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A GLOBAL OPTIMIZATION FRAMEWORK FOR STOCHASTIC INTEGRATED REFINERY PLANNING WITH NONLINEAR UNIT MODELS UNDER DEMAND AND PRICE UNCERTAINTIES

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A GLOBAL OPTIMIZATION FRAMEWORK FOR STOCHASTIC INTEGRATED REFINERY PLANNING WITH NONLINEAR UNIT MODELS UNDER DEMAND AND PRICE UNCERTAINTIES

A DISSERTATION APPROVED FOR THE

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BY

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I dedicate this dissertation to my beloved mother Mahzar Sedghi and late father Yadollah Siamizade whose unconditional love and inspirations were instrumental in my lifetime pursuit of knowledge and wisdom and my eventual success in academic endeavors.

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Table of Contents

List of Tables

List of Figures

ABSTRACT

The refining industry is facing increased volatility in the global market such as lower economic margins. In this situation, refinery production planning becomes a substantial tool to utilize all potentials to extend the economic margin to its maximum level. Classical refinery production planning models employ input-output relationships for different refinery units. However, these input-output relationships usually do not include decision making variables related to the units' operation (pressure, temperature, etc.). In addition, they fail to capture the nonlinear nature of the refinery units and the inaccuracy caused by these models may reduce the overall profitability or compromise product quality. The refinery business involves tasks spanning from unloading crude oil at the refinery's front end, generating utilities for refinery operations, blending different crudes and procuring crude blends to intermediate products, blending intermediates into final products and distributing refined products from refinery to distribution centers by means like pipelines. The traditional approach for the planning problem of these sub-systems is a sequential hierarchical approach. In reality, refinery processes are tightly interconnected and any attempt to solve this problem in a sequential push or pull manner may result in infeasible or suboptimal solutions. Eventually, the oil industry is subject to uncertainties such as unstable prices and unpredictable product demands. The existence of uncertainty in such parameters can seriously affect the optimization results and lead to inefficient operations. Nevertheless, there are challenges associated with the integrated optimization approach which arise from the difficulty of obtaining a solution with reasonable quality and time. The corresponding integrated model of the refinery operations with nonlinear unit correlations under uncertainty results in a computationally intensive nonconvex MINLP (Mixed Integer Nonlinear Programming) model due to the presence of bilinear, signomial, exponential or logarithmic terms in some of the mass

balance, product yield and quality constraints. A further complexity is introduced in attempting to obtain a globally optimal solution. The standard methods for solving this complex refinery wide optimization problem may fail to converge to a solution or lead to sub-optimal solutions. Despite these complexities, this research presents a novel optimization heuristic for the integrated supply chain model of a refinery network. The production planning model of the refinery employs two different nonlinear models for the distillation unit utilizing correlations based on the Geddes fractionation index (FI) and a swing-cut (SW) data-based model and empirical nonlinear models for the remaining refinery units. The main contribution of this research is the development of an aggregation /disaggregation methodology based on lumped variable linearization (LVL) and normalized multiparametric disaggregation (NMDT) techniques through a two-level optimization algorithm and obtaining ε-global optimal solutions. To model the uncertainties, three modeling schemes such as robust programming, fuzzy possibilistic programming and two-stage stochastic programming with financial risk management have been utilized. The results indicated the effectiveness of the nonlinear models in terms of improving the overall refinery profit margin over a linear input-output model. In addition, they substantiated the huge advantage of a nonlinear distillation model utilizing correlations based on the Geddes fractionation index (FI) over the swing-cut (SW) data-based model. The results on the integration of the refinery supply chain echelons through a deterministic refinery model reinforced that the integrated model when solved by the proposed heuristic can provide significantly better solutions than its sequential counterpart in terms of both economic and operational objectives. Eventually, the results of the stochastic refinery model represented significant economical and operational differences between the outcomes of three uncertainty quantification methodologies discussed earlier while highlighting an obvious advantage of the robust optimization scheme.

