIDES, decision-related knowledge is modeled as modular, computational templates based on the DSP constructs using ontology to facilitate execution and reuse. The advantages of PDSIDES is that it provides the functionality to capture knowledge when Template Creators create decision templates in original design, maintain consistency when Template Editor modify decision templates in adaptive design and provide a package of documented knowledge when Template Implementers executes decision templates in variant design. In Chapter 9, the efficacy of DSE process template ontology in PDSIDES is demonstrated by carrying out the decision-based design of a multi-stage hot rod rolling system in a steel manufacturing process chain. Using this industry-inspired example problem, we illustrate the utility of ternary plot feature in Post-Solution Analysis (PSA) template to explore the design space. The microstructure space solutions that satisfies the conflicting mechanical property goals in the best possible manner for the rod produced are identified by carrying out design trade-offs. The template-based ontological method for design space exploration facilitates the understanding and prediction of process behavior in design via extending designer's abilities and supporting them to make decisions with the features of robustness, flexibility and modifiability, particularly in the early stages of design.

10.2.5 Theoretical Performance Validation

As discussed in Chapter 1, theoretical performance validity involves showing that the systems-based design is useful beyond the example problems and domains discussed in this dissertation. This involves i) showing that the example problem is representative of a general class of problems and ii) strengthening confidence in the design methods and architecture proposed by generalizing the findings.

With respect to the systematic function-based approach presented in this dissertation in particular, characteristics of the example problems are:

- The system can be represented as a network of subsystems that are connected in terms of functions that they wish to satisfy and the information they share;
- A subsystem can be considered separately to formulate a problem and its relations with other subproblems temporarily suspended;
- Appropriate phenomena and solution-principles have been identified and the associated functional relationships/ technology to develop functional relationships exist;
- Solutions that best satisfy the designer's interest is selected;

With respect to the concept exploration framework, inverse design exploration with robustness presented in this dissertation, characteristics of the example problems are:

- Decisions can be formulated mathematically, and analysis models are available for design decision-making;

- Design process starts with an end goal in mind – could be an end product that needs to be supplied to customers;
- There exist models or computational tools or data that can establish the forward information workflow for the process/product that is being considered;
- Analysis models for problems are typically incomplete, inaccurate and not of equal fidelity;
- Designer's interest is in identifying satisficing robust solutions given the uncertainty in the problem and not single-point optimum solutions;
- Design is a goal-oriented activity with design requirements subject to change at any time for the problems considered;
- There are emergent properties for the system/problems being considered.

Building confidence in the applicability of the systems-based design architecture proposed in this dissertation

1) ***Robust Design of an American Football Helmet*** (**Work carried out at Mississippi State University and the Center for Advanced Vehicular Systems**)

Much has been written about brain damage to athletes who participate in contact sports in general and American football in particular. Essentially, helmet equipment has not been historically designed with the metrics directly related to the brain. By using brain damage as a performance metric, we are developing a goal-oriented, inverse decision-based design method with the end performance goal of total energy absorption so as to mitigate the possibility of brain damage to athletes.

The helmet system is partitioned into three subassemblies, namely, the helmet shell, the stress wave damper, and the helmet liner. In the shell subassembly, thickness of the paint and outer/inner shells are treated as variables. The stress wave damper is fixed to the shell and specifications (for example, base radius, length, volume, etc.) for the complex geometry are treated as variables. The liner subassembly consists of Velcro, TPU foam wrap, and the foam material with thickness and area ratio being treated as variables. Each of the subassemblies is linked via an information chain (consisting of variables and goals) beginning with the paint and ending with the liner foam. Considering the end goal of zero energy at the head, we define the forward process as an energy transfer from the external paint to the helmet liner. The subassembly specifications is solved in an inverse manner beginning with the foam liner and working backwards towards the paint. The mathematics underlying the proposed goal-oriented, inverse decision-based design method is embodied in the Concept Exploration Framework (CEF). Data from finite element analysis using ABAQUS (explicit) is garnered in which an Internal State Variable (ISV) elastic-viscoplastic material model will be used to accurately capture the constitutive behavior. The boundary conditions will include a normal load and a transverse load with velocities appropriated by the NOCSAE standard for American Football Helmets.

Background: In a head-on collision, kinetic energy is transferred to a player's head through the helmet. It is well understood that players receive concussion from high-energy impacts but can also develop degenerative brain disorders from repeated low-energy impacts. The football industry has established a set of standards for helmets which uses linear G-forces as the performance metric. However, we know that damage is correlated to energy and stress waves penetrating to the brain, not just a single G-force. We know that brain damage does not have a one to one correlation to G-forces, but we do not yet have an exact correlation between kinetic-energy or stress waves and brain damage. As such, this design problem needs to be somewhat flexible as we anticipate further research that shows the correlation between input energy and resulting brain damage.

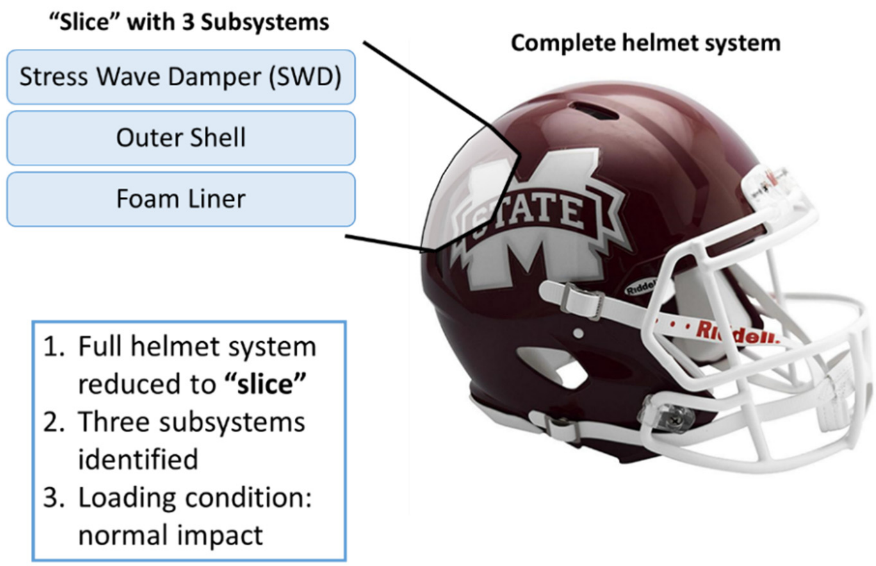


Figure 10.2: Framing the helmet design problem (Courtesy of Tate Fonville and Dr. Mark Horstemeyer, MSU)

Word Problem Formulation: The goal for this problem is to design a TPU wrapped foam liner for maximum energy absorption and minimum weight, see Figure 10.2. A previous parametric study has reduced the size of the design space to two variables, pod depth and TPU thickness. There are 6 cylindrical pods positioned in a circular array which, when combined, have a total surface area ratio of 0.73 (pod surface area/shell surface area). Having a fixed the surface area, the pod depth is allowed to vary from a minimum of 25.4 mm to a maximum of 50.8 mm. For each pod, the TPU thickness is allowed to vary from 0.1 mm to 1.3 mm. For a given pod, energy absorption is formulated as a function of the pod's depth and tpu thickness. Other parameters such as foam volume and pod weight can be determined from these two variables.

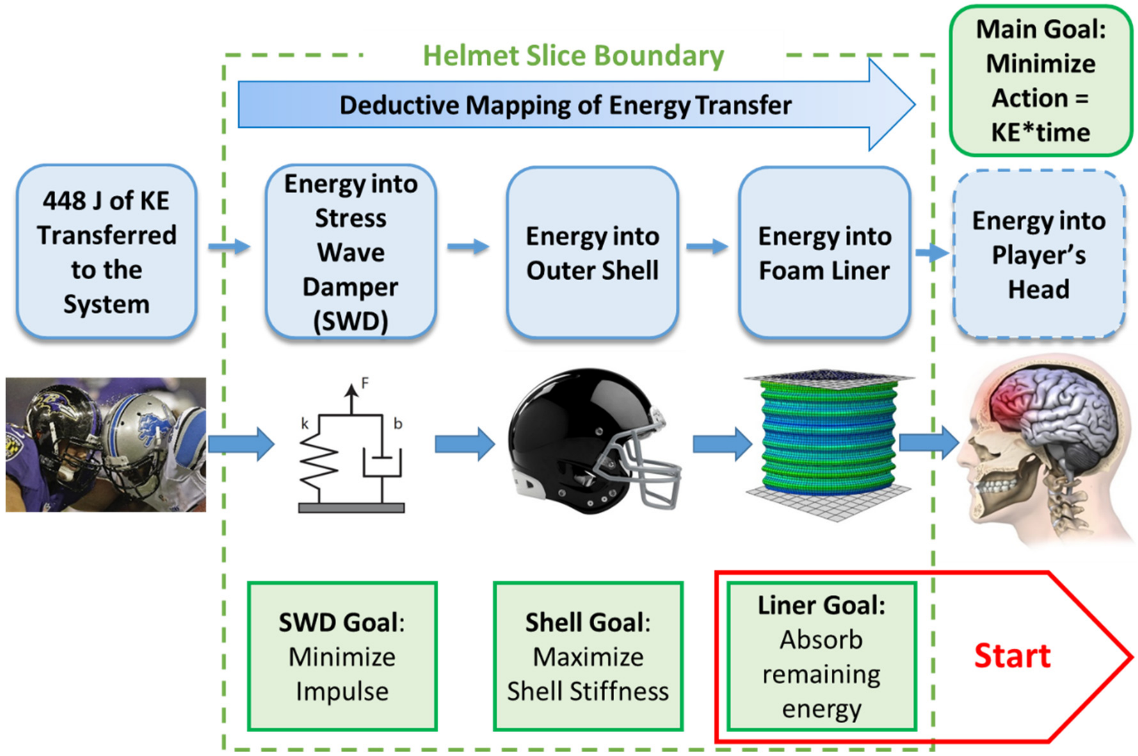


Figure 10.3: Forward information workflow for helmet design problem (Courtesy of Tate Fonville and Dr. Mark Horstemeyer, MSU)

Similiarly, the goal for pod weight can be determined from the pod depth and TPU thickness, as volume and mass can be computed from these two variables. In general, the liner cannot exceed a depth of 50.8 mm (2 in) and upon compression, the minimum thickness of the compressed liner must at least be 12.7 mm (0.5 in).

In Figure 10.3, the forward information workflow for the helmet design problem is shown. This is the first step of the GoID method proposed in this dissertation. In this step for the problem boundary considered, mathematical models are either identified or developed to establish the functional relationships for the energy transferred to the system in terms of energy into stress wave damper, energy into outer shell, energy into foam liner and finally the energy impacting the player's head. Simulations using Finite Element

Models for the subsystems are used to come up with relationships to establish the overall function structure for the problem.

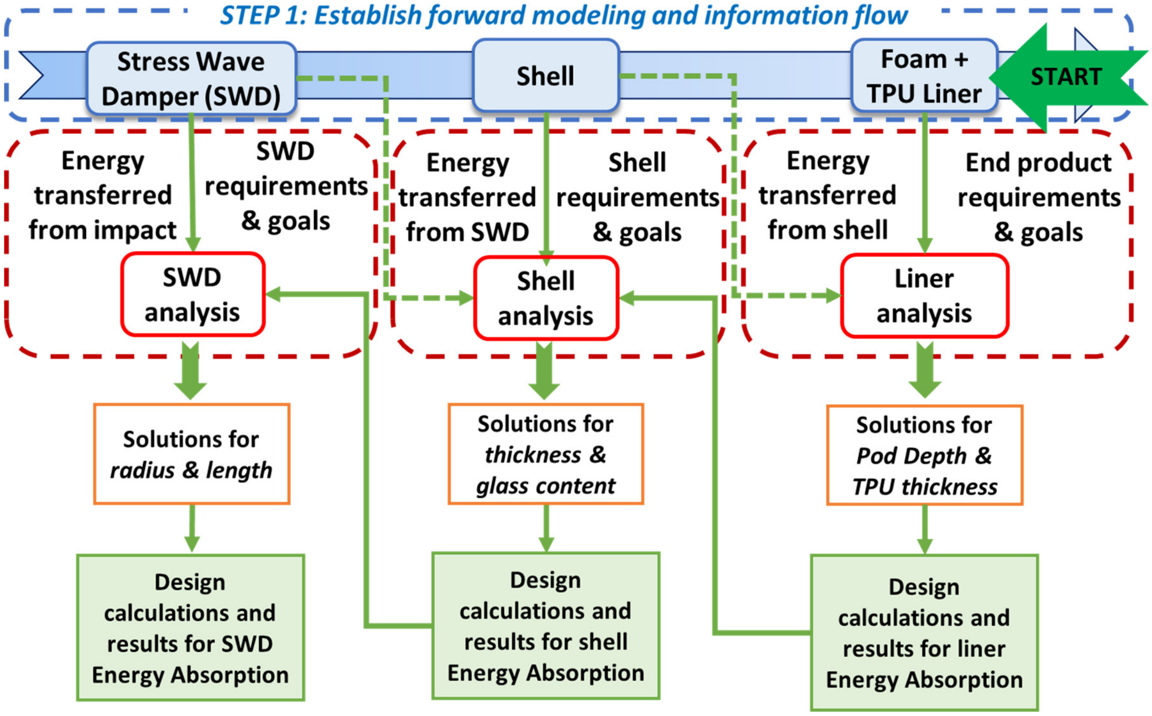


Figure 10.4: The Goal-oriented Inverse Design Method for exploring the helmet design problem (Courtesy of Tate Fonville and Dr. Mark Horstemeyer, MSU)

In Figure 10.4, the application of the GoID method proposed in this dissertation to the helmet design exploration problem is shown. The end goal is to completely absorb the energy impacting the human head/brain. With this requirement in mind, the system is designed in an inverse manner starting from the foam and TPU liner. The cDSP for foam and TPU liner is formulated and the preliminary results are obtained for the subsystem. The results obtained are presented in and is not addressed in this dissertation. In Figure 10.5, the application of the Concept Exploration Framework to formulate the cDSP for foam and TPU liner is shown.

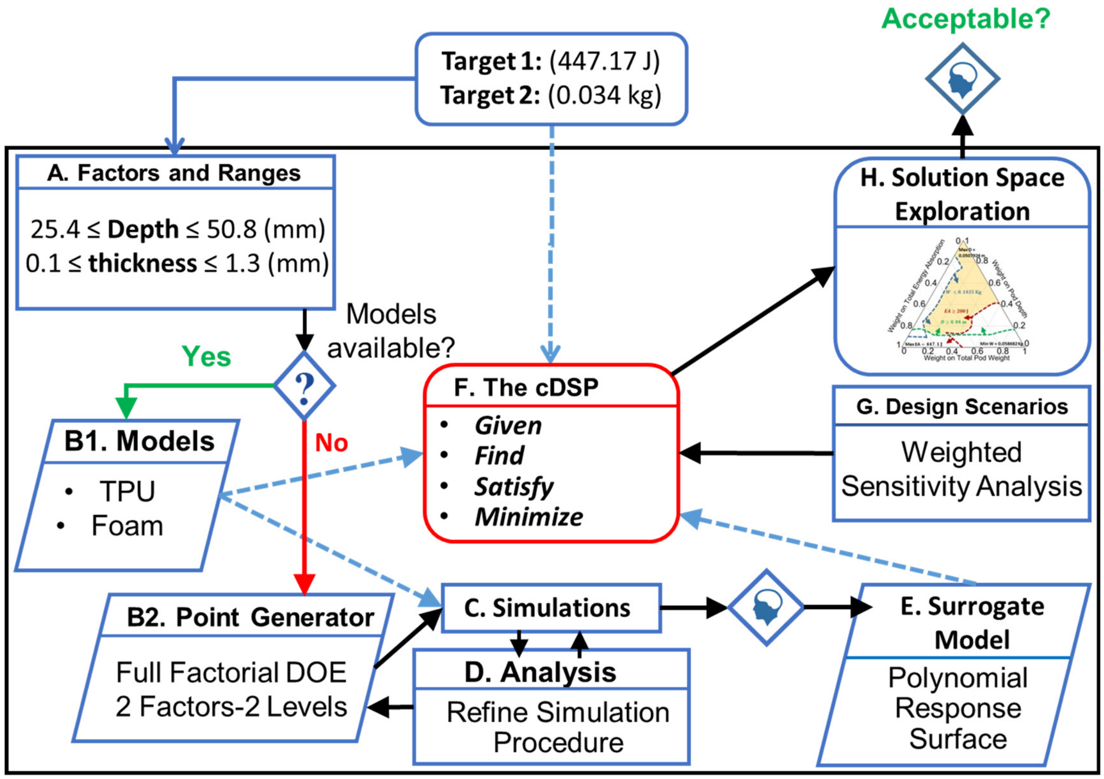


Figure 10.5: Application of the Concept Exploration Framework to formulate the cDSP for foam and TPU liner (Courtesy of Tate Fonville and Dr. Mark Horstemeyer, MSU)

The helmet design example is thus used to gain confidence in the applicability of the systems-based design architecture to example problems discussed beyond this dissertation thereby establishing theoretical performance validation of the hypotheses proposed in this dissertation.

2) ***Integrated Design of Topology and Material – Hot Stamping Example*** **(Work carried out by Beijing Institute of Technology, China and SRL@OU)**

Problem Overview: The production of high strength steel components with desired properties during hot stamping requires profound knowledge and control of the forming procedures. Depending on the temperature history and mechanical deformation, different phases evolve resulting in different mechanical properties of end product produced. The difficulty lies in establishing the processing-structure-property-performance relationship considering topology features and material behavior due to complex relationships. Therefore, the interested here is to describe the different phenomenon that happens during hot stamping so as to establish the processing-structure-property-performance relationship in an inverse manner considering topology features and material behavior.

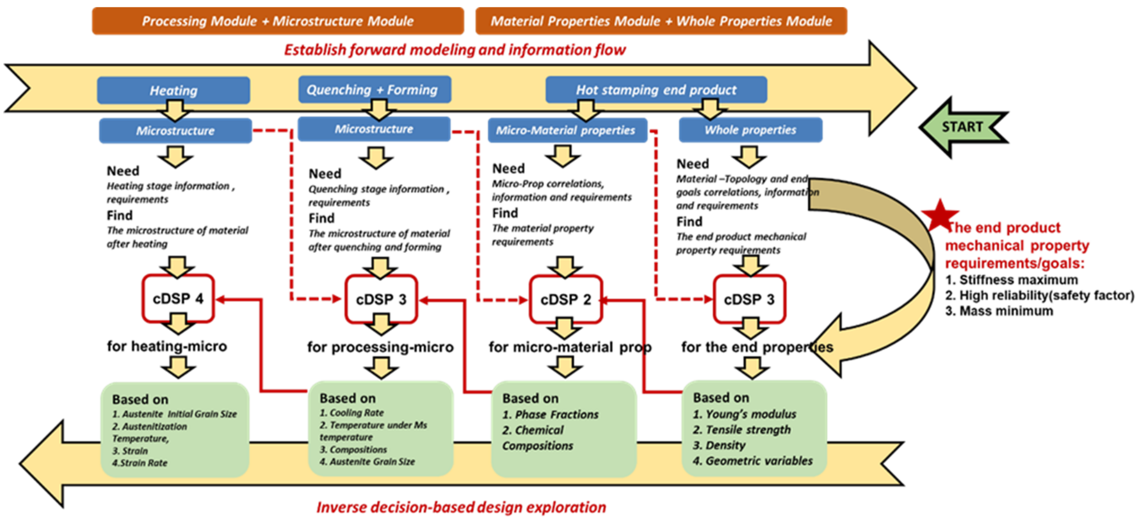


Figure 10.6: Application of GoID method for the hot stamping problem (Courtesy of Shuting Chen, Beijing Institute of Technology, China)

In Figure 10.6, the application of GoID method for the hot stamping process chain is shown. The forward information workflow for the material is established using models. The inverse design exploration starts with the cDSP for the end product mechanical properties. The GoID method is used to further design the microstructure and processing aspects of the product. In this example problem, both the topology and the material are designed in an integrated manner. The results obtained are not addressed in this dissertation. The hot stamping process chain design example is thus used to gain confidence in the applicability of the systems-based design architecture to example problems discussed beyond this dissertation thereby establishing theoretical performance validation of the hypotheses proposed in this dissertation.

3) Designing a Data Analytics Platform for Analyzing Signals (Work in initial discussion stage with TCS Research, Bangalore)

***Problem Overview*:** Fundamentally, any data analytics application requires a computational model. This computational model is in terms of a data flow and control flow. The flow graph consists of nodes and edges. The nodes are computational units. The edges are data buffers which connect the interdependent nodes. For handling dynamic environments, the data flow and control flow need to be adaptive. Towards this, there is a need for a decision support platform, which can support the designer in multi-objective decision support by taking into account data and control dependencies. The utility through the decision support is in identifying the computational nodes that best satisfy the requirements. These selected nodes when executed, can achieve a data analytics goal in the presence of constraints. In Figure 10.7, a typical data and control flow diagram with nodes and edges are shown.