Chapter 1

INTRODUCTION

1.1. Inherent Nonlinearity of Refinery Processes

Production planning is a crucial tool in today's petroleum refining industry. It aids decision making and the resource allocation process to achieve business objectives through optimal production operations.[1-3] Historically, the petroleum industry has relied on linear programming (LP) to address its planning and optimization needs.[1,4,5] The LP approach simplifies the inherent nonlinearity of the refinery processes to ensure simplicity and robustness of the models at the expense of accurate and optimal solutions to the planning model. [1] Nevertheless, the linear process models are not suitable for refinery process modeling, since refinery processes involve both physical operations (e.g., phase separations, blending operations) and chemical operations (e.g., cracking reactions, hydrotreating reactions, etc.) with nonlinear nature.[6]
In reality, the actual refinery process is highly nonlinear. Moreover, the stringent environmental regulations, product qualities, and heavier feedstocks make it necessary to develop accurate models for refinery production planning. [7,8] Consequently, the operating plans based on the linear programming technique may not be reliable and the inaccuracy caused by linear models and approximate algorithms may reduce the overall profitability or compromise product quality. [6,9]

Nonlinear approaches and specialized algorithms have also been proposed for refinery planning problems to obtain models of the refining processes while focusing on increasing the accuracy of the planning models and/or the performance of the solution algorithms.[4,7,9,10,11,13-22] These approaches can be grouped into three main categories: rigorous models, simplified or empirical models, and statistical models. The selection of which model is most suitable for a certain application depends on such issues as the amount of information that needs to be provided by the model, and the difficulty of generating, implementing and validating the model among other things. In an optimization problem, it is crucial to use models that, in addition to accurately representing the processing system, can be stable and implemented in a short period of time.[24]

Although more accurate results of processing units can be obtained by using rigorous models, their complexity and the length of the solution time prevent them from being used commonly.[4,12] The nonlinear implementation for the process units in planning models mainly rely on empirical relations.[1,23] Empirical models use empirical correlations to establish material and energy balances for refinery units. Their simplicity, relatively easy application and adequate accuracy to reflect actual conditions of a refinery unit, make them suitable candidates for refinery wide production optimization. [4]

Crude distillation units (CDUs) are the entrance and first processing unit in oil refineries.[25]. The accurate representation of the CDU in a planning model is important because the CDU model dominates the outcome of planning model optimization.[26]

Various forms of simplified CDU models have been devised over the past several decades.

One approach to simplified CDU modeling is "delta-based" models which use incremental changes to produce true boiling point (TBP) curves deviations from some base case operation. Another approach (we shall call it "full model") is to compute product TBP curves via a model which uses operating conditions, crude TBP data, and sometimes approximations of the CDU structure.

There are two types of delta-based models. One of them is to modify the back end and the front end of the product yield by adding or subtracting some delta differences. Since the CDU unit can operate under different operating modes, the deviations from the base case are not constant but depend on the operating mode. Product yields and the cut-points are calculated by using the middle point of the modified front and back ends of TBP curves of adjacent products.[25] One way to improve this model is by setting different production modes where each production mode has a different set of deltas. Unfortunately, this modified model doesn't cope well when processing different kinds of crude oil feed or crude cocktails as deltas also are dependent on the properties of the crude oil, not only CDU operation modes.[27] Figure 1.1 illustrates feed and product TBP curves for a typical crude distillation unit.