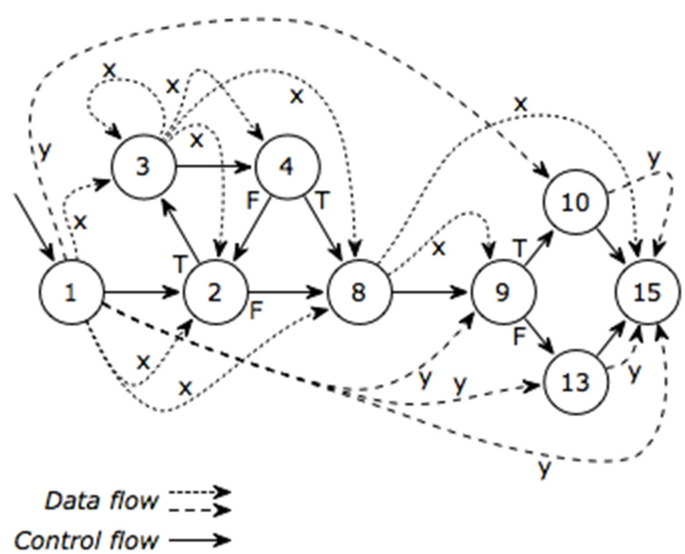


Figure 10.7: Data flow and control flow diagram (Image source: http://www.julioauto.com/project/visual-data-tracer.html)

Connecting the steel manufacturing example used in this dissertation to the problem described: The data analytics problem is tied to the steel manufacturing process chain example that we are looking at and can be explained in the context of that. In the steel manufacturing process chain example, the designer is looking at a manufacturing process chain involving the material and end product in terms of the information flow that is happening across the process chain. We capture the manufacturing process chain in terms of a network of computational models that transform information (the information is the material at each stage that gets transformed) to realize the end product. Once the designer comes up with the information flow across the manufacturing process chain via a network of models (defined as the forward material workflow), a goal-oriented, inverse design exploration is carried out starting from the end performance that is needed for the product. This is a "top-down", requirements-driven inductive/inverse design exploration, where we formulate a Decision Support Problem (DSP) starting from the end product in an inverse manner to design the whole system to meet the end requirements that are identified (defined as the inverse decision workflow). The philosophy in formulating the DSP is to find "satisficing robust solutions" rather than single point optimal solutions. This is because optimization of a complex system is not possible as the single point solutions will not be valid due to the uncertainty that is present in a complex system. So, robust solutions are sought by managing the uncertainty that is present.

The data analytics problem described is a similar problem where information is flowing via a network of computational models. The data flow here would tie to how the material flows throughout the process chain. Control flow would tie to how the material flow is controlled in the process chain. Like, say the austenite phase of iron has to completely transform into other phases, etc. This would be like setting rules based on physics of the material/problem so that we achieve the end product desired. Now for this whole forward flow chain of information, the designer can come up with an equivalent decision workflow. The decision workflow will be used by the designer to design the system to achieve certain end requirements. Now, the next part is for the decision workflow to be adaptive and reusable. This means the knowledge associated with the decision workflow needs to be captured and there should be a facility to carry out original, adaptive and variant designs as per the changes that are happening. Also, there is a need to communicate information instantly across multiple directions in a data flow network. This can be facilitated by a CB-PDSIDES (Cloud-Based Platform for Decision Support in the Design of Engineering Systems). The CB-PDSIDES is proposed in Section 10.4.

An equivalent analogy from the steel manufacturing process chain on the processing-structure-property-performance into data analytics and the application of the constructs proposed in this dissertation to this problem domain is described below.

Process Analogy: Portfolio of algorithms

Structure Analogy: Structure in data (statistial, spectral, topological)

Property Analogy: Accuracy, Consistency, Completeness, Density, Validity (Quality properties from Data analytics)

Performance Analogy: Goal relevant performance on the inferences made on the data.

Proposed Approach: In the problem described, there is data that is flowing through several computational units. The user at the end starts with certain performance characteristics desired in the data. These characteristics are transformed to certain functional requirements like accuracy, consistency, etc of the data. This is similar to defining the material properties desired for the end performance of the product. Now the goal here is to design the data structure to satisfy these property requirements. This is similar to designing the microstructure of the material to satisfy the end mechanical properties. Now, once the required data structure is designed/identified, the algorithms need to process the initial data set so that the identified data structure is achieved. This whole process is equivalent to the goal-oriented inverse design exploration of material microstructure and processing paths to satisfy product level property and performance requirements.

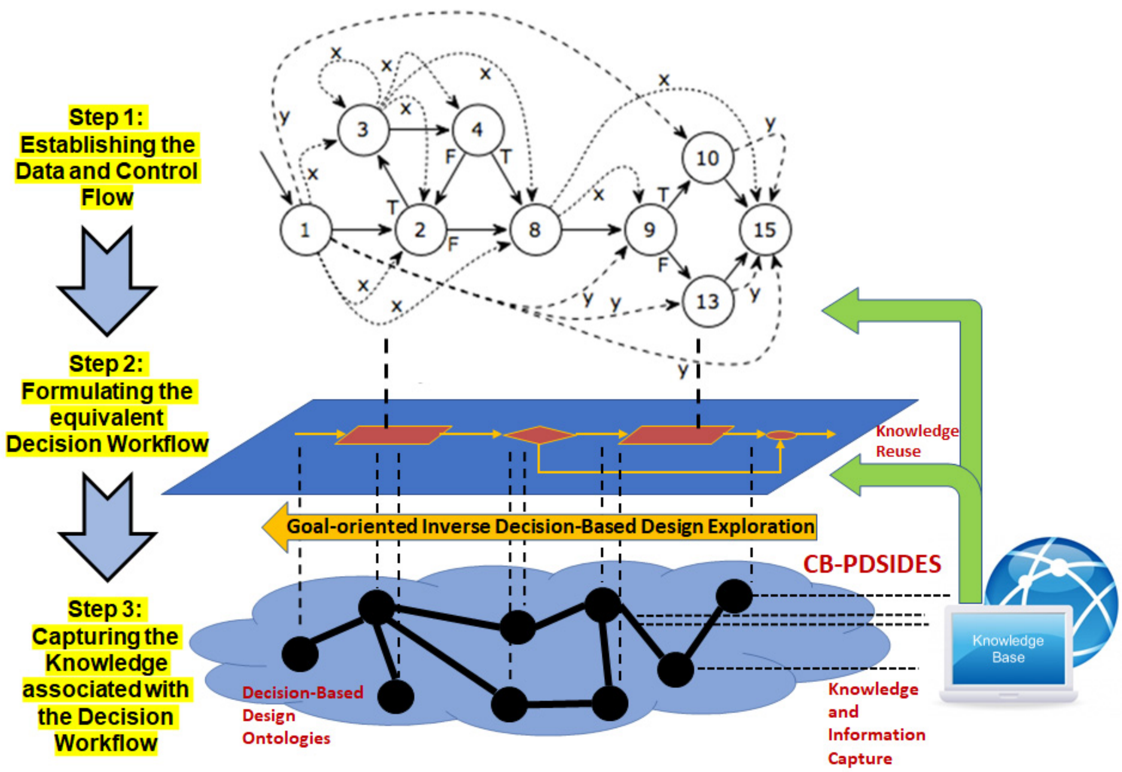


Figure 10.8: Vision to carry out the design of a data analytics platform

The application of the work proposed in this dissertation to this problem domain is explained using Figure 10.8 in three steps.

Step 1: To apply the approach proposed in this dissertation, there should be models/computational units that can establish the data/information flow across the system. The models should be able to represent/define functional relationships in terms of input factors and output responses across the whole system. This is the Step 1 of the approach.

Step 2: Once data/information via data flow diagram and control flow diagram is established, the designer can formulate the equivalent decision workflow. In the decision workflow the designer tries to capture the key information and propagation of information across the system as defined by the problem statement. This allows the designer/data scientist to carry out an inverse decision-based design exploration further to achieve end user requirements. This is by formulating specific goals and constraints relevant to the problem and exploring the solution space in an inverse manner to satisfy the end user data requirements.

Step 3: Using decision-based design ontologies associated with the Decision Support Problem constructs in PDSIDES, the knowledge associated with decision workflow for data structure is captured. The PDSIDES platform facilitates original, adaptive and variant designs and supports the designer/data scientist in reusing the knowledge and making the process adaptive to changing requirements. Since multi-way information flow is necessary and information acquisition in an instant manner to collaborating data scientists across the globe is necessary, the need for a cloud-based platform is essential. The PDSIDES platform can support this when integrated with the cloud. The initial ideas regarding PDSIDES in the cloud known as Cloud-Based Platform for Decision Support in the Design of Engineering Systems (CB-PDSIDES) is proposed in Section 10.4 and will be developed as a future work in collaboration with Beijing Institute of Technology, China.

10.3 Key Contributions and Opportunities for Improvement in this Dissertation

10.3.1 Key Contributions

The foundational premise for this dissertation is that systems-based materials design techniques offer the potential for tailoring materials, their processing paths and the end products that employ these materials in an integrated fashion for challenging applications to satisfy conflicting product and process level property and performance requirements. The primary goal in this dissertation is to establish some of the scientific foundations and tools that are needed for the integrated realization of materials, products and manufacturing processes using simulation models that are typically incomplete, inaccurate and not of equal fidelity by managing the uncertainty associated. Accordingly, the interest in this dissertation lies in establishing a systems-based design architecture that includes system-level synthesis methods and tools that are required for the integrated design of complex materials, products and associated manufacturing processes starting from the end requirements.

The contributions from the dissertation are categorized into new knowledge in four research domains: a) systematic model integration and information flow (vertical and horizontal) for integrated material and product workflows, b) goal-oriented, inverse decision support, c) robust concept exploration of process chains with multiple conflicting goals and d) knowledge-based decision support for rapid and robust design exploration in simulation-based integrated material, product and process design.

As discussed in Chapter 1, the creation of new knowledge in this dissertation is associated with the development of a systems-based design architecture involving systematic function-based approach of formulating forward material workflows, a concept exploration framework for systematic design exploration, an inverse decision-based design method, and robust design metrics, all integrated with a knowledge-based platform for decision support. The theoretical, mathematical and computational foundations for the design architecture are proposed in this dissertation to facilitate rapid and robust exploration of the design and solution spaces to identify material microstructures and processing paths that satisfy conflicting property and performance for complex materials, products and processes by managing uncertainty.

Specific contributions in this research include:

- Systematic identification and integration of material, process and product models and workflows to define processing-structure-property-performance mapping and information workflow ***(Contributions from Research Hypotheses 1)***,
- A reusable, expandable computational framework supporting vertical and horizontal integration of models to identify material structures and processing paths that satisfy ranged set of product and manufacturing process-level property and performance requirements ***(Contribution from Research Hypotheses 2 and 4)***,
- A framework supporting systematic design and solution space exploration ***(Contribution from Research Hypotheses 2)***,
- A generic method for inverse design of materials and products across process chains ***(Contribution from Research Hypotheses 2)***,
- Metrics, robust design constraints and goals for facilitating robust design across process chains for multiple conflicting goals ***(Contribution from Research Hypotheses 3)***,

- Capture knowledge in original design, maintain consistency in adaptive design and provide a package of documented knowledge in variant design ***(Contribution from Research Hypotheses 4)***,
- Template-based ontological method for systematic design space exploration ***(Contribution from Research Hypotheses 4)***.

Based on these contributions a designer now has the following abilities the baseline designer did not have before:

- Designing materials and products in a systematic fashion during the early stages of design by looking at information flow and mapping across models,
- Designing products, materials and their processing paths in a function-based, systematic, integrated fashion from a systems perspective by satisfying specific end performance requirements ***(Contribution from Research Hypotheses 1 and 2)***,
- The capability to carry out rapid, integrated design exploration of material and products using simulation models that we accept are typically incomplete and inaccurate ***(Contribution from Research Hypotheses 2)***,
- The capability to support a human designer under complex material system's random variability and/or model parameter uncertainty and/or model structure uncertainty in making decisions that satisfies multiple conflicting goals ***(Contribution from Research Hypotheses 3)***,
- The capability to model decision-related knowledge with templates using ontologies to facilitate execution and reuse ***(Contribution from Research Hypotheses 4)***,

- The capability to coordinate information and human decision making ***(Contribution from Research Hypotheses 1 to 4)***.

Therefore, crucial to this dissertation are:

i) The requirements driven, "top-down" design of system and associated subsystems by taking a goal-oriented, inverse approach which is different to the standard practice of bottom-up modeling and design of material and product systems,

ii) The management of uncertainty in the system without removing the sources and supporting in identifying satisficing robust design solutions across process chains for multiple conflicting goals that require different types of robust designs,

iii) Platformization of decision templates to support different types of users to facilitate original, adaptive and variant designs in materials and product design.

The systems-based design architecture for integrated model-based realization of materials, products and associated manufacturing processes is validated using the industry-inspired example problem from the steel manufacturing domain, namely: *the integrated design of steel (material), manufacturing processes (rolling and cooling) and hot rolled rods (product) for automotive gears*.

However, potential applications are numerous and compelling, and not limited to the one addressed in this dissertation. The framework and method developed in this dissertation is generalizable for industries in which mechanical, structural, and thermal systems are essential. The applications include the manufacturing of lightweight, high performance, low cost and reliable parts and machine components, for example automobile gear box, shafts, etc.

10.3.2 Opportunities for Improvement in Current Work

Opportunities for improvement in Research Area 1 based on Research Hypotheses 1 proposed in this dissertation

- The assumption in Research Hypotheses 1 is that models are available, or data/simulations are available to come up with functional relationships for the problems that are being tackled. However, in reality this is not the case and thus further research need to be carried out to address situations when there is not enough information available to come up with function structures.
- Opportunities to address beyond concept generation and early stages of design needs to be explored.
- Improvements in design catalogs to update instantly and provide information instantly via online and cloud-based resources needs to be explored.

Opportunities for improvement in Research Area 2 based on Research Hypotheses 2 proposed in this dissertation

- Automation of the design exploration process by using rules and improved algorithms that uses machine learning and artificial intelligence techniques is required to improve the design and solution space exploration process.
- Improved visualization and post processing tools needs to be developed to handle *n* number of goals while exploration.

- Different surrogate modeling techniques needs to be explored and used depending on the size, accuracy and computational complexity of the problem/data being considered.
- Iterative loops and feedback loops need to be included into the GoID method to ensure the identification of satisficing solutions that best meets the requirements.
- The GoID method in the form presented in this dissertation only supports sequential flow of information. However, most complex problems will have information flow in the form of network or hierarchy where information flow is non-sequential. Exploring opportunities to address situations with non-sequential flow of information is essential to address a wide range of complex problems.

Opportunities for improvement in Research Area 3 based on Research Hypotheses 3 proposed in this dissertation

- Capturing the designer's preference via EMI and DCI is not fully possible due to the mathematical form of the metrices. This necessitates the need to reformulate the robust design goals in terms of mean and variance separately. This, however limits the exploration process as more than three goals needs to be explored due to the reformulation. Hence opportunities for capturing the designer's preference needs to be explored in Research Hypotheses 3. This also demands the need for exploration and visualization techniques when there are more than three goals.
- Another assumption is that the mean model truly represents the mean value of the variability associated with the model. This, however is not true. Hence, there is a need to accurately formulate and capture mean response models from a given set of

data so as to be considered for robust design using the approach proposed in this dissertation.

Opportunities for improvement in Research Area 4 based on Research Hypotheses 4 proposed in this dissertation

- Opportunities need to be explored for integrating PDSIDES platform with the cloud to facilitate smart product realization in the globalized 21st century.

10.4 A Vision for Future Research in Robust Product Realization via a Cloud-Based Platform for Decision Support in the Design of Engineered Systems (CB-PDSIDES)

A revolution is happening with the advent of Industry 4.0 where the different elements of an industrial system is integrated and connected with smart, internet communication technologies resulting in smart and intelligent manufacturing procedures for product realization. As discussed by Thames and Schaefer (Thames and Schaefer 2017), Industry 4.0 and its associated technologies such as cloud-based design and manufacturing systems, the Internet of Things (IoT), the Industrial Internet of Things, and Social-Product Development are driven by technologies and innovations that are disruptive leading to massive creation of value to those involved in the market sectors. This new revolution is a result of the convergence of industrial systems with advanced computing technologies, sensors and ubiquitous communication systems. The IoT started when there began efforts to integrate the computing and communication technology into many "things" that people use at home and work. The Industrial IoT is defined as a subset of IoT with very similar characteristics, especially the presence of embedded computing and communication technology. Now, in this section we address how these technologies are going to change the way we realize materials and products and the way they are designed. One major change that has happened with these new technologies is the power shift from the hierarchical business models that used to exist in industry to cooperative collaboration networks. Now this will impact the way products are designed and developed in the 21st Century and has thus paved way for some new product development paradigms.

10.4.1 The Traditional Product Design Paradigms and Need for a Change

The two widely accepted design approaches both in academia and industry are the Pahl and Beitz (Pahl and Beitz 1996) systematic design approach and Suh's Axiomatic Design (Suh 1990). Both of these are reviewed in detail in Chapter 3. Pahl and Beitz describe the process of product development as a series of core transformations. The core transformations start from problem description to requirements list to principal solutions and working structures, to preliminary design, to detailed design and final manufacturing specifications. The whole product design activities are classified into product planning, conceptual design, embodiment design, and detail design.

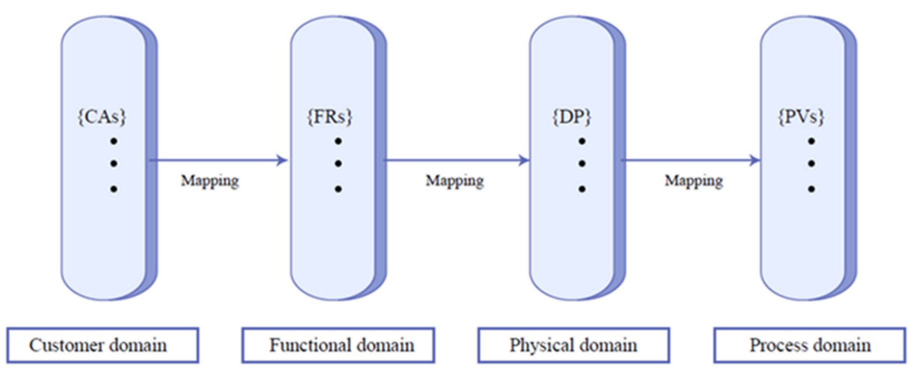


Figure 10.9: Suh's Axiomatic Design domains and one-way mapping across domains

Suh's Axiomatic Design is a systematic design approach that uses a design matrix to analyze the transformation of customer needs into functional requirements, design parameters and process variables. Thus, there is a one-way mapping across these four design domains in Suh's Axiomatic Design from customer domain to functional domain to physical domain to process domain, see Figure 10.9.

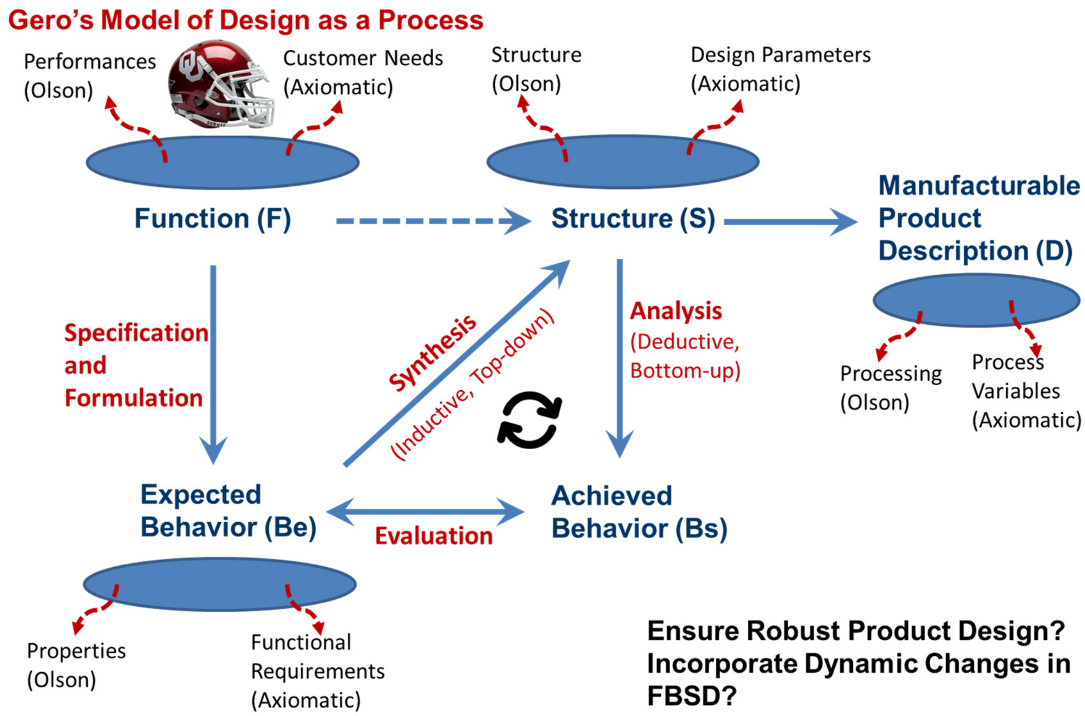


Figure 10.10: Gero's model of design as a process for coming up with manufacturable product descriptions and questions to be addressed

The model of design as a process proposed by Gero (Gero 1996) to come up with manufacturable product descriptions also can be tied to Suh's Axiomatic Design. Gero uses Function-Behavior-Structure-Description model where the function is equivalent to customer domain, the behavior equivalent to functional requirements, the structure equivalent to design parameters and the product descriptions equivalent process variables, see Figure 10.10.

However, these traditional design paradigms are not competent to address the changing needs and technologies associated with product realization in the 21st Century. Neither Pahl and Beitz design method nor Suh's Axiomatic Design (or even Gero's model of design) offers a framework that facilitates seamless information, knowledge and resource sharing, or aids participants of global value co-creation networks in identifying potential collaboration partners or resource providers (Franke, Von Hippel and coauthors 2006, Thames and Schaefer 2017)***. The need therefore is for a network of participants who share information, knowledge and manufacturing resources so as to facilitate co-creation of value in a more cost-effective manner. Thus, traditional product development methods need to be updated and bridged to the new developments happening in the globalized world, such as crowd-sourcing, mass collaboration and social product development.***

We tie this product development paradigms to the research addressed in this dissertation. We focus on the end product goals that need to be satisfied and try to design the system starting with these end goals in an inverse manner to design explore the material microstructures and processing paths, see Figure 10.11. In Figure 10.11, a quadrant is shown. The quadrant captures the domains of product development. In the lower right quadrant is the production domain involving process variables and their relationship to design parameters. In the upper right quadrant is the engineering domain involving design parameters and functional relationships. In the upper left quadrant is the customer domain involving functional relationships and their dependencies to customer requirements.