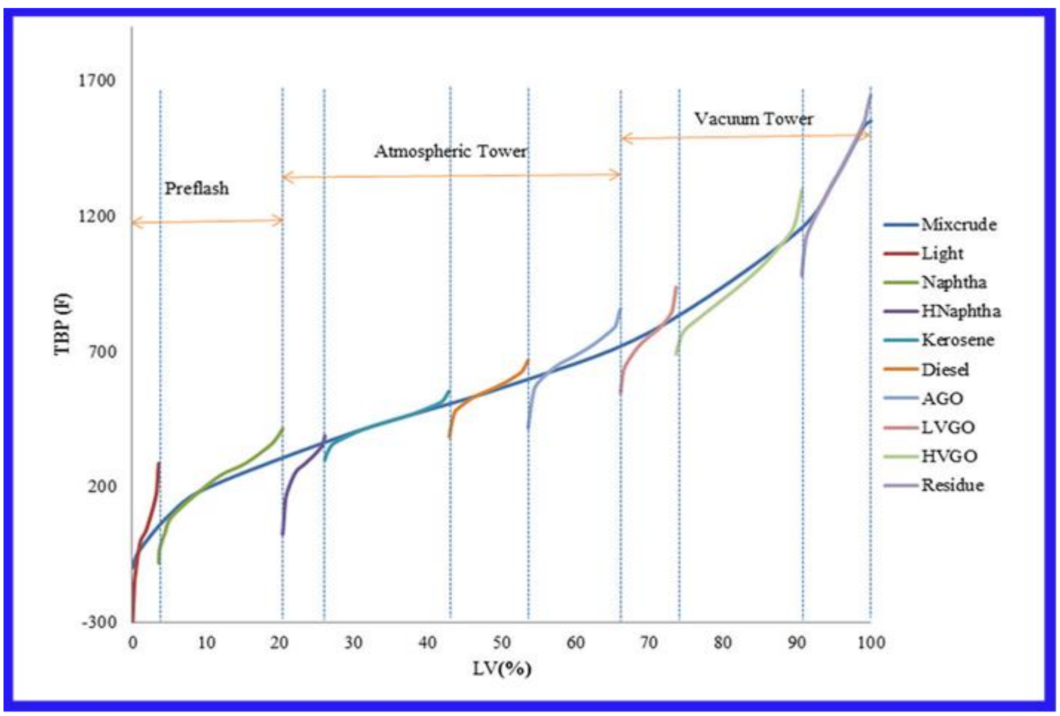

Figure 1.1. Feed and product TBP curves for a crude distillation unit [25]

The second type of delta-based models are swing-cut methods. A swing-cut is the volume fraction of crude where two adjacent petroleum fractions' boiling range overlap. It can be split disproportionally or completely shifted to either light or heavy fraction's yield by adjusting the cut point temperature. In these models the swing-cut size and TBP range are estimated for each product. Based on the swing-cut information and crude properties in their respective TBP range, product properties are computed. The traditional swing-cut model assumes the size of the swing-cut is fixed and that the properties of the swing part are constant across the cut which can cause inaccuracies in the predictions of both its quantity and quality.[28,30] However in the flexible swing-cut method the swing-cut is calculated based on different operating modes (max naphtha, max diesel, or max gasoline) based on a "weight transfer ratio" concept and the properties of swing-cut and fractions were determined by regression models according to the crude properties.[29] The traditional swing-cut model can be further improved by separating the swing-cut into two parts (light and heavy part). The properties of these two parts are calculated by interpolating qualities correspondent to their light and heavy swing-cut quantities.[30] To account for the nonlinearity of the distillation process, some attempts are made based on swing-cut methods by fitting CDU data for a large pool of crude oils and using polynomial regression.[31] Figure 1.2 demonstrates the cut-points and swing cuts of a distillation fraction.