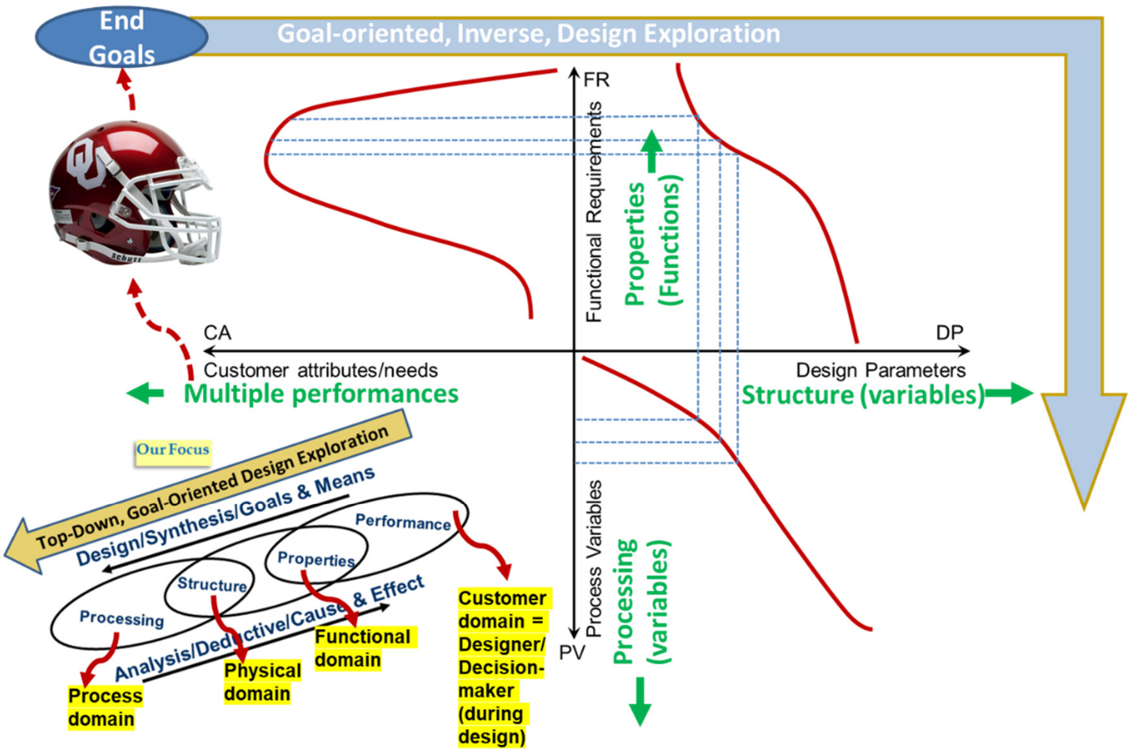


Figure 10.11: The customer-centric product realization process – tied to the research addressed in this dissertation

Thus, we adopt a customer-centric perspective towards product realization where the customer attributes/needs are the performance desired for the product. The product/material properties are the functional requirements, the microstructure of material are the design parameters in physical domain and the processing variables are the process variables in process domain, see Figure 10.11. Currently, based on the research addressed in this dissertation and the systems-based design architecture proposed, we are able to carry out a one-way mapping starting from the end performance of the product to the initial processing of the material using models and are able to identify robust satisficing solutions across the different domains. Using the knowledge-based platform PDSIDES we are also able to capture, store and reuse the information and knowledge generated. However, in the current form the systems-based design architecture proposed do not facilitate the opportunity for a network of participants/designers to share information, knowledge and manufacturing resources instantly and collaborate so as to facilitate co-creation of value in a more cost-effective manner thereby supporting open innovation. This needs to be addressed and the hypothesis is that *a cloud-based platform for decision support (CB-PDSIDES) that has all the features and functionalities of PDSIDES integrated in the cloud will provide this opportunity for mass collaboration and open innovation there by supporting product realization needs in 21st century.*

We start with the key functionalities needed for product realization in 21st century globalized world in Section 10.4.2. This is followed by defining the cloud-based platform for decision support in design of engineering systems (CB-PDSIDES) and key functionalities that CB-PDSIDES offers.

10.4.2 Key Functionalities Needed for Product Realization in 21st Century Globalized World

- **Integration of models and simulation tools** spanning processes and length scales (the different domains in axiomatic design),
- **Define computational workflows** involving decision making, spanning multiple activities and users; define modular, reusable sub-workflows for specific processes,
- Ability to **connect to external databases** on materials, products and processes,
- **Knowledge-guided assistance** to different types of users in design-related decision making,
- **Collaborative, multidisciplinary design** and privacy control,
- **Management of Complexity** (Reduced cost of computation),

- **Exploration and Visualization** of the design and solution space,
- **Dynamic** and **cost-efficient reconfiguration** and **integration** of design decision templates to explore different **robust design** strategies.

PDSIDES has the potential to provide these functionalities when integrated with the cloud. Figure 10.12 illustrates the concepts underlying the foundations and principles of CB-PDSIDES as proposed in this dissertation. To integrate PDSIDES with cloud and bring-in the concepts of cloud computing and collaboration into product design and manufacturing, we adopt a definition for Cloud-Based Design and Manufacturing as proposed by Wu and co-authors (Wu, Thames and coauthors 2012).

"Cloud-Based Design and Manufacturing refers to a product realization model that enables collective open innovation and rapid product development with minimum costs through a social networking and negotiation platform between service providers and consumers. It is a type of parallel and distributed system consisting of a collection of inter-connected physical and virtualized service pools of design and manufacturing resources (e.g.: parts, assemblies, CAD/CAM tools) as well as intelligent search capabilities for design and manufacturing solutions."

From the context of PDSIDES, the platform integrated to cloud has in its core a decision support tool. This could be cDSP, sDSP or any other decision support tools that the designer prefers. In Figure 10.10, we show the CB-PDSIDES with the cDSP construct at its core as the fundamental decision support construct. The cDSP will have problem specific information captured via the keywords. The analysis codes and simulations associated with the problem framed are also communicated to the decision support construct, see Figure 10.12.

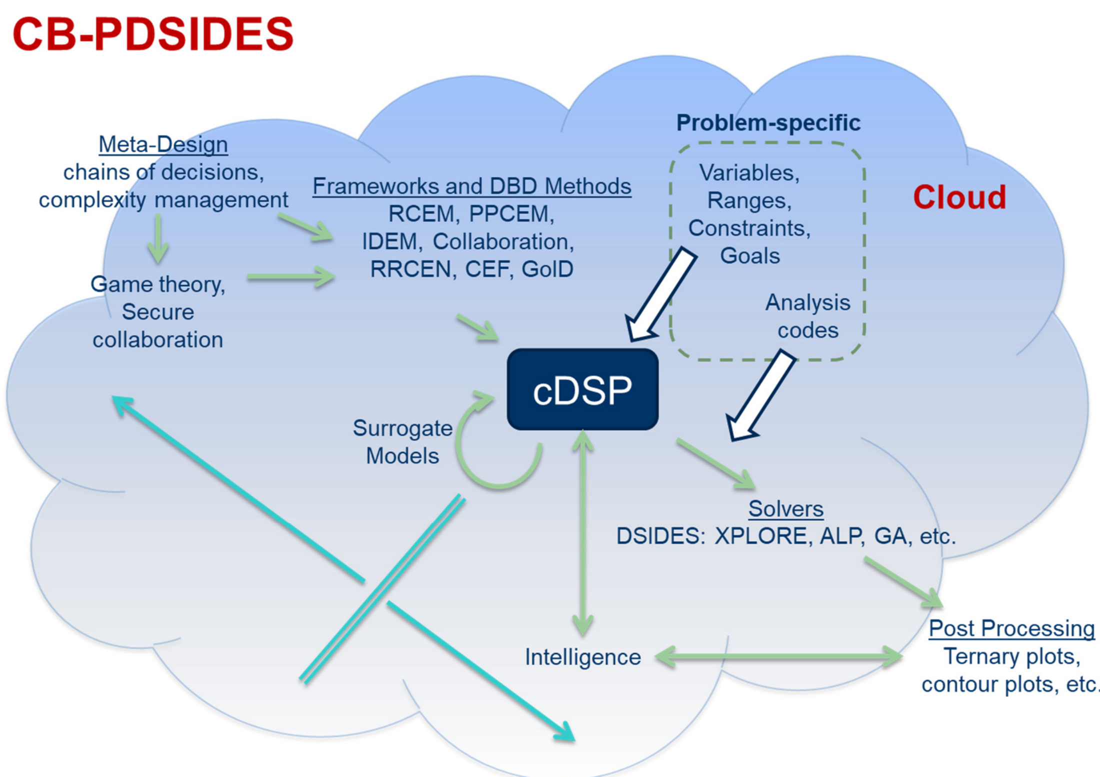


Figure 10.12: An illustration of the Cloud-Based Platform for Decision Support in the Design of Engineering Systems concept

All the frameworks and decision-based design methods, constructs and tools developed over the years are available to support the designer to formulate and execute the design problem systematically. This includes Robust Concept Exploration Method (RCEM), Product Platform Concept Exploration Method (PPCEM), Inductive Design Exploration Method (IDEM), Concept Exploration Framework (CEF), Goal-oriented Inverse Design (GoID) Method, etc. The solvers associated with the execution of problem formulated like DSIDES for cDSP construct is available to be accessed in the cloud. Post-processing tools like ternary plots, contour plots etc. that are automated with rules to help the designer easily explore the solution space will be available to access. Machine learning techniques can be used to bring in intelligence into the exploration process there by supporting the designer in making "intelligent" design decisions. Surrogate modeling techniques and tools are available in the platform to support the designer in managing the complexity and coming up with reduced order models. The issues of collaboration and information sharing is also addressed as collaboration and communication is key in the cloud-based PDSIDES. The key functionalities of CB-PDSIDES to facilitate robust product design is addressed in Section 10.4.3.

10.4.3 Key functionalities needed in cloud-based computer platform (CB-PDSIDES) to facilitate robust product design

❖ ***Modular reuse of design workflows along a design process***

- Designing the workflows by reusing past knowledge from similar design problems. Specifically,
  - Support for reusing and reconfiguring workflows for different conditions and problems
  - Reconfiguring the computational workflow developed for one product to the design of another product, see Figure 10.13.

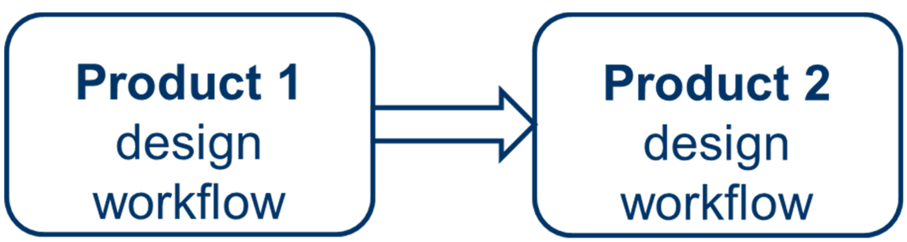


Figure 10.13: Modular reuse of reuse of design workflows along a design process

  - Example: Design of gears to design of shafts
  - Support for uncertainty and complexity management in design workflows
  - Uncertainty propagation in design workflows
  - Model management and knowledge-based idealizations

The focus is on concurrently exploring the design space of both the products and the materials and narrow the set of possible options in the shortest possible time and minimum expense. Hence, instead of exploring the complete design space from first principles using detailed models, the focus is on simplified models that are good enough to compare different design alternatives. Additionally, the notion of designing the workflows by reusing past knowledge from similar design problems is important because of:

i) evolving simulation models, resulting in multiple fidelities of models at different stages of a design process, and

ii) significant model development and execution costs, necessitating judicious use of resources.

Moreover, the needs for accurate information depend on whether the goal is to narrow down the alternatives to a specific class of materials (i.e., during early design phase) and products or to design the composition and structure of a specific material system (i.e., during the later stages of design). In order to support the need to generate information at variable fidelities during the design process, the following requirements must be satisfied by CB-PDSIDES:

i) Support for reusing and reconfiguring workflows for different conditions and problems

ii) Support for complexity and uncertainty management: Need computational techniques to measure how complexity and uncertainty changes by replacing different components of the workflow

iii) *Model management and knowledge-based idealizations: Representation of models at different levels of abstraction, along with information about their accuracy.*

❖ ***Design workflows in distributed collaborative settings***

- Collaborative design workflows

A scenario where components (gear and shafts) are designed by one organization, and materials (steel) are designed by another organization.

Assume that materials designers have proprietary models. They do not want to share (explicitly or implicitly) their own models with the component designers. Similarly, the product designers do not want to share the details of their cDSP.

However, both parties would like to jointly design the product and the material and are connected with each other via cloud.

The collaborative nature of the design process induces additional requirements on the management of design workflows.

Key issues in collaborative workflow management

i) The potential for inconsistencies among collaborating entities. These inconsistencies can be in requirements, assumptions about the system, levels of fidelity of models, and the manner in which resources are allocated. Hence, ensuring consistency across the parts of workflows developed by different collaborative entities is an essential feature of a platform for integrated product and materials design.

ii) Issues in collaborative design exploration during the early stages of design due to intellectual property protection, different parties may be reluctant to share information with each other. Before parties have decided whether the collaboration would be meaningful, designers generally need to exchange information about capabilities and sub-system behaviors. Such information can either be in terms of performance curves and datasheets, or test results from independent entities. For complex systems such as integrated materials and products design, systems designers may need detailed mathematical models encapsulating the behavior to ensure that the collaborative design would meet the desired performance objectives. Such behavioral models embody significant knowledge and have the potential to reveal confidential information about the subsystem. In such cases, designers may be reluctant to share the models for collaborative exploration of design spaces. In such cases, the platform should enable collaborative design while preserving privacy of the individual models.

The requirements to be addressed in CB-PDSIDES includes:

i) Collaborative authoring of workflow templates

ii) Privacy-preserving collaboration in integrated products and materials design

❖ ***Reduce cost of computation and management of complexity***

There are several methods for simulating various aspects of materials manufacture and product design. However, it can be very costly and time consuming to compute and re-compute these simulations in the process of design, especially in the early stages of design where it is desirable to explore a wide range of options rather than developing detailed designs. For situations like this, there are several ways of developing surrogate models (metamodels) which rapidly provide design information, each of these will give metamodels of different degrees of accuracy at different costs which may be used at different stages of design. There is thus a need to assess the benefits of using different metamodels in different stages of design and compare these with the costs of developing these metamodels. Using metamodels of increasing fidelity in a design process is one way of exploring the design space, an alternative way is by using robust design with decreasing bands of robustness. The advantages and limitations of each of these approaches will be considered. The requirements thus to be addressed in CB-PDSIDES include:

i) *Develop reduced order models of various degrees of fidelity using simulations and assess reductions in computational costs when using these models.*

ii) *Combine the use of metamodels with varying degrees of robust design and assess tradeoffs between accuracy and computational costs.*

❖ ***Cost-efficient integration of templates for product development – Carry out meta-design***

- Changing the outcome of design process by changing the ways in which templates are integrated.
  - Exploring the effect of changing the ways in which templates are integrated on the outcomes of the design workflows (i.e., meta-design)

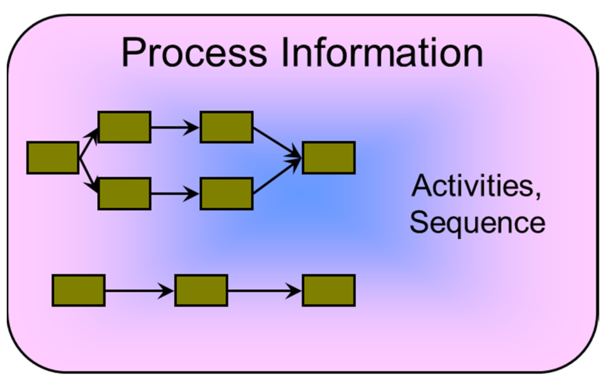


Figure 10.14: Meta-design - Changing the outcome of design process by changing the ways in which templates are integrated

Many different strategies can be adopted for integrated design of products and materials. The outcomes of the design process change by changing the ways in which templates are integrated, see Figure 10.14. Two examples of such strategies include sequential design and set-based design. In the sequential design scenario, the decisions are made in a sequential order, e.g., the material may be designed before the product designer finalizes the geometry. On the other hand, in the set-based design scenario, designers consider sets of design alternatives rather than pursuing one alternative directly. The strategy is to gradually narrow down the design space until a final solution is achieved. In the materials-product design scenario, this may be implemented as one designer (materials or product) coming up with a range of design parameters and then passing on this range to another designer to select the best value in that range. Since the designers do not pick a single alternative, the designers develop multiple alternatives. Although this approach is more likely to result in designs that show superior performance with regard to both the material and product considerations, the design effort involved in developing all alternatives is higher.

- ***Systematic design and solution space exploration considering system uncertainty***

Design and solution space exploration by considering system uncertainty is essential for the model-based realization of complex engineered systems. As discussed in this dissertation in previous chapters, the models that are available are typically incomplete, inaccurate and not of equal fidelity. Hence, seeking single point optimum solutions are not valid in this case as these solutions are not more valid if any variations occur. This necessitates the need for systematic design and solution space exploration to identify satisficing solutions that perform well and are relatively insensitive to the uncertainty present in the system. Using the cloud-based platform CB-PDSIDES, designers can collaborate from different parts of the world in formulating design problems and exploring the design and solution space using rules defined in the platform for exploration of solution space and post-solution analysis. The exploration of the solution space provides designers with knowledge to refine or improve the model especially at early stages of design.

❖ ***Cloud-based design communication – Instant feedback across design workflows***

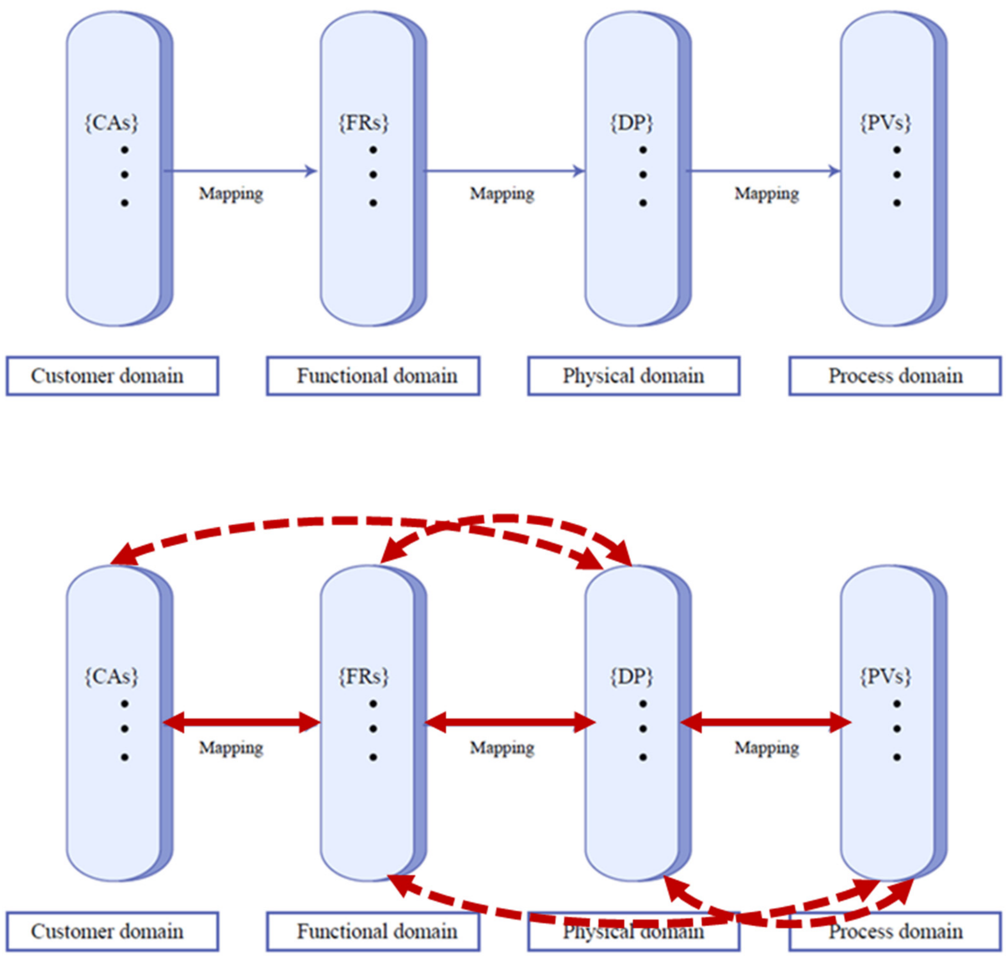


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Figure 10.15: Communication in traditional design (top) and communication via information channels using cloud-based design (bottom)

- Multiple information channels and communication across design workflows (can be related communication between axiomatic design domains),
- Communication across multiple directions – dynamic product updates, design changes and feedback.

Communication of design process is a very important goal in engineering design. Improving design communication requires addressing of the key issue which is the extent to which design engineers fully understand a complex design process. This includes design tasks that need to be completed, the source for specific information that is needed for design, the individual to be contacted for the right information, the extent of distortion in the information available, the extent to which the distorted information affects design (Wu, Rosen and coauthors 2015). In traditional design paradigms discussed in Section 10.4.1, the communication is a one-way mapping in a linear sequence of design phases/domains as can be seen in Figure 10.15.

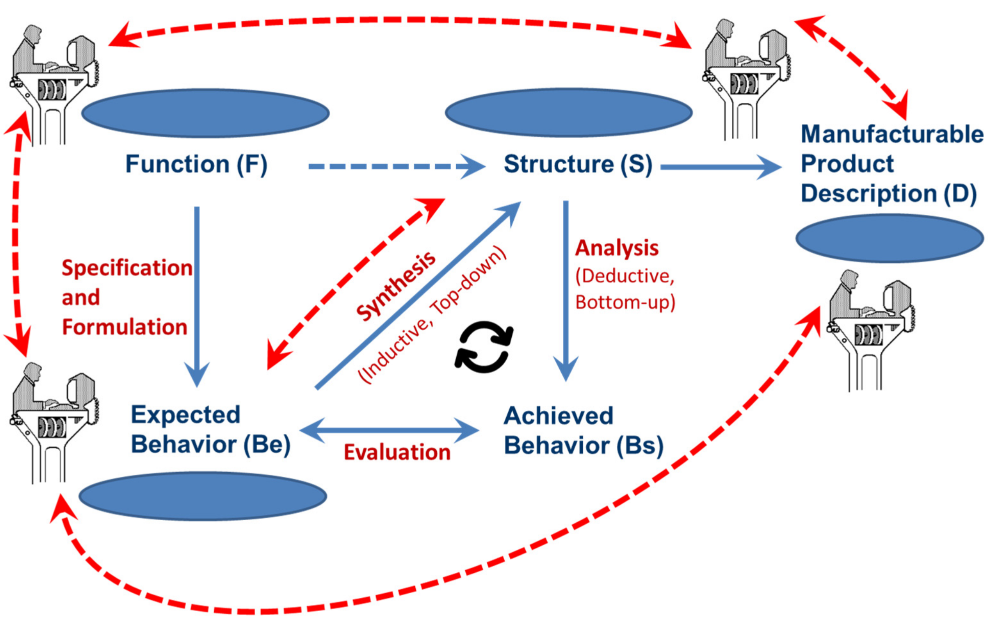

Figure 10.16: Implication of CB-PDSIDES in product realization process

PDSIDES has the potential to facilitate this communication via decision workflows in its current stage. Integrating PDSIDES in the cloud settings will improve design communication through multiple information channels facilitated by cloud. This will allow for information flow in multiple directions as shown in Figure 10.15. This will facilitate dynamic changes during product development and instant communication between the different design domains like customer and physical domains or functional and process domains; as shown in Figure 10.15. The implication of CB-PDSIDES in product realization process is explained using Gero's model of design in Figure 10.16. Assuming that each stage of product realization starting from function to final manufacturable product descriptions involve distributed designers as shown in Figure 10.16. In the traditional way PDSIDES facilitates a decision network where information is shared in a one-way fashion. CB-PDSIDES however can facilitate collaboration and can result in a two-way and multi-way network for product realization where the distributed designers are connected through the cloud. This facilitates dynamic product updates, design changes and feedback in the product realization process.

10.4.4 Transitioning to Industry using CB-PDSIDES – Interface TCS PREMΛP with CB-PDSIDES

The PREMΛP—Platform for Realization of Engineered Materials and Products is developed by TCS Research, Pune as a comprehensive IT platform that facilitates the integration of models, knowledge, and data for designing both the material and the product (Gautham, Singh and coauthors 2013). PREMΛP is developed as a platform to help address problems related to,

i) new product design;

ii) material and/or process substitution;

iii) new material development;

iv) developing materials for special performance needs;

v) develop and/or enhance specifications

in an industrial environment. The platform is developed for different types of users like expert users, non-expert end user and for researchers. The PREMΛP includes several components which are both domain dependent and domain independent as shown in Figure 10.17.

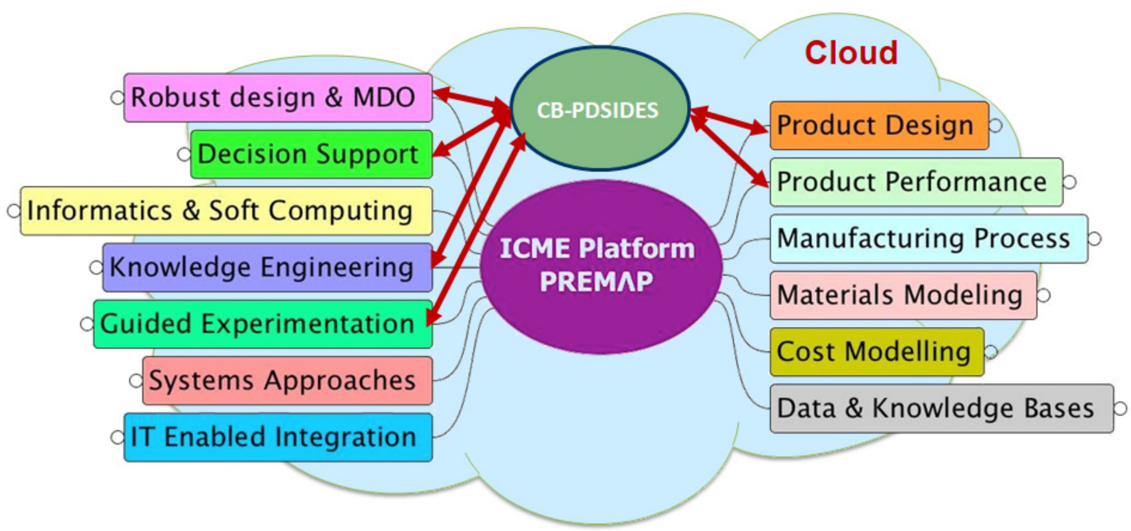

Figure 10.17: Interfacing CB-PDSIDES with TCS PREMΛP. The domain independent (left) and domain dependent (right) components of the platform are shown.

The CB-PDSIDES proposed in this dissertation has the potential to support PREMΛP with several of its components. Based on the key functionalities proposed for CB-PDSIDES in Section 10.4.3, it is envisioned that CB-PDSIDES can support PREMΛP in *Robust design and MDO, Decision Support, Knowledge Engineering; Guided Experimentation, Product Design* and *Product Performance*. Discussions along these lines with TCS Research, Pune has resulted in the experimentation of implementation of models and framework proposed in this dissertation on PREMΛP. Key concepts in terms of the Concept Exploration Framework, Goal-oriented Inverse Design method and the proposed CB-PDSIDES platform from this dissertation are being tested for incorporation into the TCS Platform for the Realization of Engineered Materials and Products. The hot rod rolling example problem will be used in the beginning to test the platform PREMΛP. Further examples will be used in later stages. The focus in this collaboration is on scholarship with idea of publishing high-quality journal papers focused on showcasing the utility of the proposed systems-based design architecture in this dissertation for supporting industry-inspired problems.

10.5 *"I"* Statement

Having discussed specific opportunities for future work, long-term research goals and the author's vision for research in design based on the foundations laid in this dissertation are addressed in this section. In this section, the author uses "I" statements to assert about the feelings, beliefs, values, and the author's future vision for research.

10.5.1 Self-Reflection

The author reflects on the technical and career goals,

"My long-term goal is to establish a strong academic career focused on discovery, learning, and engagement in Simulation-Based Multi-level "Intelligent" Design of Complex Engineered Systems. The foundational question that I plan to address as a faculty member is: ***What are the principles underlying rapid and robust concept exploration of complex engineered systems involving the material, product and***

manufacturing process when simulation models are typically incomplete and inaccurate?

Towards this long-term goal, I plan to focus on three research thrusts as a faculty member: *i) Robust Design Exploration of Materials and Products by Managing Uncertainty, ii) Collaborative, Multidisciplinary, Robust Design Exploration for Products and Materials, iii) Design and Solution Space Exploration (DSSE) using Knowledge-Based Platform PDSIDES.*

Accordingly, my research interest lies in establishing system-level synthesis methods and tools that are required for the integrated robust design of complex materials, products and associated manufacturing processes. The emerging area of materials design—a multidisciplinary field for developing general methods for designing materials with preferred functional characteristics—is an important component in a comprehensive systems design approach and a particularly intriguing opportunity for applying my systems design research. My research interests and expertise are grounded in this doctoral dissertation, in which I am establishing the foundations of:

1. Integrated design of materials, products and associated manufacturing processes,
2. Knowledge-based platform for decision support to realize the simulation-based design of complex engineering systems.

Both these areas as discussed in this dissertation are summarized in this section. These two areas will be foundational to a strong long-term career in simulation-based multi-level design of complex engineering systems. The key foundational elements of the systems-based design architecture proposed in this dissertation and my future research focus is shown in Figure 10.18. Further discussion will be based on these foundational elements of the systems-based design architecture proposed.

Integrated Design of Materials, Products and Associated Manufacturing Processes: In my PhD research, the core of materials design is recognized as the interplay of hierarchical systems-based design of materials and multiscale/multilevel modeling methodologies, embedded within a computational framework that supports coordination of information and human decision making. The underlying philosophy here is that design is basically a decision-making process and the fundamental role of a human designer is to make decisions given the information available. In this regard in my PhD dissertation, I adopt the definition for the term materials design as the top-down driven, simulation-supported, decision-based design of material hierarchy to satisfy a ranged set of product-level performance requirements.

In this dissertation, I address the integrated design of materials, products and processes as fundamentally an inverse, goal-oriented synthesis activity in which the designer (decision-maker) aims at identifying material structures and processing paths that achieve/satisfy certain required product and process-level properties and performances. My research focus in this dissertation is distinct from the multiscale materials modeling efforts, where the emphasis is on developing problem specific links between models at multiple scales to accurately predict the system behavior.

Why is this research essential? In this PhD dissertation, I introduce elements of Decision-Based "Integrated" Design (DBID) of materials, products, and processes from a systems perspective to the current developments in the materials design domain.

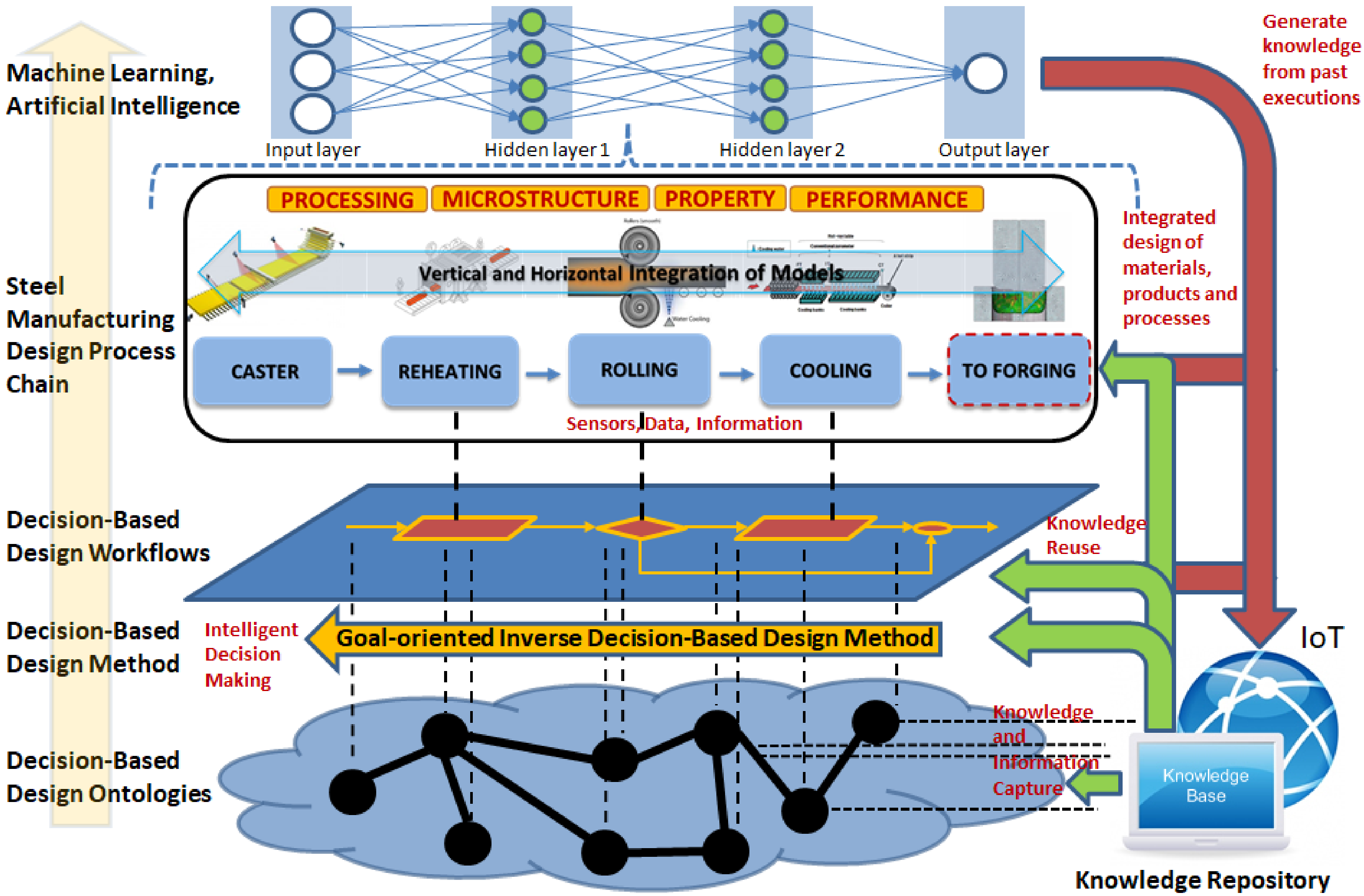

Figure 10.18: An overview of the systems-based design architecture proposed in this dissertation and future vision

Even though there have been significant advances in approaches for modeling and simulation of material behavior starting from atomic to continuum scale, the inherent uncertainty associated with these approaches/models needs to be managed while predicting the material microstructures that meets specified properties so as to facilitate robust design decision-making. The gaps associated with integrating such models that are typically at different length and time scales across the manufacturing process chains need to be addressed so as to concurrently design the material, product, and process.

Knowledge-Based Platform for Decision Support to Realize the Simulation-Based Design of Complex Engineering Systems: The design decisions and information generated from a complex material system needs to be stored and the knowledge associated should be captured. In this PhD dissertation, I address the following research question: *How can structural consistency of the decision-based design workflow for the manufacturing process chain involving the material and product be maintained while incorporating newer data, information and knowledge associated with the material system?* This challenge is addressed using a "Knowledge-Based" Platform for Decision Support in the Design of Engineering Systems (PDSIDES) that is anchored in modeling decision-related knowledge with templates using ontologies to facilitate execution and reuse. This work is carried out in collaboration with Dr. Zhenjun Ming, Dr. Ru Wang, Dr. Guoxin Wang and Professor Yan Yan from Beijing Institute of Technology, China who are developing the platform, PDSIDES. The two primary constructs required for the realization of decisions within PDSIDES are: 1) Decision Support Problem (DSP) construct and 2) Ontology. Three types of platform users are defined according to the amount of knowledge they have for operating the decision template, namely, Template

Creators, Template Editors and Template Implementers. Template Creators are domain experts, and responsible for creating decision templates for original design, which requires the greatest novelty. Template Editor are senior designers who have sufficient knowledge and experience in a specific domain and are responsible for editing (or tailoring) existing decision templates in adaptive design, this requires the original templates to be adapted for new applications. Template Implementers are designers who have basic knowledge and typically little knowledge or interest in the analysis embodied in the template, they are responsible for executing existing decision templates that result in variant designs that require only parametric changes in the original decision templates.

Test Example for PDSIDES and Potential Benefits: The performance of the platform, PDSIDES is tested using the steel manufacturing process chain problem addressed in this dissertation. The performances of PDSIDES in terms of 1) template creation, 2) consistency checking, and 3) post-solution analysis, is tested respectively for the three different types of users defined. The potential of PDSIDES for bringing benefits to engineering enterprises (involving material and product) mainly lies in two aspects: 1) document the decision related knowledge (key intellectual capital of enterprises), and reuse it in multiple situations, 2) rapid decision making. Enterprises can rapidly response to the dynamic market shifts (requirement changes) by modifying and executing the documented decision templates.

Future Research Vision - Simulation-Based Multi-level "Intelligent" Design of Complex Engineering Systems

In the context of the emerging Integrated Computational Materials Engineering (ICME) domain and Industry 4.0 domain, I plan to pursue my vision, that is, to collaboratively (with academic and industrial partners) define the emerging frontier for simulation-based multi-level "intelligent" design of complex engineered systems when the computational models are incomplete and inaccurate. In the long term, my major focus will be on ***multilevel complex material systems***.

The prospect of materials design sparks compelling systems design research questions, such as: ***Given material simulation models at different time and length scales and with differing levels of accuracy, how can these models be exercised strategically, efficiently, and simultaneously, along with models of the rest of the system (product, manufacturing process, and environment), for rapid, concurrent, virtual design of complex systems?*** The methods needed for designing complex products and materials have much in common when viewed from a systems perspective, independent of the domain of application. My intention is to establish intellectual and computational foundations for supporting teams of product and material designers who are faced with a set of fundamental challenges associated with product and material design.

Specifically, I am interested in the following **three research thrusts** that I plan to pursue as my future research.

Research Thrust 1: Robust Design Exploration of Multi-Scale Materials and Products by Managing Uncertainty

Research Thrust 2: Collaborative, Multidisciplinary, Robust Design Exploration for Products and Materials

Research Thrust 3: Design and Solution Space Exploration (DSSE) using Knowledge-Based Platform PDSIDES

<u>Research Thrust 1: *Robust Design Exploration of Multi-Scale Materials and Products by Managing Uncertainty*</u>

As in product design, uncertainty and variability are prevalent in materials modeling and design. Examples include bias and uncertainty in simulation models themselves, broad ranges of operating conditions, design changes during a material/product development process, and processing-induced variability in many aspects of a multi-scale material structure.

Research question: ***What are the requirements for an inverse, goal-oriented design approach for realizing the robust design exploration of multiscale material, products and processes as a system by managing the associated uncertainties?***

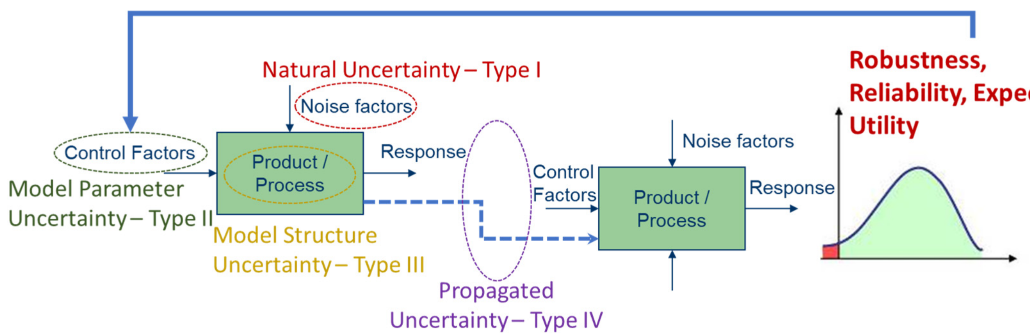

Figure 10.19: Uncertainty Types for Simulation-based Design

Research Plan: I plan to look at the different types of uncertainties defined (Type I to IV) and the corresponding robust designs associated with a complex multiscale system. In my doctoral research, I focused on information flow across scales and not on multi-scale modeling efforts. In this research thrust, I plan to look at uncertainty associated with multi-scale modeling of materials. This includes uncertainty due to noise factors (Type I), control factors (Type II), the models themselves (Type III) and their propagation as models interact (Type IV) at multiple length scales, see Figure 10.19. Robust product and material design methods are needed to ensure design feasibility and to minimize the sensitivity of performance objectives with respect to variations in either a product or a material.

Anticipated Outcome: Mathematical models for characterizing variability in materials design and establishing robust material design techniques for assessing and managing the impact of uncertainty and variability on the performance of multiscale materials and parent products.

Key Activities Involve: Developing techniques for characterizing variability, accounting for all four types of uncertainty and methods to assess and manage the same in multiscale material and product design.

Research Thrust 2: *Collaborative, Multidisciplinary, Robust Design Exploration for Products and Materials*

Complex product and material systems are characterized by a number of interdependent subsystems associated with categories of computational product and material simulation models. It is essential to distribute analysis and synthesis activities since material and product simulations are often computationally intensive and highly specialized according to length and time scales.

Research Question: *What are the requirements for a collaborative, multidisciplinary, robust design approach that facilitates the leveraging of the extensive domain-specific knowledge and expertise of various material and product designers in establishing tractable design spaces for which solutions can be achieved in reasonable time periods?*

Research Plan: To address the design of such multi-level material systems, there is a need for adopting a combination of approaches from different domains such as multi-attribute decision-making, multidisciplinary design analysis, utility-based design, meta-modeling, etc. I plan to define and implement a robust design exploration approach that eliminates the need of a central decision-maker. This collaborative robust design exploration approach facilitates the designer to identify adjustable ranges of design variables that satisfy a set of performance requirements across different length and time scales and across processing, microstructure, property spaces despite noises in system by managing the uncertainty, see Figure 10.20. ***By generating broad ranges of design variable values (rather than point solutions) for design parameters that are shared with other designers, design freedom is preserved for another collaborating designer who can make changes to a design—within the specified ranges—without compromising design requirements.***

Anticipated Outcome: Synthesis techniques and computational methods need to be established to facilitate (1) generation, communication, and acceptance of solutions that consist of ranges of design variable and performance parameter values, (2) systematic narrowing of the design space by multiple designers, and (3) translation of design information between designers on multiple length scales. ***As a result, it should be possible to achieve greater independence and concurrency of materials design activities and to accommodate distributed analysis and synthesis activities in materials design***.

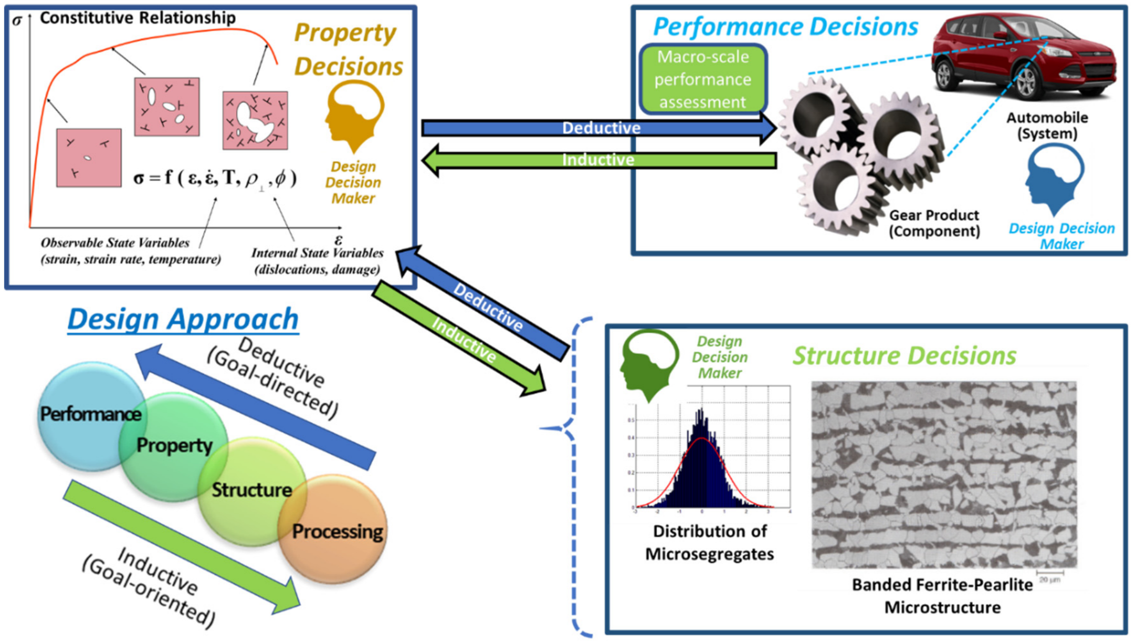

Figure 10.20: Collaborative, Multidisciplinary, Robust Design Exploration for Products and Materials

Key Activities Involve: Define collaboration between designers operating at different levels of material systems starting from processing to performance space; Frame decisions and model designer's preferences under risk involving multiple stakeholders; Identification of solutions and communicating across scales.