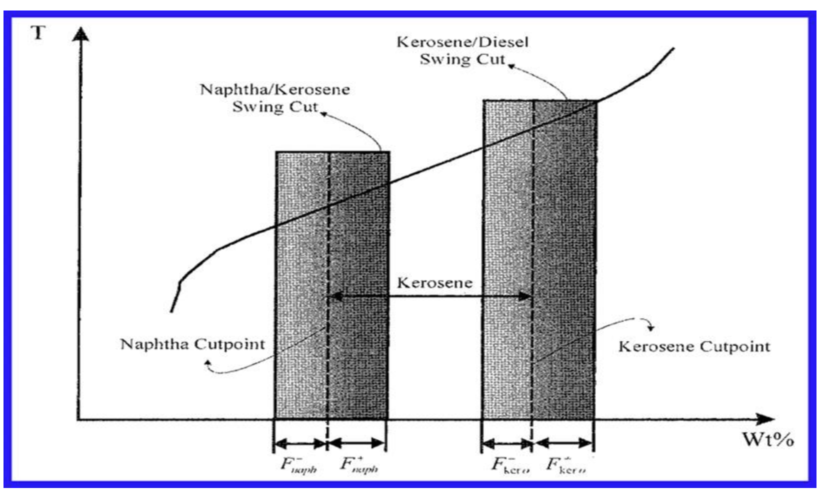

Figure 1.2. Cut-points and swing cuts of a distillation fraction [28]

Another approach in empirical CDU models has been devised based on an aggregated model for the CDU and using a cascade column to represent the stripping and rectifying sections of this complex distillation column. Based on the cascade structures, the nonlinear model of distillation unit is represented as a sequence of flash processes using the fractionation index to determine the separation in each section.[1,32-34] Figure 1.3 illustrates cascade representation of CDU based on the FI model.

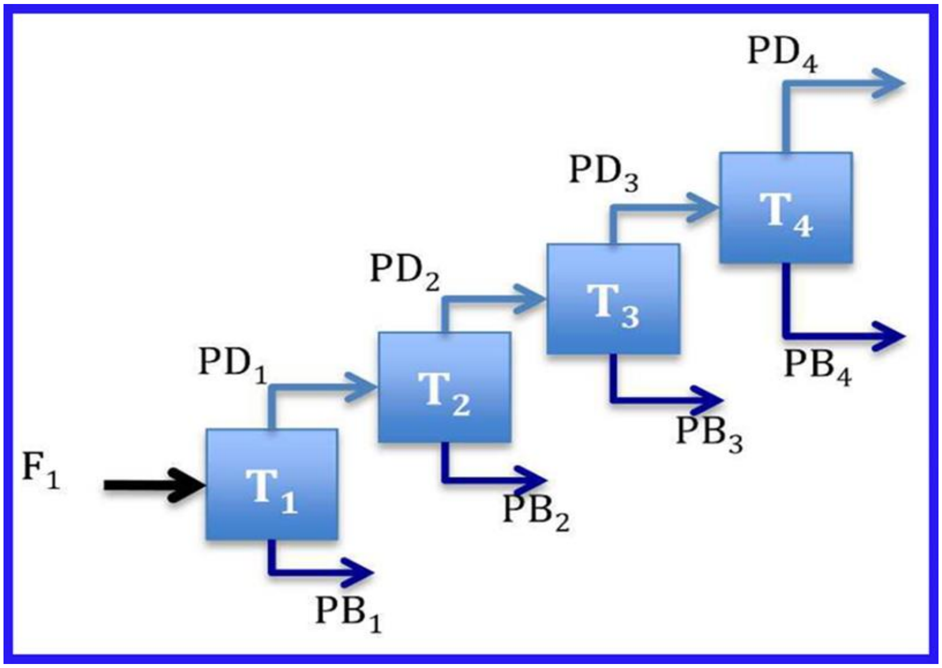

Figure 1.3. CDU representation for the FI model.[1]

The fractionation index (FI) is a quantitative criterion for sharpness of fractionation with complex mixtures by a fractionator.[35] The index is the equivalent number of theoretical plates, operating at total reflux, which would affect the same component separation as the fractionator. In the case of crude oils, the number of components is numerous and the data have been broken down into short fractions which have then been treated as pseudocomponents in subsequent column calculations.[36] The FI model is a more accurate nonlinear model for the complex crude distillation unit (CDU) than the fixed yield or the swing cuts models and optimizes the crude cuts quantities and temperature while being independent from crude type, characteristics of the CDU, and readily calculated.[34]