<u>**Research Thrust 3:** ***Design and Solution Space Exploration (DSSE) using Knowledge-Based Platform CB-PDSIDES***</u>

To further the work on PDSIDES and address the need for effective design and solution space exploration techniques, I plan to collaborate with my PhD advisors Professors Janet K. Allen and Farrokh Mistree and colleagues from Systems Realization Laboratory @ OU, Beijing Institute of Technology, China and Purdue University (**International Systems Realization Partnership**) in developing template-based ontological methods using the knowledge-based platform PDSIDES for design and solution space exploration

(DSSE) in the cloud. In Figure 10.21, I illustrate the application of the knowledge-based platform CB-PDSIDES in design space exploration which includes the exploration of design space for metamodels and problem formulated followed by exploration of solution space for different design scenarios. All these are achieved using the Design and Solution Space Exploration (DSSE) Process Templates in PDSIDES. The main contents of DSSE process template include the three sub-templates: *Problem Model* (PM), *compromise Decision Support Problem* (cDSP), and *Post-Solution Analysis* (PSA). The PM sub-template has two modules: *Theoretical and Empirical Model* and *Surrogate Model*. The PSA sub-template has five modules: *Weight Sensitivity Analysis* (WSA), *Constraint Sensitivity Analysis* (CSA), *Additional Requirement Analysis* (ARA), *SSE_Experiment* (Solution Space Exploration Experiment), and *Deviation Response*, see Figure 10.21.

Anticipated Outcome: ***The anticipated outcome of this work is the designer's ability to adjust the design space (including design space for metamodels and design space for the problem formulated) to achieve robust, reliable, flexible solutions (using solution space exploration) and manage the risk of the propagation of undesirable solutions during multi-stage process, product and material design thereby improving the designer's capabilities to communicate, understand and facilitate the management of reusable information***. The template-based ontological method for design space exploration facilitates the understanding and prediction of process behavior in design via extending designer's abilities and supporting them to make comprehensive material, product and process level decisions with the features of robustness, reliability, flexibility and modifiability, particularly in the early stages of design.

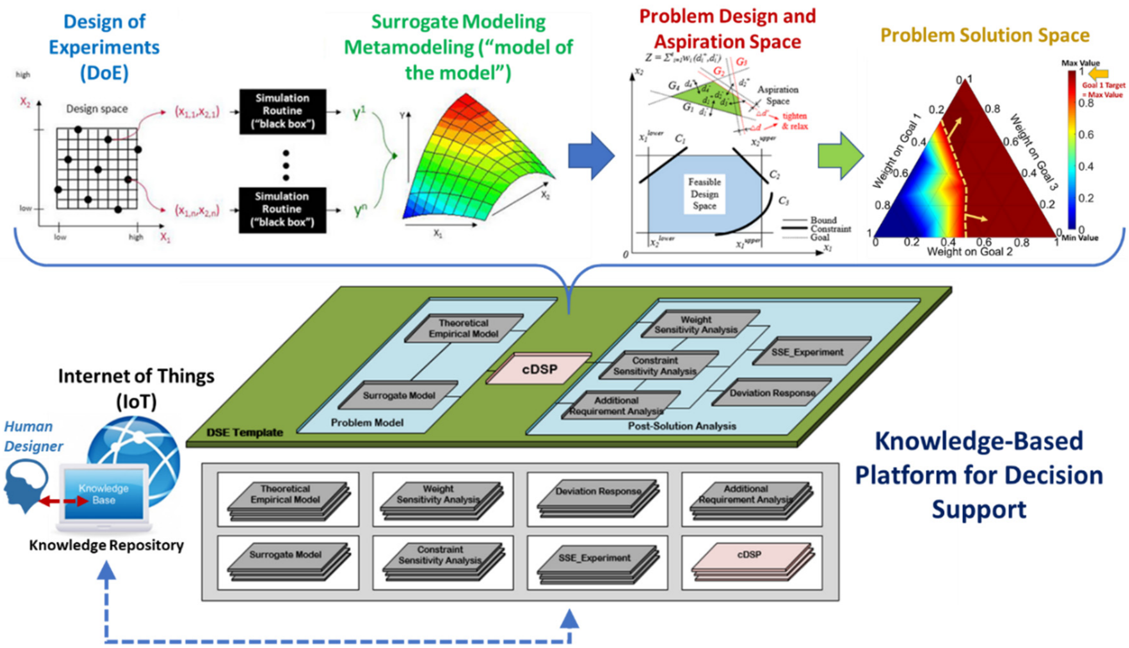

Figure 10.21: Knowledge-Based Platform in Cloud for DSSE and Decision Support

Key Activities Involve: Defining the ontology for inverse decision-based design exploration, developing template-based ontological methods that support systematic design and solution space exploration of material systems

I believe that these three research thrusts are intended:

1) to impact our ability to realize the integrated simulation-based multi-level design of complex material, product and process systems and
2) to contribute to the theoretical and computational foundations necessary for comprehensive simulation-based product-process-material system development.

I anticipate extensive multidisciplinary collaboration with experts in related research areas such as materials science and engineering, industrial and systems engineering. As a future faculty member, I look forward to developing formal foundations for simulation-based multi-level design of complex material systems by establishing a focused research program and working together with industrial and academic colleagues with a broad spectrum of backgrounds. Through these partnerships, I envision leading a new research laboratory on Simulation-Based Design of Complex Engineered Systems that will be invited to join the International System Realization Partnership (ISRP) that currently consists of the Systems Realization Laboratory @ OU (University of Oklahoma), the Design Engineering Laboratory (Purdue University) and the Institute of Industrial Engineering (Beijing Institute of Technology).**”**

The author reflects on personal goals, experiences and achievements,

“During my PhD, under the mentoring of my advisors in the Systems Realization Laboratory @ OU, I have gained the knowledge and skills essential to be a successful faculty. This includes**: *i) writing scholarly papers, ii) writing research proposals, iii) mentoring graduate and undergraduate students and helping them to achieve their learning goals, iv) orchestrating graduate and undergraduate level courses, v) presenting research at international conferences and vi) establishing long-term collaborations with the mindset of sharing to gain***.

The SRL@OU is a multicultural, multidisciplinary academic family focused on educating the next generation of professors. The mentoring at SRL is focused on developing career sustaining competencies and providing an opportunity for the individual to learn, unlearn and relearn. The career sustaining competencies include: *(1) to continue learning through reflection on doing and the associated creation and articulation of knowledge; (2) to speculate and identify gaps that foster innovation; (3) to ask questions, actively listen, reflect, and identify gaps and opportunities worthy of further investigation; (4) to make decisions using incomplete information; and (5) to think critically (deductive reasoning and inductive speculation) and identify a way forward – speculate the future*. The family mission of SRL@OU is to provide an opportunity for each person to learn how to dream and rise to his/her full potential and contribute to the scholarship associated with the realization of complex engineered systems with the mindset of sharing to gain. The whole experience at SRL@OU has made me realize that '***the best job in the world is to be a professor'***. The fundamental principles embodied within the Systems Realization Laboratory is to focus on scholarship and critical thinking, viewing students as colleagues, and creating a family environment where everyone rises to their full potential. These principles have impacted me a lot and I plan to abide to these when I start my own research laboratory in future. The two quotes that I take away from SRL into my personal life are **'*Happy people are always successful; Successful people are not necessarily happy*'** and **'*Focus on things that you can control and do not worry about things that you cannot control*'**. Both are wonderful philosophies that were revealed to me by my advisors and have impacted my life and thinking in a positive manner as I started to practice.

The competencies that I developed during my doctoral studies include:

- *Ability to identify a research problem by defining boundary around the area of interest;*
- *Ability to carry out literature search based on the boundary defined and frame a problem in terms of dilemmas that exists;*
- *Ability to pose questions worthy of investigation based on the identified dilemmas;*
- *Ability to propose a plan by identifying the associated tasks for addressing the questions posed;*
- *Ability to verify and validate the plan so that the knowledge gap is filled;*

- *Ability to communicate a research proposed;*
- *Ability to teach, mentor and collaborate with a mindset of sharing to gain."*

10.5.2 Self-Assessment on the competencies

Table 10.1: Self-assessment of competencies developed

Competencies Developed	**Justification**
Ability to identify a research problem by defining boundary around the area of interest	*To ascertain my ability for this competency, in my doctoral dissertation, I have framed three problems by defining a boundary around the multistage hot rod rolling process in the steel making manufacturing chain. The boundary is apt to test the research hypotheses proposed in this dissertation. The hot rod rolling process chain problem is a complex, multistage manufacturing process chain problem which requires vertical and horizontal integration of models across process chains. Moreover, the problem is suitable for demonstrating the different aspects of integrated materials, product and manufacturing process design. The integrated design of material (steel), product (rod) and associated manufacturing processes (hot rod rolling and cooling) example consists of decisions related to product and materials design.*
Ability to carry out literature search based on the boundary defined and frame a problem in terms of dilemmas that exists	*To frame the problems for the hot rod rolling process, I carried out extensive literature search that are related to modeling of the hot rod rolling process, the complexities, requirements and challenges involved with the process, the methods used to design rolling systems, etc. Based on the complexities that I identified for the hot rod rolling problem, I formulated three research problems worthy of investigation. In the first one, I addressed macrostructural design of rod and design of rolling passes. In the second example, I focused on designing material microstructure for target mechanical properties of rod. In the third comprehensive example, I addressed the integrated design of material (steel), product (rod) and associated manufacturing processes (hot rod rolling and cooling). The core research papers related to research hypotheses framed are identified and categorized (around 300 key papers). The problems framed are addressed in Chapters 5 and 6 of this dissertation.*
Ability to pose questions worthy of investigation based on	*Based on the key challenges identified in this dissertation and the research hypotheses framed to address the challenges and requirements, I frame a primary research question and four secondary research questions that are worthy of*

the identified dilemmas	*investigation. Each of those secondary research questions, are associated with a research area. These areas include: Systematic model integration and establishment of information workflow, Systematic concept exploration and inverse design exploration, Systematic robust concept exploration and Knowledge-based platform for decision support. The details are available in Chapter 1 of this dissertation.*
Ability to propose a plan by identifying the associated tasks for addressing the questions posed	*In context of these research questions, I propose a plan by identifying the tasks for addressing the questions posed. The need for a systems-based design architecture to systematically achieve the integrated design of materials, products and processes is identified at first. I identified that there needs to be a systematic method for integrating models and establishing the information workflow – addressed as tasks in RQ1. The need for a framework for concept exploration and a generic method of inverse design exploration are identified and addressed as tasks in RQ2. The need for robust design metrics, goals and constraints are identified and the associated tasks are identified and addressed in RQ3. Finally, the need for a platform for decision support in facilitating knowledge capture, storage, and reuse is identified and the associated tasks are identified and addressed in RQ4. Thus, the tasks that needs to be carried out for answering the research questions so as to realize the systems-based design architecture are identified and a research plan is put forward for accomplishing the same.*
Ability to verify and validate the plan so that the knowledge gap is filled	*I propose to verify and validate the proposed systems-based design architecture using the verification and validation square framework and is addressed as a part of this. The design architecture is checked for internal consistency by carrying out theoretical structural validity. The appropriateness of the example problems to test the utility of the design architecture is checked using empirical structural validity. The availability of practical results for the example problems using the design architecture is checked using empirical performance validity and the ability of the design architecture to produce practical results for other problems is checked using theoretical performance validity. The validation square framework and the way of using it to verify and validate the plan is described in Chapters 1 and 10.*
Ability to communicate a research proposed	*This competency is evaluated based on the papers that I have published during my doctoral studies. Based on this dissertation, I have 7 journal papers (5 published, 2 under review), and 6 conference papers (all published). Thus, a*

	total of 13 journal and conference papers are the outcome of this dissertation. Apart from these, 6 papers are in progress and these papers will be submitted by end of this year to selected journals and conferences. Further, I am in the final stages of submitting a proposal to Springer/CRC Press to publish my dissertation as a monograph. The papers based on this dissertation are listed in Section 10.5.3.
Ability to teach, mentor and collaborate with a mindset of sharing to gain	*I had a chance to mentor one graduate student and two undergraduate HERE scholars during my doctoral studies. I also received the opportunity to co-orchestrate two graduate-level engineering design courses. With each teaching and mentoring experience, I learned how to empower students to learn which has further increased my passion for entering academia. From this experience, I was able to see the need for establishing context in a course, providing structure and scaffolding for students, and connectivity throughout the curriculum. Through my mentoring and collaboration experience, I realized how weekly meetings and weekly reports play a key role in making sure that the students/project goals are in the right track. The importance of starting from an end goal and working backwards to achieve the same is something I find successful for every project I have been part of. I have realized the importance of competency-based learning where the student focuses on the competencies that he/she wishes to develop by carrying out a task. The overall experience has made me realize the importance of contextual assessment of student learning through reflection on doing. Several papers are co-authored with the students I mentored, and these are listed in Section 10.5.3.*

10.5.3 List of Publications based on this Dissertation

Book (Monograph)

B1. Nellippallil, A.B., Gautham, B.P., Singh, A.K., Allen, J.K., and Mistree, F., 2019, "Integrated Realization of Materials, Products and Associated Manufacturing Processes," Springer Monograph, Proposal to Springer by October 2018. Work in progress.

Refereed Journal Publications

J1. Nellippallil, A.B., Rangaraj, V., Gautham, B.P., Singh, A.K., Allen, J.K., and Mistree, F., 2018, " An Inverse, Decision-Based Design Method for Integrated Design Exploration of Materials, Products and Manufacturing Processes," *ASME Journal of Mechanical Design*. vol.140, no. 11, pp. 111403-111403-17.

J2. Nellippallil, A. B., Song, K. N., Goh, C.-H., Zagade, P., Gautham, B., Allen, J. K., and Mistree, F., 2017, "A Goal-Oriented, Sequential, Inverse Design Method for the Horizontal Integration of a Multi-Stage Hot Rod Rolling System," *ASME Journal of Mechanical Design*, vol. 139, no. 3, pp. 031403.

J3. Nellippallil, A.B., De, P.S., Gupta, A., Goyal, S., and Singh, A.K., 2016, "Hot Rolling of a Non-Heat Treatable Aluminum Alloy: Thermo-Mechanical and Microstructure Evolution Model", *Transactions of the Indian Institute of Metals*, vol. 70, no. 5, pp. 1387-1398.

J4. Wang, R., **Nellippallil, A.B.**, Wang, G., Yan, Y., Allen, J.K., and Mistree, F., 2018, "An Ontology-Based Design Space Exploration Process Template in Model Based Realization of Complex Engineered Systems," *Advanced Engineering Informatics*, vol. 36, pp. 163-177.

J5. Ming, Z., **Nellippallil, A.B.**, Yan, Y., Wang, G., Goh, C.-H., Allen, J.K., and Mistree, F., 2018, "PDSIDES – A Knowledge-based Platform for Decision Support in The Design of Engineering Systems," *ASME Journal of Computing and Information Science in Engineering*. Vol. 18, no. 4, pp. 041001.

J6. Nellippallil, A.B., Mohan, P., Allen, J.K., and Mistree, F., 2018, "An Inverse, Robust Design Exploration Method for Managing Uncertainty in Process Chains," *ASME Journal of Mechanical Design*. **Under Review.**

J7. Nellippallil, A.B., Shukla, R., Ardham, S., Goh, C-H., Allen, J.K., Mistree, F., 2018, "Exploration of Solution Space to Study Thermo-Mechanical Behavior of AA5083 Al-Alloy During Hot Rolling Process", *ASME Journal of Mechanical Design*. **Under Review.**

Refereed Conference Publications

C1. Nellippallil, A.B., Mohan, P., Allen, J.K., and Mistree, F., 2018, "Robust Concept Exploration of Materials, Products and Associated Manufacturing Processes," *ASME Design Automation Conference*, Quebec City, Canada. Paper Number: DETC2018-85913.

C2. Nellippallil, A.B., Rangaraj, V., Gautham, B.P., Singh, A.K., Allen, J.K., and Mistree, F., 2017, "A Goal-Oriented, Inverse Decision-Based Design Method to Achieve the Vertical and Horizontal Integration of Models in a Hot-Rod Rolling Process Chain," *ASME Design Automation Conference*, Cleveland, Ohio, USA. Paper Number DETC2017-67570.

C3. Ming, Z., **Nellippallil, A.B.**, Yan, Y., Wang, G., Goh, C.-H., Allen, J.K., and Mistree, F., 2017, "PDSIDES – A Knowledge-based Platform for Decision Support in The Design of Engineering Systems," *ASME Design Automation Conference*, Cleveland, Ohio, USA. Paper Number DETC2017-67562.

C4. Nellippallil, A.B., Shukla, R., Ardham, S., Goh, C-H., Allen, J.K., Mistree, F., 2015, "Exploration of Solution Space to Study Thermo-Mechanical Behavior of AA5083 Al-Alloy During Hot Rolling Process", *ASME Design Automation Conference*, Cleveland, Ohio, USA. Paper Number DETC2017-68173. **Recognized as Paper of Distinction**.

C5. Nellippallil, A.B., Song, K.N., Goh, C-H., Zagade, P., Gautham, B.P., Allen, J.K., Mistree, F., 2016, "A Goal Oriented, Sequential Process Design of a Multi-Stage Hot Rod Rolling System", *ASME Design Automation Conference*, Charlotte, NC, USA. Paper Number DETC2016-59402.

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PP2. Fonville, T.R., **Nellippallil, A.B.**, Horstemeyer, M.F., and Mistree, F., 2019, "A Decision-Based Design Approach for Robust Design of an American Football Helmet," Planned for *The 5th World Congress on Integrated Computational Materials Engineering (ICME 2019)*. **Status: Paper writing in progress. Shot version.**

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PP5. Ming, Z., **Nellippallil, A.B.**, Guoxin, W., Yan, Y., Allen, J.K., and Mistree, F., 2018, "An Ontological Computational System for Robust Design of Process Chains under Uncertainty," Planned for *Advanced Engineering Informatics*. **Status: Paper writing in progress.**

PP6. Nellippallil, A.B., Allen, J.K., and Mistree, F., 2018, "A Function-based Approach for Systematic Model Integration for the Design of Materials and Products," Planned for *ASME Design Automation Conference 2019*. **Status: Paper writing in progress.**

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APPENDIX A

A.1: cDSP Formulation for Pass 2 (Chapter 5)

In this section we describe the mathematical formulation of the compromise decision support problem (cDSP) for Pass 2 of rod rolling. The cDSP for Pass 2 incorporates the design information passed from Pass 3 and Pass 4. The cDSP reads as follows:

Given:

1) Design information passed from Pass 3 and Pass 4
2) Requirements at Pass 2

- Achieve target throughput (results obtained from Pass 4 design)
- Achieve target rolling load
- Target value for throughput, $T_{p4,Target} = 0.0006\ m^3/sec$
- Target value for rolling load, $P_{Target} = 40\ t$
- Minimum value of rolling load, $P_{min} = 35\ t$
- Maximum value of rolling load, $P_{max} = 45\ t$
- Minimum value of throughput, $T_{pmin} = 0.0001\ m^3/sec$
- Maximum value of throughput, $T_{pmax} = 0.0008\ m^3/sec$

3) Initial billet size = 42 × 42 mm
4) Other parameter values for passes
5) The regression equations and well established empirical and theoretical correlations for the oval to round pass for Pass 2
6) Variability in system variables

   The ranges identified for the system variables are provided in Table A.1.

Table A.1: System variables and ranges for Pass 2 cDSP

Sr. No	Variables	Ranges
1	X_1, diameter of rod after Pass 2 (h_2)	0.03-0.04 m
2	X_2, the coefficient of elongation for Pass 2 (λ_2)	1-3
3	X_3, the spread occurring in Pass 2 (β_2)	1-2
4	X_4, the exit velocity for Pass 2 (w_2)	0.5-3 m/sec
5	X_5, the maximum radius of roll in Pass 2 ($R_{max,2}$)	0.155-0.2 m
6	X_6, the roll gap (G_2)	0.0035-0.0055 m
7	X_7, the coefficient of friction (μ_2)	0.3-0.45

Find:

System Variables

X_1, diameter of rod after Pass 2 (h_2)

X_2, the coefficient of elongation for Pass 2 (λ_2)

X_3, the spread occurring in Pass 2 (β_2)

X_4, the exit velocity for Pass 2 (w_2)

X_5, the maximum radius of roll in Pass 2 ($R_{max,2}$)

X_6, the roll gap (G_2)

X_7, the coefficient of friction (μ_2)

Deviation Variables

d_i^-, d_i^+, *i =1,2*

Satisfy:

System Constraints

- Minimum coefficient of elongation constraint: $\lambda_2(X_2)$-1.2≥ 0
- Maximum coefficient of elongation constraint: $2 - \lambda_2(X_2)$≥ 0
- Minimum spread constraint: $\beta_2(X_3)$-1.1≥ 0
- Maximum spread constraint: $1.7 - \beta_2(X_3)$≥ 0
- Exit speed constraint: $w_2 - v_r(X_i) \geq 0$
- Minimum load constraint: $P(X_i) - P_{min}$≥ 0
- Maximum load constraint: $P_{max} - P(X_i)$ ≥ 0
- Maximum wear constraint: 0.0001 - $\Delta R(X_i)$ ≥ 0

System Goals

Goal 1:

- Maximize Throughput:

$$\frac{T_p(X_i)}{T_{p,Target}} + d_1^- - d_1^+ = 1$$

Goal 2:

- Minimize Rolling Load:

$$\frac{P_{Target}}{P(X_i)} - d_2^- + d_2^+ = 1$$

Variable Bounds

Defined in Table A.1

Bounds on deviation variables

d_i^-, d_i^+≥ 0 and d_i^-*d_i^+ = 0 , i=1,2

Minimize:

Minimize the deviation function

$$Z = \sum_{i=1}^{2} W_i(d_i^- + d_i^+); \sum_{i=1}^{2} W_i = 1$$

A.2: Design Calculations (Refer to Figure 5.2)

In this section, we describe the design calculations carried out for each pass based on the cDSP results obtained that are showcased in Tables 5.4 and 5.5. The design process is carried out following the sequential relationships that exist between passes ensuring the flow of information pattern shown in Figure 5.3.

Step 1: Formulation of cDSP for roll Pass 4 using the information from the end product to be realized and the sequential relationship existing between roll Pass 3 and 4

The cDSP for Pass 4 is formulated in terms of the end requirements of minimizing ovality, maximizing throughput and minimizing rolling load within the system constraints and bounds defined. The cDSP is exercised for different scenarios and ternary plots are used to identify best region and the results are summarized in Table 5.4.

Step 2: Design of Passes 4 and 3 using the design and operating set points identified and the information available from end product requirements

We calculate the area of the round rod using the height value obtained for rod from cDSP results. Cross-sectional area of material after Pass 4:

$$F_4 = \frac{\pi h_4^2}{4} = 532.26\ mm^2$$

Entry speed of material for roll Pass 4:

$$v_4 = \frac{w_4}{\lambda_4} = 0.8671\, m/sec$$

Throughput achieved in Pass 4:

$$T_{p4} = F_4 \times w_4 = 0.0005999\, m^3/sec$$

We carry out the design calculations for Pass 3 based on the cross-sectional area of rod and elongation coefficient (cDSP result) obtained after Pass 4. We also define some requirements for Pass 3 such as meeting the throughput same as that of Pass 4.

Cross-sectional area of material after Pass 3:

$$F_3 = F_4 \times \lambda_4 = 691.93\, mm^2$$

Theoretical width of oval pass after Pass 3:

$$b_{3w} = \sqrt{4.35 \times F_3} = 54.86\, mm$$

Height of material after Pass 3 (assuming b/h ratio = 3):

$$h_3 = \frac{b_{3w}}{(b/h)} = 18.28\, mm$$

Radius of curvature of oval Pass 3:

$$R_3^* = \frac{b_{3w}^2 + h_3^2}{4h_3} = 45.72\, mm$$

Exit speed of material for roll Pass 3:

$$w_3 = v_4 = 0.8671\, m/sec$$

Throughput to be maintained in Pass 3 (Given):

$$T_{p3} = T_{p4} = 0.0005999\, m^3/sec$$

We carry out design calculations for Pass 4 now with the new information generated for Pass 3.

Width of round profile (approximated rectangle) after Pass 4:

$$b_4 = \beta_4 \times h_3 = 21.03\ mm$$

Mean height after Pass 4:

$$h_{4m} = \frac{F_4}{b_4} = 25.31\ mm$$

Theoretical diameter of roll for Pass 4:

$$D_{t4} = 2\left(R_{max,4} + \frac{G_4}{2}\right) = 314\ mm$$

Effective diameter of roll for Pass 4:

$$D_{w4} = D_{t4} - h_{4m} = 288.7\ mm$$

Step 3: Formulation of cDSP for roll Pass 2 using the design information generated for Passes 3 and 4; and the sequential information existing between Passes 1 and 2; along with information on input material (billet)

The designer formulates the cDSP for Pass 2 after finding the results from Passes 3 and 4. For example, the range of the height of rod for Pass 2 is identified based on the dimensions achieved in Passes 3 and 4. Another example is the rolling load target value. Since there is a chance of having higher rolling load during Pass 2 due to larger stock that is being rolled than Pass 4, the target, minimum and maximum values for Pass 2 are fixed after looking at the rolling load value obtained in Pass 4. The designer also fixes the target throughput value for Pass 2 after analyzing the throughput achieved in Passes 3 and 4. Thus the designer makes judgements based on the information obtained from the information as it develops.

Step 4: Design of roll Passes 2 and 1 using the design and operating set points identified; the information available from input material and the information from Passes 3 and 4

The cDSP results for Pass 2 presented in Table 5.5 are used to design Pass 2.

Cross-sectional area of material after Pass 2:

$$F_2 = \frac{\pi h_2^2}{4} = 755.07\ mm^2$$

Entry speed of material for roll Pass 2:

$$v_2 = \frac{w_2}{\lambda_2} = 0.611\ m/sec$$

Throughput achieved in Pass 2:

$$T_{p2} = F_2 \times w_2 = 0.0005997\ m^3/sec$$

Next, the design calculations for Pass 1 is carried out using Pass 2 design results and initial billet information from caster.

Cross-sectional area of material after Pass 1:

$$F_1 = F_2 \times \lambda_2 = 981.59\ mm^2$$

Theoretical width of oval pass after Pass 1:

$$b_{1w} = \sqrt{4.35 \times F_1} = 65.345\ mm$$

Height of material after Pass 1 (assuming b/h = 3):

$$h_1 = \frac{b_{1w}}{(b/h)} = 21.78\ mm$$

Radius of curvature of oval Pass 1:

$$R_1^* = \frac{b_{1w}^2 + h_1^2}{4h_1} = 54.45\ mm$$

Exit speed of material for roll Pass 1:

$$w_1 = v_2 = 0.611\ m/sec$$

Given Initial billet size from caster:

$$h_0 \times b_0 = 42 \times 42\ (mm)$$

Cross-sectional area of initial billet:

$$F_0 = 42 \times 42 = 1764\ mm^2$$

Coefficient of elongation for Pass 1:

$$\lambda_1 = \frac{F_0}{F_1} = 1.797$$

Width of oval profile (approximated rectangle) after Pass 1 (assuming $\beta_1 = 1.4$):

$$b_1 = \beta_1 \times b_0 = 58.8\ mm$$

Mean height of material after Pass 1:

$$h_{1m} = \frac{F_1}{b_1} = 16.69\ mm$$

Effective diameter of roll for Pass 1 (Assuming a theoretical diameter for rolls in Pass 1, $D_{t1} = 350\ mm$):

$$D_{w1} = D_{t1} - h_{1m} = 333.3\ mm$$

Entry speed of material for roll Pass 1:

$$v_1 = \frac{w_1}{\lambda_1} = 0.3401\ m/sec$$

Throughput to be maintained in Pass 1:

$$T_{p1} = T_{p2} = 0.0005997\ m^3/sec$$

The design calculations for Pass 2 are carried out next using Pass 1 information generated followed by collecting all the results for Passes 1 and 2.

Width of round profile (approximated rectangle) after Pass 2:

$$b_2 = \beta_2 \times h_1 = 26.14\ mm$$

Mean height after Pass 2:

$$h_{2m} = \frac{F_2}{b_2} = 28.88\ mm$$

Theoretical diameter of roll for Pass 2:

$$D_{t2} = 2\left(R_{max,2} + \frac{G_2}{2}\right) = 314\ mm$$

Effective diameter of roll for Pass 4:

$$D_{w2} = D_{t2} - h_{2m} = 285.1\ mm$$

With the information generated for Passes 1 and 2 the design calculations for Passes 3 and 4 are carried out completing design results for Passes 1, 2, 3 and 4.

Coefficient of elongation for Pass 3:

$$\lambda_3 = \frac{F_2}{F_3} = 1.091$$

Width of oval profile (approximated rectangle) after Pass 3 (assuming $\beta_3 = 1.5$):

$$b_3 = \beta_3 \times b_2 = 39.2\ mm$$

Mean height of material after Pass 3:

$$h_{3m} = \frac{F_3}{b_3} = 17.65\ mm$$

Effective diameter of roll for Pass 3 (Assuming a theoretical diameter for rolls in Pass 1, $D_{t3} = 314\ mm$):

$$D_{w3} = D_{t3} - h_{3m} = 296.35\ mm$$

Entry speed of material for roll Pass 3:

$$v_3 = w_2 = 0.7943\ m/sec$$

Exit speed of material for roll Pass 3:

$$w_3 = v_3 \times \lambda_3 = 0.867\ m/sec$$

This completes the design of the rolling passes with the determination of all the key dimensions presented in Figures 5.4a and 5.4b.

APPENDIX B: IDEM Based Exploration of Solution Space – Utility and Limitations of IDEM

Abstract

The Inductive Design Exploration Method (IDEM) is used to explore the solution space of a metallurgical process with an aim to foster material innovation through simulation-based design. The efficacy of the method is demonstrated in the context of hot rolling of the AA5083 alloy. The set-based design approach is employed to predict the process parameters of rolling operation for a given set of specified requirements. Critical process parameters such as strain rate, temperature, heat transfer coefficient and strip width are only considered in the design study. Ternary plots are constructed and utilized to explore the solution space obtained and thereby identifying feasible regions of process operation wherein the specified requirements are satisfied. Since plant data is not available for the study, Finite-element (FE) analysis is carried out as a means to validate the results obtained using aforesaid design method. The utility of the method and its limitations are identified and reported in this appendix.

B1. Frame of Reference

In machine design, typically a designer is required to determine the geometry, materials, and dimensions of a part that satisfies a set of target requirements. Designers tend to solve the forward problem iteratively and arrive at a utopian solution that meets the specified target requirements. Striving to identify a utopian solution for design problems in the real scenario is impractical due to complexity and cost and time involved in solving the forward problem iteratively. However, this limitation can be overcome if the focus is shifted to formulating and solving the inverse problem, i.e., to identify design set points for a specified set of requirements.

Next, when we talk about constructing and solving the inverse problem, managing the uncertainties becomes critical. No computational/empirical models are correct and we have uncertainties associated with each of them, which tend to propagate as the inverse process chains are constructed and solved. One of the methods that is used to solve inverse problems in the presence of uncertainty is the Inductive Design Exploration Method (IDEM) (Choi, Mcdowell and coauthors 2008). The method uses the forward problem process chain to obtain the solution for the inverse problem by using an error metric known as the Hyper Dimensional Error Margin Index (HD_EMI). The focus of here is on formulating and solving an inverse problem using the concept of Hyper Dimensional Error Margin Index (HD_EMI). The efficacy of the method is demonstrated in the context of hot rolling of the AA5083 alloy. The limitations associated with IDEM is also identified. The key question anchored in the inverse problem is to predict the critical design set points of rolling operation in order to meet a specified set of requirements. Results predicted using this approach are validated using FE analysis.

Appendix B is organized as follows. In Section B2 we briefly describe the hot rolling operation and provide a glimpse of past work. Problem statement and underlying models are presented in Section B3. Details of IDEM and problem formulation are provided in Section B4. Results and post-solution analysis are discussed in Section B5 and B6 respectively. Section B7 summarizes the key findings and closing remarks.

B2. The Hot Rolling Problem for testing the Utility of Method

Hot rolling is considered to be one of the most important and complex metal forming unit operation in steel and aluminum industries. The complexity arises due to the need of precise control of the process parameters in order to obtain the desired microstructure and properties in the final product. Owing to the increasing competition faced by steel and aluminum manufacturers from advanced materials, there is an increasing demand to make the rolling operation more flexible, agile and energy efficient. Process designers are thus required to come up with rapid and cost effective solutions to assist in decision making and improve the efficiency of the rolling operation. In this paper, we are demonstrating the design exploration for aluminum alloy, so next we explain the process and critical process parameters of rolling of aluminum. We are selecting AA5083 as the material in the study due to its wide application in pressure vessels for oil industries and body parts for automotive industries.

The process of hot rolling of aluminum involves the deformation of a pre-heated ingot from an initial thickness of 500-600 mm to around 2-5 mm in the temperature range of 300-500 °C (Ahmed, Wells and coauthors 2005). Plasticity, heat flow and microstructural changes (recovery and recrystallization) occur during the process which is influenced by the strain, strain rate, and temperature. These microstructural changes can be predicted using physics-based models for recovery and recrystallization, details of which are provided in the reference (Nellippallil, De and coauthors , Wells, Maijer and coauthors 2003). Also, heat transfer coefficient (htc) along the roll gap governs the temperature profile, thereby influencing microstructural changes and deformation during rolling operation. Because of the importance of aforesaid parameters (strain rate, temperature, width, and htc), these have been considered as critical parameters and included in the design study as exploratory variables. Rolling power and factor of safety are the two parameters considered in the current study to assess the efficiency of rolling operation. The factor of safety is computed based on the stress developed along the strip, which in turn is calculated using a mean strain value and varying strain rate and temperature along the strip. Rolling power is computed based on the rolling load applied during the operation. Thus, the factor of safety and rolling power are the final requirements, which are computed based on intermediate parameters (stress developed and rolling load) of the process.

Assumptions:

1. Mean strain value: We have assumed a mean strain value as the parameters on which the strain depends, namely the initial and final thicknesses of the strip and roll diameter are fixed parameters in our study.
2. Heat Transfer Coefficient: Literature study on htc shows different ranges used for hot rolling. We have taken data on htc from published literature and have assumed two levels (low and high) of htc for our study (Nellippallil, De and coauthors , Pietrzyk and Lenard 1989, Devadas, Samarasekera and coauthors 1991, Chen, Thomson and coauthors 1992, Hlady 1994, Hlady, Brimacombe and coauthors 1995, Fletcher, Li and coauthors 1998, Wells, Maijer and coauthors 2003). Low level corresponds to htc values in range 20-50 kW/m^2K whereas the high level corresponds to 200-450 kW/m^2K. These values are used subsequently in our study and difference in the level of satisfaction of requirements for two cases are established.

3. Temperature: We have selected two temperature ranges, i.e., low (250-370 ºC) and high (370-550 ºC). The reason for this selection is due to the occurrence of a change in slope of yield stress v/s temperature plot for AA5083 alloy at 370 ºC (Canas, Picon and coauthors 1996).
4. Stress Range: Stress range of 70-200 MPa is considered based on the stress regimes reported in literature during rolling of AA5083 (Shahani, Nodamaie and coauthors 2009).
5. Rolling Power: Precise computation of rolling power is highly complex if we go to microstructural level and bring in the effects of friction and other rolling parameters. Since the focus is on demonstrating the method and not the accuracy of results, for simplicity we use rolling power as a function rolling load per unit width. The rolling load per unit width is fixed in the range 0-8 kN/mm with a resolution of 0.5 kN/mm (Duan and Sheppard 2004). In the next sections, we talk about the problem statement and the adapted solution strategy. The problem statement and underlying models have been discussed in the subsequent section.

B3. Problem Statement

We have explained about the critical process parameters and parameters to assess the efficiency of rolling operation of AA5083 alloy in Section 2. The objective here is to minimize the power required for rolling and maximize factor of safety of the strip for a given process window while maintaining the processing constraints. Set-based inverse design approach using IDEM and Hyper-Dimensional Error Margin Index (HD_EMI) is used to explore the solutions space with an objective *to find the feasible set points of* *temperature, strain rate, heat transfer coefficient and width in order to maximize the factor of safety of strip at roll exit and minimize the power required during rolling.*

Given:

Rolling Power ≤ 20 kW

Factor of Safety ≥ 1.5

Thickness of strip: Initial = 50 mm and Final = 47.13 mm (Duan and Sheppard 2004)

Roll Radius = 460 mm (Duan and Sheppard 2004)

The values (ranges) of other independent and dependent parameters are summarized in Table B1 and B2. The modules to which these parameters serve as inputs are represented in the table. Since we have two ranges of temperature (low and high) and two ranges of htc (low and high), we explore the possibility of four different scenarios of process operation (see Table B3).

Table B1: The different models along with the parameters and the identified ranges

Model	Parameter	Range	Resolution	Constraints	Module
f1	σ (Stress)	[70, 200] MPa	20 MPa	N/A	1
f2	F (Rolling load per width)	[0, 8] kN/mm	0.5 kN/mm	N/A	1
g1	FS (Factor of Safety)	[1, 10]	1	≥ 1.5	2
g2	P (Power)	[0, 40] kW	1 kW	≤ 20	2

Table B2: The independent parameters along with the identified ranges

Parameter	Range	Resolution	Input Model	Input Module
$\dot{\varepsilon}$ (strain rate)	[0.5, 20] s^{-1}	0.1	f1, g2	1,2
w (width)	[75, 200] mm	10 mm	g2	2
T (temperature)	[250, 370] °C	10°C		
	[370, 500] °C	10°C	f1	1
h (heat transfer coefficient)	[10, 50] $kWm^{-2}K^{-1}$	5 $kWm^{-2}K^{-1}$	f1	
	[200, 450] $kWm^{-2}K^{-1}$	50 $kWm^{-2}K^{-1}$		1

Forward Problem

Since the proposed method uses forward problem process chain to obtain a solution for the inverse problem by using an error metric known as the Hyper Dimensional Error Margin Index (HD_EMI). First, we explain formulation of the forward problem (see Figure B1). We have divided the entire process into processing, structure, property and performance space and established the connectivity between the spaces by means of different modules. The processing space comprises of independent process parameters, namely strain rate ($\dot{\varepsilon}$), temperature (T) and heat transfer coefficient (h). The width of the strip (w) is a part of structure space, rolling stress ($\bar{\sigma}$) and rolling load per unit width (F) is a part of property space and a factor of safety (FS) and rolling power (P) are considered to part of performance space. The reason for choosing rolling stress and rolling load as a part of property space is due to the presence of different material properties parameters like yield stress etc. in the calculation of these parameters. Both structure space and property space server as the intermediate level between processing and performance spaces. Module 1 connects processing and property space using the transformation functions f1 and f2 whereas Module 2 connects property, structure and performance space using the transformation functions g1 and g2 (see Figure B1). Next, we describe the details of the underlying transformation functions (models).

TABLE B3. Identified scenarios that need to be explored

Scenarios	Parameters	Ranges	Remarks
S1	Strain rate ($\dot{\varepsilon}$)	[0.5, 20] s^{-1}	S1 deals with low temperature-low heat transfer coefficient ranges
	Width (w)	[75, 200] mm	
	Temperature (T)	[250, 370] °C	
	Heat transfer coefficient (h)	[10, 50] kW/m^2 K	
S2	Strain rate ($\dot{\varepsilon}$)	[0.5, 20] s^{-1}	S2 deals with low temperature-high heat transfer coefficient ranges
	Width (w)	[75, 200] mm	
	Temperature (T)	[250, 370] °C	
	Heat transfer coefficient (h)	[200, 450] kW/m^2 K	
S3	Strain rate ($\dot{\varepsilon}$)	[0.5, 20] s^{-1}	S3 deals with high temperature-low heat transfer coefficient ranges
	Width (w)	[75, 200] mm	
	Temperature (T)	[370, 550] °C	
	Heat transfer coefficient (h)	[10, 50] kW/m^2 K	
S4	Strain rate ($\dot{\varepsilon}$)	[0.5, 20] s^{-1}	S4 deals with high temperature-high heat transfer coefficient ranges
	Width (w)	[75, 200] mm	
	Temperature (T)	[370, 550] °C	
	Heat transfer coefficient (h)	[200, 450] kW/m^2 K	

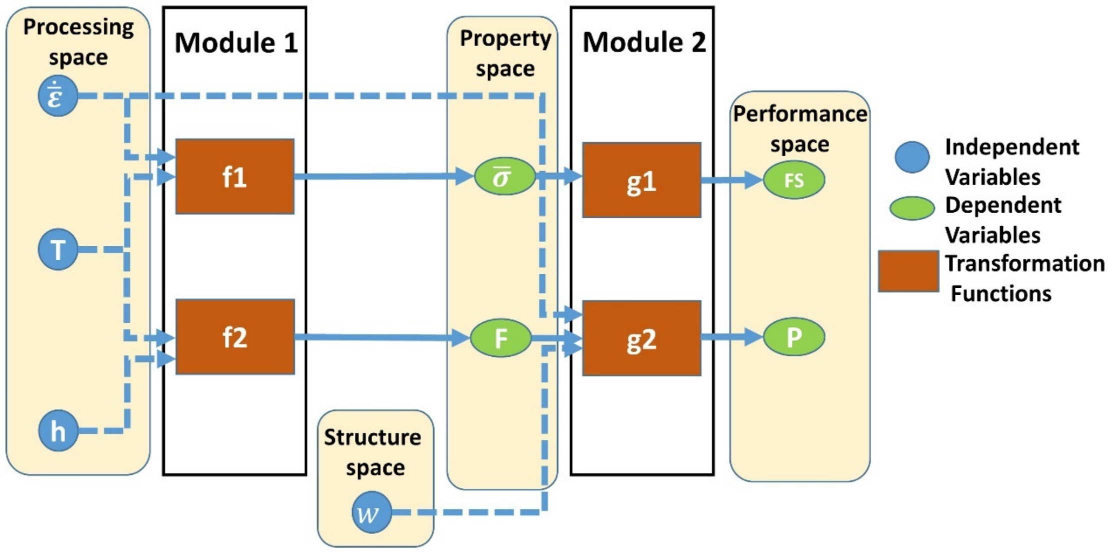

Figure B1: Schematic of the identified spaces (processing, structure, property and performance) and the transformation functions

f1: Flow Stress Prediction Model

Hot deformation studies of aluminum alloy show a huge dependence of flow stress on strain rate and temperature. There are different viscoplastic flow rules such as Norton-Hoff law (Norton 1929), hyperbolic sine function (Duan and Sheppard 2004) and Hensel-Spittel flow formulation (Hensel and Spittel 1978) that define the material behavior during deformation. In the current study, we have used Hensel-Spittel flow formulation which is given as (Duan and Sheppard 2004):

$$\overline{\sigma} = Ae^{m_1 T}\bar{\varepsilon}^{m_2}\dot{\bar{\varepsilon}}^{m_3}e^{m_4/\bar{\varepsilon}} \tag{1}$$

where, A, m_1, m_2, m_3, m_4 are constants and values of these for AA5083 alloy are 953.655 MPa, -0.00524, 0.01407, 0.11 and -0.00913 respectively (Duan and Sheppard 2004). The other parameters in the equation are the equivalent strain ($\bar{\varepsilon}$), strain rate ($\dot{\bar{\varepsilon}}$) and temperature (T). The equivalent strain is a function of initial and final thickness (H_0 and H_1) and is given as (Duan and Sheppard 2004):

$$\bar{\varepsilon} = \frac{2}{\sqrt{3}} \ln \frac{H_0}{H_1} \tag{2}$$

The strain rate term in the expression is given as (Duan and Sheppard 2004):

$$\dot{\bar{\varepsilon}} = \frac{2\pi N}{60} \sqrt{\frac{R}{\Delta H}} \ln \frac{H_0}{H_1} \tag{3}$$

where R is the roll radius, H_0 and H_1 are initial and final thickness respectively and ΔH is the difference between initial and final thickness.