In a distillation unit, the distribution of a component *i* in the top and bottom product streams, expressed as molar fraction y_i and x_i, are related to the relative volatility α_{io} of component *i* to reference component *o* for fractionation at total reflux operation through the following equation:

$$\frac{y_i}{x_i} = \alpha_{io}^{n} \frac{y_o}{x_o} \quad (1.1)$$

Geddes[35] plotted the component product composition ratio versus the relative volatility on a logarithmic scale as seen in Figure 1.4, intersecting straight lines with two slopes, changing the slope at the reference component used for the relative volatility calculation. Geddes observed that the resulting slope reflects the fractionation power of the column. On the other hand, two different slopes means unequal fractionation power in the column. Geddes named the slope of the line the "fractionation index" (FI).

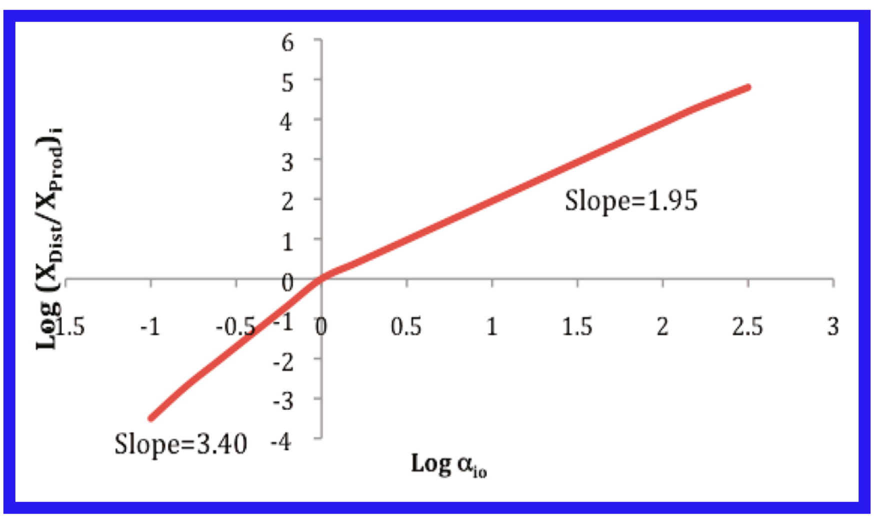

Figure 1.4. Component distribution ratios for a fractionation column [19]

He also suggested using it in other calculation methods used at the time, including Thiele-Geddes:

$$\frac{y_i}{x_i} = \alpha_{io}^{FI} \frac{y_o}{x_o} \quad (1.2)$$

Gilbert et al.[36] extended the use of FI to crude distillation units (CDU). Jakob[37] suggested using the component equilibrium constant K in the FI equation as an acceptable simpler approximation for the relative volatility term α.

To use the FI method, Alattas et al.[1,34] model the complex CDU as a series of flash single-stage fractionation units, knowing the feed crude oil assay and rate, FI values, and the temperature ranges for the cuts. Each unit has top and bottom product streams. The top product is fed to the next unit, except for the last unit where it is the CDU overhead product. The bottom product of each unit is withdrawn as one of the CDU product streams. The temperature used for the FI equation at every unit is the cut point temperature of the unit product limited to a predefined range. This range represents the overlap or gap temperature of adjacent crude cuts.