f2: Rolling Load per Width Prediction Model

The rolling load per unit width in this study is defined in terms of the rolling pressure. We then relate the relationship between rolling pressure and heat transfer coefficient (Hlady, Brimacombe and coauthors 1995) into this expression. Thus we calculate rolling load per unit width as a function of heat transfer coefficient. The equation of rolling load in terms of rolling pressure is given as (Hlady 1994)

$$F = P_r \sqrt{R\Delta H} \tag{4}$$

where F is the rolling load per unit width, P_r is the rolling pressure, R is the roll radius and ΔH is the difference between initial and final thickness The rolling pressure, in turn, can be expressed in terms of heat transfer coefficient as per the expression below (Hlady, Brimacombe and coauthors 1995):

$$P_r = H \left(\frac{hC}{k}\right)^{\frac{1}{m}} \tag{5}$$

where H is the surface hardness of workpiece, h is interface heat transfer coefficient, C is a general roughness term, m is a constant with value 1.59 for AA5XXX series (Hlady, Brimacombe and coauthors 1995), k is combined conductivity of roll, k_r and workpiece, k_{wp}. The interface heat transfer coefficient is expressed as [2]:

$$h = \frac{q_{strip}}{T_{strip} - T_{roll}} \quad (6)$$

where q_{strip} is the heat flux, T_{strip} and T_{roll} is the temperatures of strip and roll respectively. Local indentation tests show that the full plastic deformation of material happens when the applied pressure is approximately three times the yield stress (Williamson and Hunt 1972, Mikić 1974, Hlady 1994). Therefore, the surface hardness is calculated as function of yield stress, Y as

$$H = 3Y \quad (7)$$

The yield stress, Y for AA5083 is represented in terms of temperature, T using regression curves based on data from literature (Canas, Picon and coauthors 1996) as shown

$$Y = (-0.44T + 186.17)\ N/mm^2,\ \ if\ 100\ °C < T < 370\ °C \quad (8)$$

$$Y = (-0.107T + 65.367)\ N/mm^2,\ if\ 370\ °C < T < 600\ °C \quad (9)$$

The combined conductivity term k is defined as (Hlady, Brimacombe and coauthors 1995)

$$k = \frac{k_r k_{wp}}{k_r + k_{wp}} \quad (10)$$

where k_r is the conductivity of roll which is assumed to be 14 W/mK (Shahani, Nodamaie and coauthors 2009). The conductivity of the work piece, k_{wp} is represented as a function of temperature, (Shahani, Nodamaie and coauthors 2009) as:

$$k_{wp} = 2E\text{-}05\ T^2 + 0.092\ T + 142.33 \quad (11)$$

Using equations 4-11, we get transformation function for rolling load per width as a function of temperature, T and heat transfer coefficient, h as represented in Figure 1.

g1: Factor of Safety Prediction Model

The factor of safety (FS) of the strip rolled can be defined as:

$$FS = \frac{UTS}{\bar{\sigma}} \tag{12}$$

where UTS is the ultimate tensile strength of material and is taken as 325 MPa for AA5083 and $\bar{\sigma}$ is the flow stress as calculated by the Hensel-Spittel flow formulation (Equation 1).

g2: Rolling Power Prediction Model

Rolling power is expressed as a function of rolling load per unit as:

$$\text{Power} = F * w * L * \omega \tag{13}$$

where F is the rolling load per unit width, w is the width of the strip, L is the length of contact and ω is the angular velocity. The length of contact L is equal to $\sqrt{R\Delta H}$ and the angular velocity ω is given by the following expression

$$\omega = \dot{\varepsilon}/\sqrt{\frac{R}{\Delta H}} \ln \frac{H_0}{H_1} \tag{14}$$

where $\dot{\varepsilon}$ is strain rate, R is the roll radius, H_0 and H_1 are initial and final thickness respectively and ΔH is the difference between initial and final thickness.

B4. IDEM for Solution Space Exploration

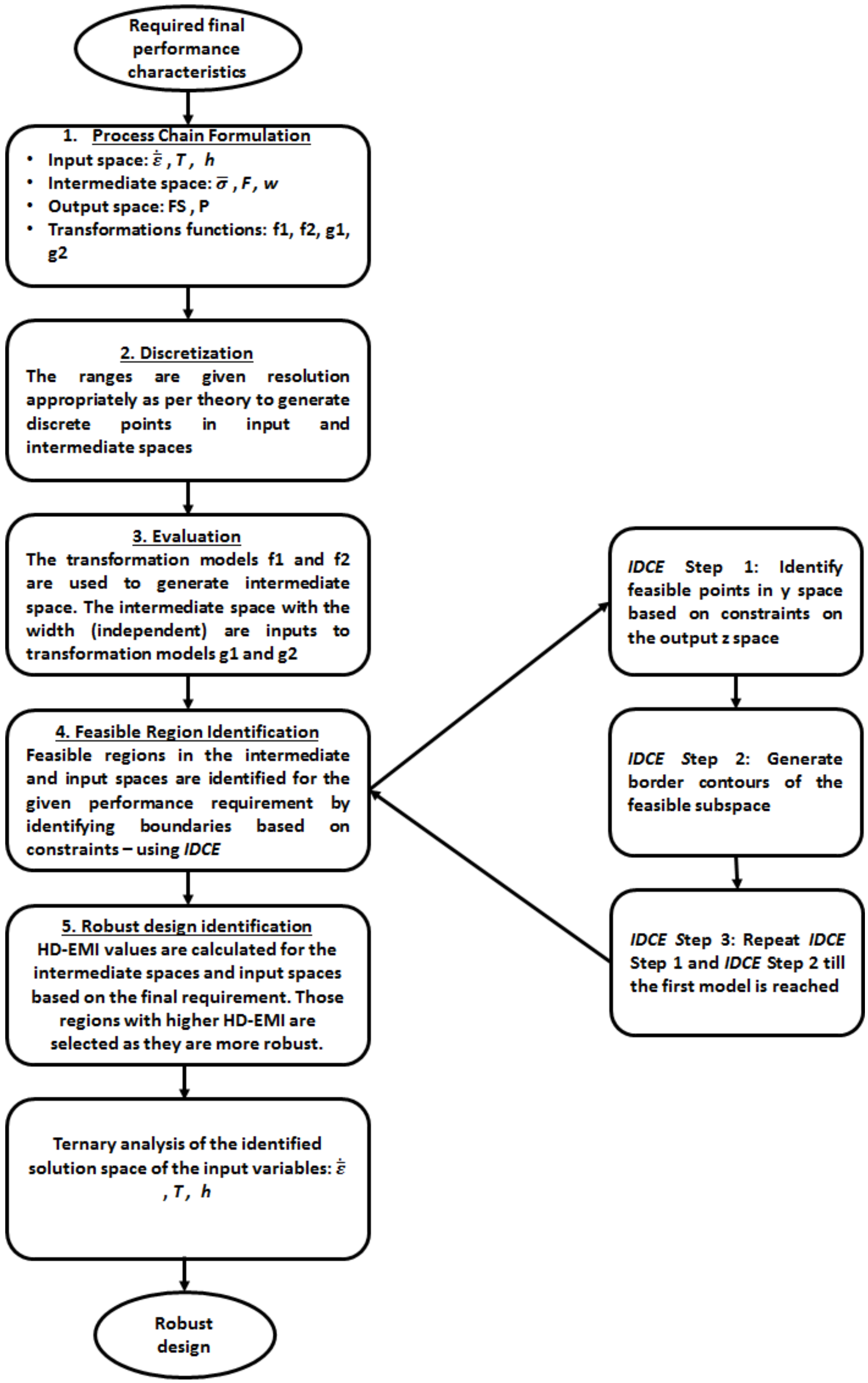

Figure B2: Steps of IDEM

The steps involved in the IDEM is depicted in Figure B2 and the details of procedural steps are present in (Choi, Mcdowell and coauthors 2008, Kulkarni, Gupta and coauthors 2014).

Step 1: Process chain formulation: A step by step forward problem process chain is generated taking into account all the inputs, constraints and desired outputs. All process models are identified in this stage.

Step 2: Discretization: At the input level (x level) and the intermediate levels (y level - can be more than one) a group of discrete points is generated in the design space. Discretization consists of discretizing, grouping, mapping, and merging:

Step 2.1: Discretizing: All the probable combinations of discrete points are generated.

Step 2.2: Grouping: Points obtained in step one are grouped and used as mapping models. Any duplicate groups are eliminated.

Step 2.3: Mapping: Grouped points are evaluated subject to their respective models and results are stored in a mapping array.

Step 2.4: Merging: The final mapping results are combined with the original input points and stored for evaluation.

Step 3: Evaluation: Mapping models are used to evaluate the discrete points and a database of the input and the corresponding output is created.

Step 4: Determination of the feasible region: For the desired range of output performance, feasible regions are obtained in the intermediate and input levels. IDCE (Inductive Discrete Constraint Evaluation) is used to determine the feasible boundaries at the different levels. Border contours of these feasible boundaries are created with the help of discrete satisfying points and discrete unsatisfying points. The steps involved in IDCE are presented in Figure B3 and described below:

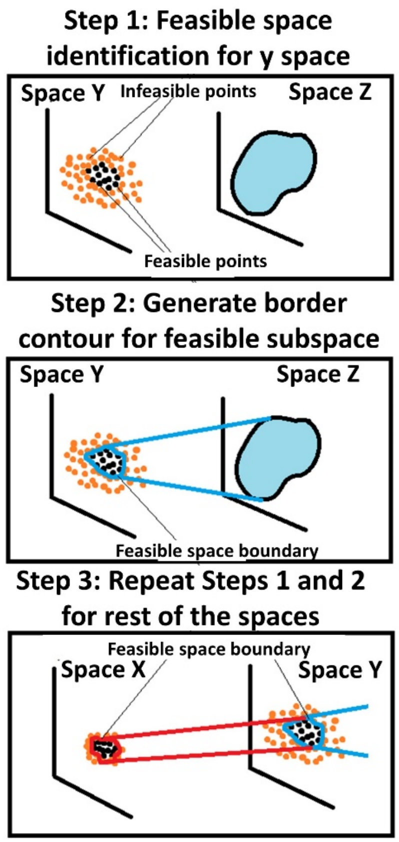

Figure B3: Schematic of IDCE for Feasible Space Identification

IDCE Step 1: Generating feasible points in input space with the help of given constraints in the output space. This step involves the use of HD_EMI (described later).

IDCE Step 2: Creating the boundary or feasible region in the input space utilizing the satisfying and non-satisfying points. The boundary is created at the point where the satisfying and non-satisfying points meet.

IDCE Step 3: Steps 1 and 2 are repeated till the first input space is reached.

Step 5: Identification of robust region: Robust regions in the output space are identified using the HD_EMI values.

Step 6: Identification of overall robust solution: The robust region found out in the output space is corresponded to the intermediate and ultimately the input space for finding the respective solution space. Ternary plots are used to explore the solution space and identify robust regions of interest.

Next, we explain the concept of HD_EMI which is an error metric used to check the feasibility of a design point. The concept of HD_EMI is used in the Inductive Design Exploration Method (IDEM) (Choi 2005, Choi, Austin and coauthors 2005, Choi, McDowell and coauthors 2008, McDowell, Panchal and coauthors 2009). For any given point there will be HD_EMI values in all the given output directions. This checks the feasibility of the mean value of an output range as to whether it is in the range or not. The process involves the identification of all the neighboring points near to the mean and checking whether more than half of them are in the feasible region. If so, then the mean is considered to be in the feasible region. If a mean point is not in the feasible region then the corresponding HD_EMI value is assigned a value of -1.

For a mean point that lies inside the feasible region, HD_EMI_i (i^{th}) is calculated with the help of discrete boundary points (B_i) and output range ($mean_i$). For a given mean value of the output range, the HD_EMI value will be the minimum of all the HD_EMIs calculated for that direction. The schematic showing the calculation of HD_EMI is in Figure B4 (Choi 2005, McDowell, Panchal and coauthors 2009). The higher the value of

HD_EMI_i means that it is farther from the constraint boundary in the i^th^ direction and hence is a more robust and better solution.

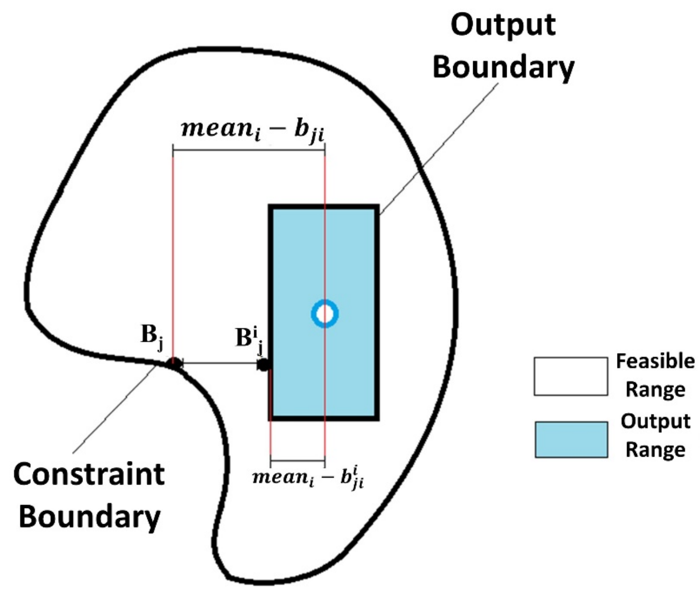

Figure B4: HD_EMI calculation showing the feasible region and output range (Choi, McDowell and coauthors 2008).

$$HD\_EMI_i = min\left(\left|\frac{mean_i - b_{ji}}{mean_i - b^i_{ji}}\right|\right) \tag{15}$$

where (Choi, Mcdowell and coauthors 2008, Kulkarni, Gupta and coauthors 2014),

$i = 1, \ldots n$, number of directions,

$j = 1, \ldots n$, number of discrete points on constraint boundaries

mean is the mean vector of output range

$mean_i$ is a vector component of the mean in an output range in i^{th} direction.

B_j is a discrete point vector on constraint boundary

$b_{j,i}$ is the i^{th} component of B_j

B^i_j is the projected vector of B_j onto the nearest boundary of output range along i^{th} direction

$b^i_{j,i}$ is the i^{th} component of B^i_j

The exploration of the solution space using proposed design method is discussed in the next section. We try to address the following questions in our design analysis:

1. *How to identify a feasible range of processing (input) variables – strain rate, temperature and heat transfer coefficient for a given set of requirements?*

2. *How are the 4 scenarios different that have been considered?*

3. *How to predict process parameters for specified requirements from the results obtained using HD_EMI analysis?*

4. *What possibilities does this method offer to a designer that can be applied to other processes or engineering systems?*

Questions 1, 2 and 3 are answered in Section B5. Question 4 is answered in the "Closing Remarks" section.

B5. Exploration of Solution Space using IDEM

The proposed method (see Figure B2) is applied to the hot rolling problem (see Figure B1) and a database for input-output sets using the transformation functions f1, f2, g1 and g2 are generated which is then used to explore the 4 scenarios and address the aforesaid questions (Section B4). The difference between the 4 scenarios is due to availability of different process window with respect to temperature and htc. Using the database generated, we will check if both the requirements (FS and Power) can be achieved in different scenarios or not and if yes, what are the feasible spaces.

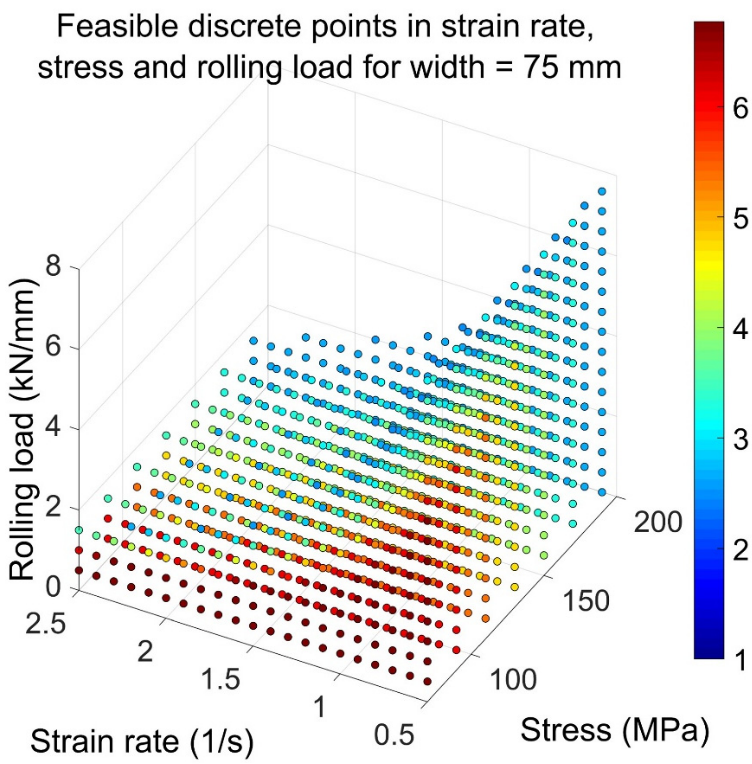

Figure B5. Feasible region for intermediate level

We first identify the feasible space for the intermediate level (stress, rolling load, strain rate and width) that satisfy the requirements defined for power and FOS. The feasible space for the intermediate level is shown in Figure B5. On analyzing the results, we observe that the width of the strip should be minimum for achieving the performance target that we have defined. The lower range value of width that satisfies this for our problem is 75 mm. Since the parameters strain rate, rolling load and stress are not varied, the identified feasible space at the intermediate level remains the same for all the four scenarios. In Figure B5, the red color indicates higher robustness in desirable solution spaces by definition. On analyzing the feasible region shown in Figure B5, we see that a strain rate in the region [0.5, 1.5] s-1 with stress in the region [80, 120] MPa and rolling load [0, 2] kN/mm forms a good robust region for the target performance. Lower rolling load along with lower strain rate values satisfy the performance target in the best manner as indicated by the red regions in Figure B5.

Next, we explore the feasible regions of processing space (strain rate, temperature, and heat transfer coefficient) for the four scenarios identified. The feasible space for intermediate level (stress, rolling load, width and strain rate) remains the same for all four scenarios.

Scenario 1

For Scenario 1 (see Figure B6, HD_EMI values are shown on the color bar) the available feasible space is prominent. We also observe that as we go towards higher temperature regions, the point with higher values of HD-EMI is more which emphasizes the significance of temperature on influencing rolling power and factor of safety.

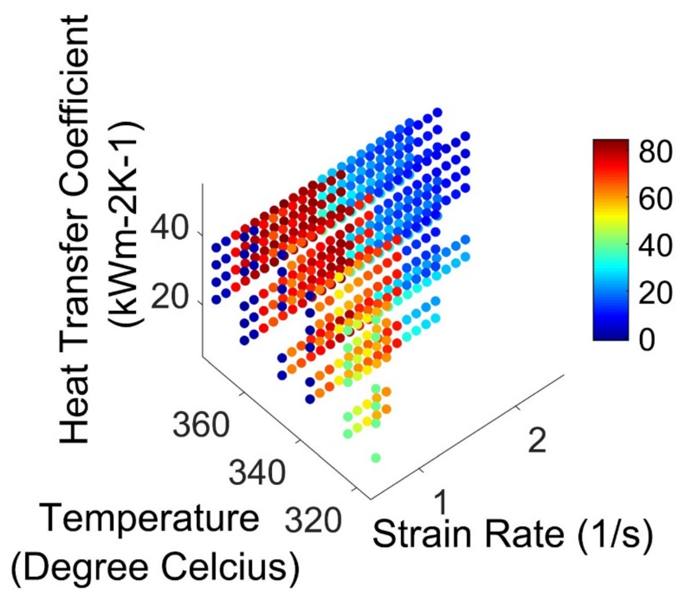

Figure B6. Feasible Region for processing space in Scenario 1

Scenario 2

For Scenario 2 (see Figure B7, HD_EMI values are shown on the color bar.) only one set of feasible space is available which is for the maximum temperature available in the process window (370 °C, see Figure B7). This indicates that achieving requirements on rolling power and FS is not possible for lower temperature and high heat transfer coefficient. This is line with expectation because: 1) it is difficult to roll the material at a lower temperature and hence higher rolling power will be needed to facilitate the same, and 2) occurrence of the high-stress region is more at a lower temperature, thereby resulting in reduced FS.

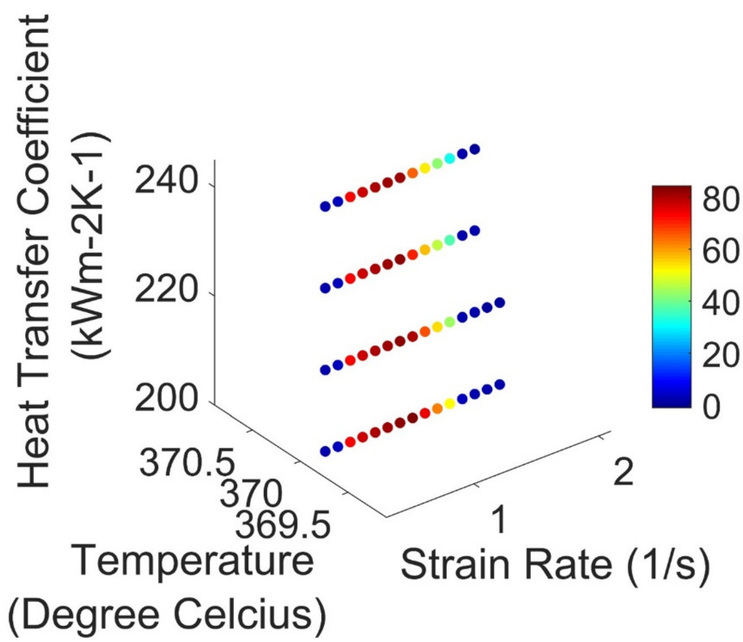

Figure B7. Feasible region for processing space in Scenario 2

Scenarios 3 and 4

For Scenario 3 and 4 (see Figure B8 and B9) the available feasible space is prominent, which indicates that achieving requirement on FS is easily possible for both ranges (low and high) of htc in the higher temperature range. This is in line with expectation as the same has been reported in the literature as well that high in the range of 450-550 °C is best suited for hot forming operations (Agarwal, Krajewski and coauthors 2008).

Using the IDEM framework, we have created a database of inputs and outputs which is then utilized to identify the feasible input space for different scenarios for a specified set of requirements. However, this information only tells us the feasible input space and does not *predict the process design set points for specified requirements.* To answer this question, the designer needs to visualize the effect of process parameters on different requirements by exploring various scenarios. Data generated by exploring different scenarios are used to construct Ternary plots, which assist a process designer in making informed decisions and identifying the design set points. Shukla and co-authors (Shukla, Goyal and coauthors 2014, Shukla, Goyal and coauthors 2015, Shukla, Kulkarni and coauthors 2015) and Nellippallil and co-authors (Nellippallil, Song and coauthors , Nellippallil, Song and coauthors 2016, Nellippallil, Allen and coauthors 2017, Nellippallil, Vignesh and coauthors 2017) have used ternary plots to predict design set points of different unit operations in steel manufacturing, namely, ladle refining, tundish, casting and rolling operations. We have already identified feasible space using IDEM (described above). Among the identified feasible space, regions having higher HD_EMIs are selected and these data points are used to construct ternary plots. Ternary plots are then used to predict design set points for a given set of requirements and for demonstration purpose we will discuss the analysis only for Scenario 3 (a similar study can be done for other scenarios as well).

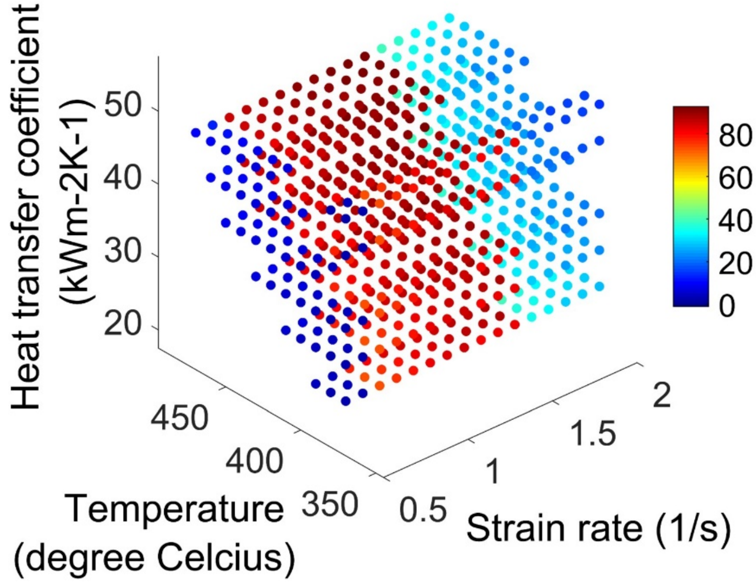

Figure B8. Feasible region for processing space in Scenario 3

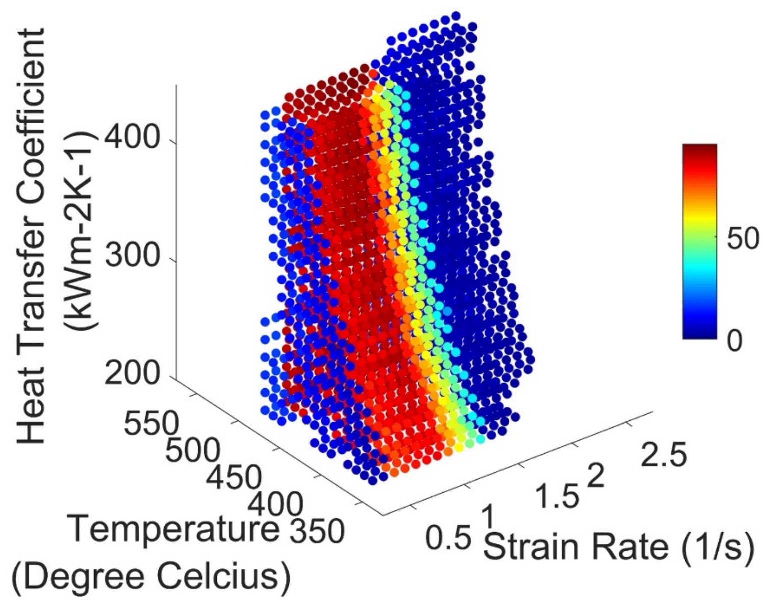

Figure B9. Feasible region for processing space in Scenario 4

Table B4: Scenarios Explored for Ternary Plots

Weights			Values					Normalized Values	
			Input Variables			Performance/ Output			
Strain Rate	Temperature	Heat transfer coefficient	Strain Rate (1/s)	Temperature (°C)	Heat transfer coefficient (kW/m^2K)	Power (kW)	FS	Power	FS
1	0	0	1.5	420	45	3.510495	3.494706	1	0
0	1	0	0.8	470	45	1.380131	4.866604	0	1
0	0	1	0.8	420	50	2.000531	3.744905	0.291218	0.182374
0.5	0.5	0	1.15	445	45	2.337418	4.102008	0.449354	0.442673
0.5	0	0.5	1.15	420	47.5	2.784472	3.598355	0.659203	0.075551
0	0.5	0.5	0.8	445	47.5	1.682273	4.269071	0.141827	0.564448
0.25	0.75	0	0.975	457.5	45	1.831829	4.459941	0.212029	0.703576
0.25	0	0.75	0.975	420	48.75	2.399632	3.664293	0.478557	0.123615
0.75	0	0.25	1.325	420	46.25	3.154836	3.542721	0.833052	0.034999
0.75	0.25	0	1.325	432.5	45	2.896954	3.782538	0.712002	0.209805
0	0.75	0.25	0.8	457.5	46.25	1.529164	4.558056	0.069957	0.775094
0	0.25	0.75	0.8	432.5	48.75	1.839411	3.998408	0.215588	0.367157
.33	0.33	0.34	1.031	436.5	46.7	2.255381	3.970739	0.410846	0.346989

Sabeghi and co-authors (Sabeghi, Smith and coauthors 2015) propose a method that embodies ternary plots, to explore the solution space. We have employed a similar approach which allows us to perform process parameter sensitivity analysis and to visualize the effect of process parameters on individual requirements and thereby predicting design set points (process parameters) for specified set of requirements. The three axes of the ternary plot represent normalized value of process parameters (strain rate, temperature and heat transfer coefficient) and fourth axes (represented by color contour) is the achieved value of a particular requirement.

To start the analysis, we identify feasible regions having highest HD_EMIs for Scenario 3 and which gives us a range of temperature from 420 to 470 °C, strain rate from 0.8 to 1.5 s^{-1}, and heat transfer coefficient from 45 to 50 kW/m^2K.

Ternary plots for rolling power and FS are constructed based on the data generated in Table B4. Suppose, we have requirement of having a power of 2 kW or less and FS as 1.5 or more (the values are not sacrosanct and are taken only for demonstration purposes).

In Figure B10, the region bounded by the axes and red dashed line in the direction of the arrow is the feasible region. If we chose a combination of temperature, strain rate and htc from this region and carry out the rolling operation, we will satisfy the requirement of having power equal to or less than 2 kW.

In Figure B11, the region bounded by axes and blue dashed line in the direction of the arrow is the feasible region. If we chose a combination of temperature, strain rate and htc from this region and carry out the rolling operation, we will satisfy the requirement of having FS equal to or more than 4.3.

We superimpose the feasibility region of the two plots to identify if both the requirements can be simultaneously achieved or not for the given set of requirements.

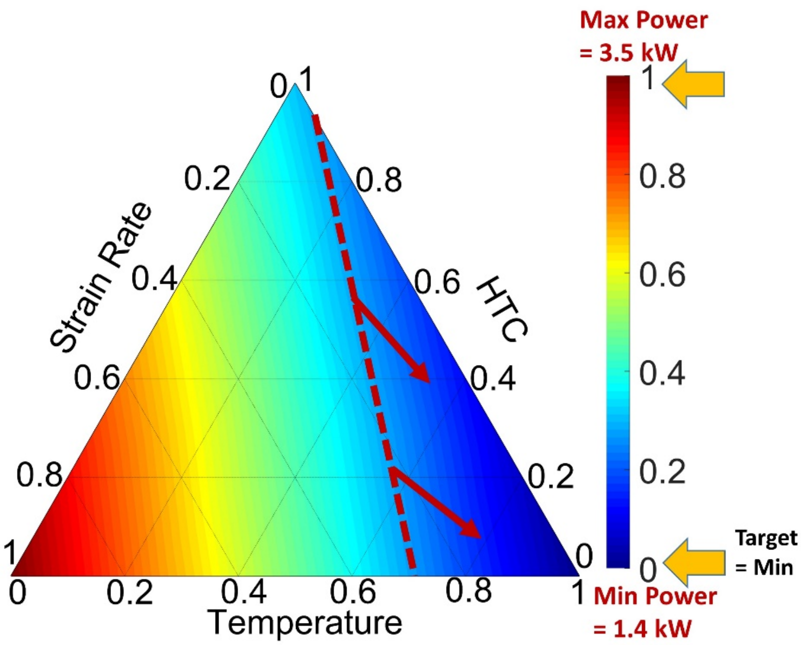

Figure B10. Ternary plot for Rolling Power

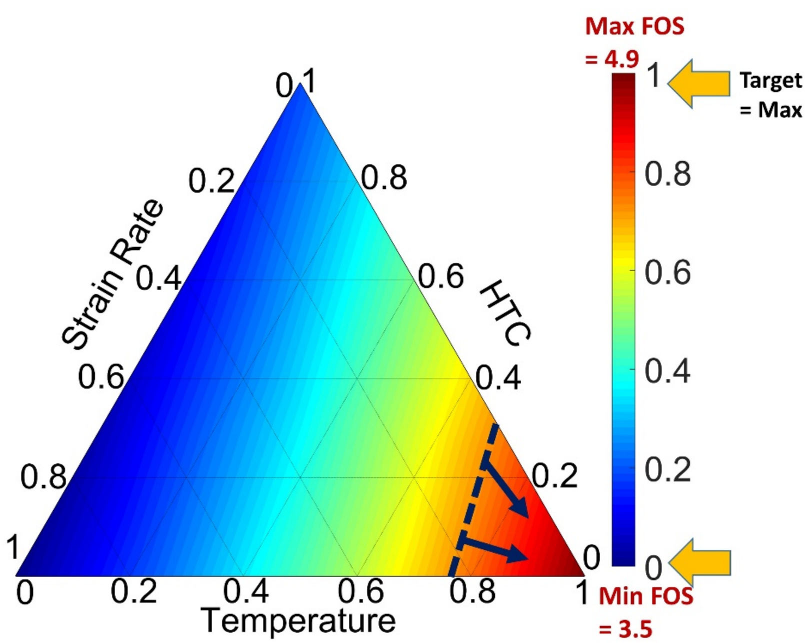

Figure B11. Ternary plot of Factor of Safety

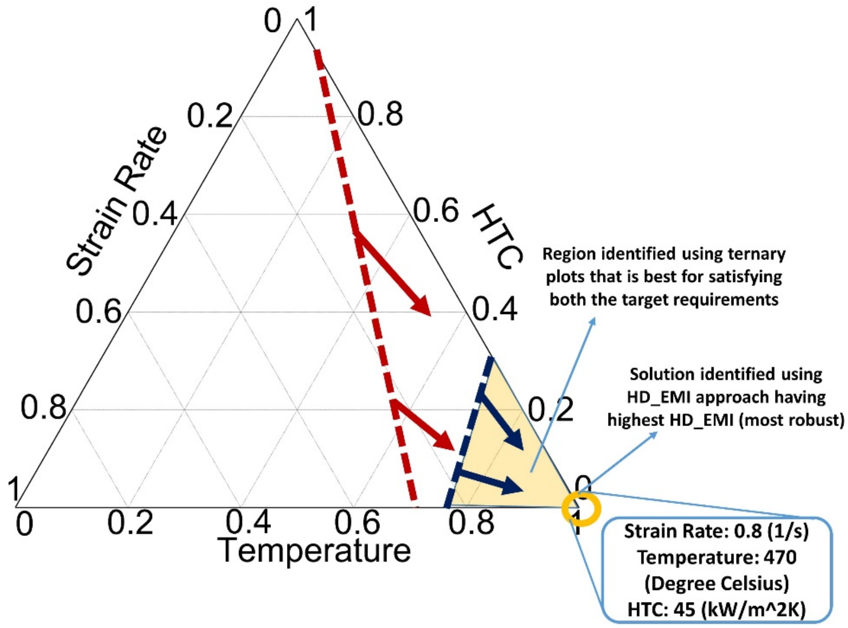

Figure B12. Superimposed Ternary Plot

For the given case, we observe an overlap of the feasibility region exists and is shown in orange color, which is the feasible solution space for which both the requirements will be achieved (see Figure B12). If we choose a combination of temperature, strain rate and htc from this region and carry out the rolling operation, we will satisfy the requirement of having power equal to or less than 2 kW and FS equal to or more than 4.3. One such point is point indicated by the orange dot, having strain rate 0.8 s^{-1}, temperature 470 °C, and heat transfer coefficient 45 kW/m^2K. The importance of ternary analysis is that a designer can identify whether a set of requirements can be achieved and therefore predict the design set points. The ternary plots serve as a look-up table to be used by a process designer to make informed decisions without actually running the simulations repeatedly, which in turn saves computational time and cost.

B6. Verification

Since we have considered a simplified rolling process for the purpose of demonstrating the utility of our method and owing to unavailability of plant/lab data, we cannot directly validate our design predictions with experimental or industrial data. However, to give a reasonable verification of our method, we carry out FEM analysis of the rolling model and check if the design set points predicted using the proposed method gives us desired stress state in the strip or not. Next, we explain the FEM model and the subsequent analysis.

Finite Element Model

A finite element model for the hot rolling of AA 5083 alloy is developed in ANSYS to verify the predicted results. A plane strain condition is assumed and only half strip is modeled because of the symmetric conditions. The details on the formulation of the FE model, the initial and boundary conditions used, the details on the material model, etc. are available in reference (Nellippallil, De and coauthors). Friction coefficient and heat due to plastic deformation value are taken as 0.3 and 0.9 respectively for AA 5083 alloy. Heat transfer coefficient is defined between roll gap and air and flow behavior of the material is modeled using Perzyna viscoplasticity model. The angular velocity of the roll is applied based on strain rate applied. The FEM model along with the mesh developed for the problem under consideration is depicted in Figure B13.

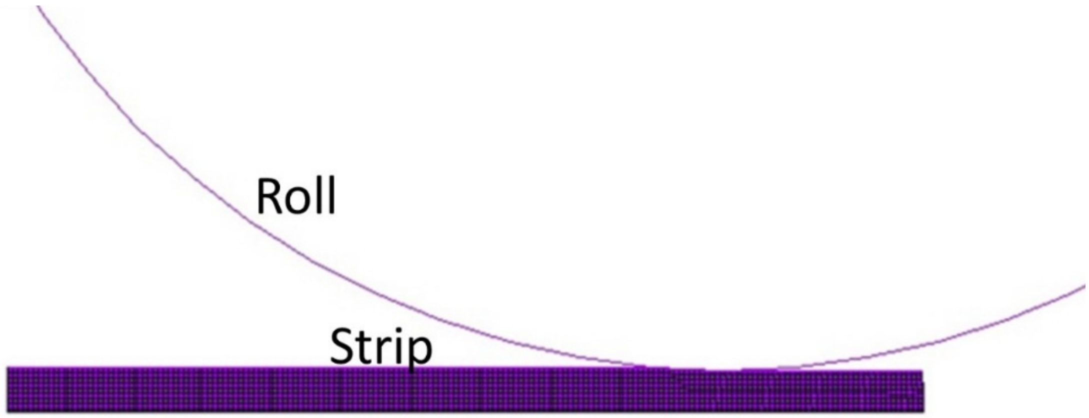

Figure B13. FEM model showing the mesh developed for hot rolling of AA 5083 in ANSYS

The values of initial temperature, heat transfer coefficient, and strain rate are selected from the feasible solution space that we obtain using ternary plot, which corresponding to the ternary plot's vertex point (see Section 5, Scenario 2 in Table B4) is provided in Table B5.

Table B5. Design Set Points Identified for Scenario 2

Scenario 2 HD_EMI max	**Strain rate (1/s)**	**Temperature (°C)**	**Heat transfer coefficient (kW/m^2K)**
	0.8	470	45

The values provided in the table are input to the FE model. The angular velocity of the roll is calculated for the strain rate of 0.8 s^{-1} using Equation 13. Temperature (470 °C) is input as an initial condition to the strip and heat transfer coefficient (45 kW/m^2K) is applied in the region where the strip comes in contact with the roll. The FEM results for stress during rolling are then analyzed and are shown in Figure B14.

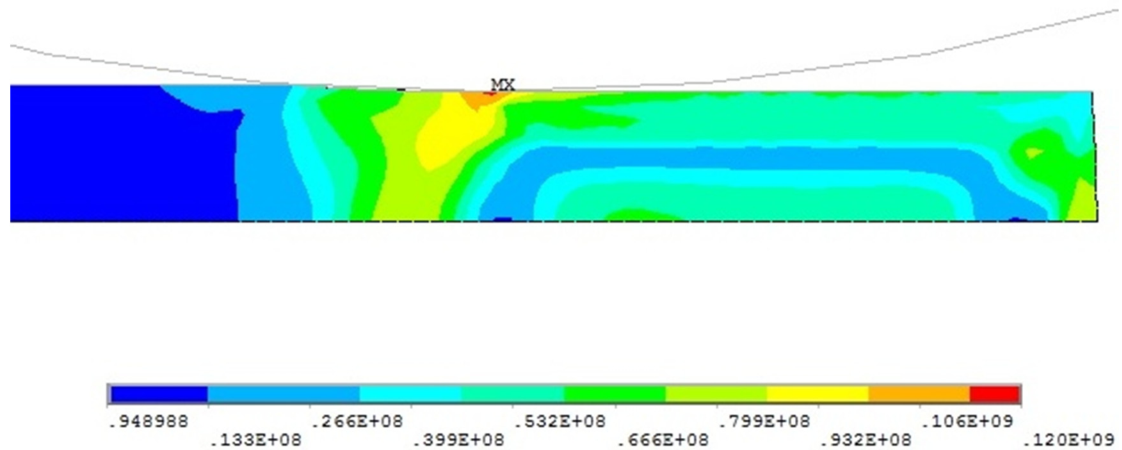

Figure B14. Finite element model stress plot

We see that the strip during rolling achieves a peak stress value in the range of 80-100 MPa. Computing the FS and rolling power based on this stress value along with the combination of other input parameters, we get FS more than 4.3 and rolling power less than 2 kW, which is exactly what is specified as our requirements (see Section B5). Using FEM analysis, we verified that the predictions using our method of IDEM followed by ternary plots analysis predict the design set points which will lead to meeting the specified performance requirements.

B7. Closing Remarks

It is critical for a designer to identify the design variables that satisfy a particular output performance target that is desired. In Appendix B, we illustrate the efficacy of the IDEM that uses the HD_EMI metric as a tool to explore the solution space by defining performance-properties-structure and processing relations in an inductive manner and by identifying robust design specifications that take into account the uncertainty involved.

This is an inductive approach since we are identifying a feasible range in lower processing level from a desired range in higher performance level. The method is used to identify feasible and robust solutions for the problem chain constructed using the HD_EMI metric. Through this method, the designer is able to manage the uncertainty that occurs due to propagation and this ensures the identification of robust set points for the input parameters that satisfy a desired output performance. We demonstrate the efficacy of the method by applying it to a hot rolling inverse problem formulated. The hot rolling process chain formulated takes into account the thermo-mechanical behavior of the alloy. HD_EMI metric based IDEM approach is used to find the feasible space of initial process parameters of rolling operations. We have then constructed ternary plots and used the same to predict the design set points for a given set of requirements from the feasible space predicted by IDEM. FEM analysis is carried out to verify the predictions on design set points using our proposed method.

The utility of the method is that it helps a process designer to predict the design set points at which a unit operation should be operated in order to meet the specified requirements. This method has been applied to a simplified rolling operation for the purpose of demonstration of the utility of the method. However, the same can be applied to a much more complex rolling or any other systems, given that the underlying models are available.

Limitations of IDEM based on the study carried out

The following limitations are identified in IDEM based on the study carried out using the hot rolling problem. These include:

- Error due to discretization of design space – IDEM uses discretization of design space and further inductive discrete constraints evaluation for mapping from one space to another – this leads to discretization errors and also inability to capture the feasible boundary accurately – resulting in loss of information affecting system performance.
- Increasing accuracy by increasing the resolution of discrete points results in highly computationally expensive IDEM runs for evaluating feasible spaces.
- There is limitation in terms of the number of design variables that can be used in IDEM for a design problem under study. The number of design variables increases the discrete points to be evaluated in the order of power – virtually impossible to evaluate beyond 9 variables for an IDEM study.
- Limitation in terms of exploration and visualization – IDEM uses a three-dimensional visualization space using HD-EMI metric for exploration where only a maximum of 3 design variables can be studied at a time with the others variables taking defined values – this limits the scope of the simulation study and results.
- Issue of flexibility in design – IDEM do not allow designers to incorporate new goals or requirements at different levels during the process of design as the method is based on mapping to feasible spaces of 'Y' and 'X' for a given 'Z' space.

Hence, due to these limitations a new method for robust, top-down design exploration is needed that addresses these limitations so as to applied for the design of complex systems. In Chapter 8, we propose our approach of Robust Concept Exploration using the CEF and cDSP construct with EMI and DCI metrics for measuring robustness.

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