One of the first academic contributions to consider nonlinearity in production planning is that of Moro et al.[13] Their model represented a processing unit employing a general nonlinear model with the following variables: feed flow rate, feed properties, unit operating conditions, product flow rates, and product properties. Pinto and Moro [14] developed a nonlinear planning model for production planning which allows for the implementation of nonlinear process models and blending relations. Li et al.[4] presented a refinery planning model utilizing simplified empirical nonlinear process models with considerations for crude characteristics, product yields and qualities. Alhajri et al. [31] developed a nonlinear model to represent the refinery processes to address the refinery planning problem. The resulting model is able to predict the operating variables such as the Crude Distillation Unit (CDU) cut-point temperatures and the conversion of the Fluid Catalytic Cracking unit (FCC) and evaluate properties of the final products to meet the market specification as well as the required product demands. Alattas et al. [34] developed a fractionation index (FI) based nonlinear model for crude distillation units (CDUs). In contrast to the swing cut methods, the fractionation index model incorporates thermodynamic principles such as relative volatility and phase equilibrium. Alattas et al. integrated the FI-based nonlinear model into the linear refinery planning model, solving it with nonlinear programming (NLP) solvers without guaranteeing global optimality. Alattas et al.[1] presented a multiperiod MINLP model for the refinery planning problem by modifying their previous NLP model in Alattas et al.[19] to a mixed-integer nonlinear programming (MINLP) model to determine the sequencing, changeovers, and processing times of crude oils over multiple time periods.

Menezes et al.[21,30] used the improved swing cut approach to introduce a new and relatively simple improvement to the conventional swing-cut modeling. In their improved model, the usual assumption that the swing-cut properties flowing from the swing-cut to the light and heavy final-cuts (or product-cuts) are the same, has been extended or modified to account for the fact that they vary according to their proportions between the light and heavy interfaces. Zhang et al. [22] developed a multiperiod MINLP model that aims to optimize the production plan of a refinery site accounting for the material and energy requirements. Nonlinearities appear in the pour point blending equations.

Li et al. [9] proposed a global optimization-based planning formulation with data-driven model development and integration of nonlinear models to predict product yields and properties in refinery production units. The yield and property prediction models for the crude distillation and vacuum distillation units are developed using swing-cut theory based on crude assay data. Empirical nonlinear models are developed for other processing units, including bilinear, and quadratic terms. Moreover, property indices in blending units are linearly additive and calculated on weight or volume basis, which introduce bilinear and trilinear terms.

Lopez et al.[29] presented a new NLP optimization model for a CDU system that includes the energy restriction of plants and utilizes the metamodel approach to represent the non-linear phenomenon of distillation and attempted to obtain the optimum operational conditions for each atmospheric tower, calculating products yields and their properties, temperatures and duties of exchangers responsible for crude pre-heating.

One of the main issues is that none of the literature mentioned thus far explicitly accounts for the operating variables or provides an option for the refinery planner to adjust the operating variables or the process severity within the refinery units to obtain desired yields and product quality. In addition, most of the literature mentioned does not include all major refinery units in their model and therefore present a partial production planning. The other main issue is that the empirical nonlinear models of refinery units are nonconvex; therefore, traditional convex optimization techniques are not suitable if the global optimum is required and most of the literature dealing with nonlinear models mentioned thus far, do not guarantee the global optimality. [9,11]

1.2. Integrated Decision Making in Refining Industry

The second subject addressed in this study is the integration of activities across the refinery supply chain. Refining is a divergent process industry which adds value mainly by performing spatial transformations on petroleum (e.g., lifting crude oil to the surface; transporting crude oil from oil fields to refineries; procuring crude blends to intermediate products, blending intermediates into final products, distributing refined products from refinery to distribution centers by means like pipelines). The primary economic objective in refining is to generate maximum profit and responsiveness by sustaining high production levels in order to satisfy the demand for products while reducing costs, inventories and environmental impact.[38-40]

However, the refining industry is under immense pressure to produce eco-friendly products and facing increased volatility in the global market such as crude supply and demand fluctuations, and lower economic margins because of stiffer competitions, stricter environmental regulations on harmful gas emissions and depressed market demand.

This volatility forces refiners to make complex and agile decisions to adapt to dynamic market conditions. Therefore, optimization of the refinery operations is essential for the economic success of a refinery to maintain its competitive edge. In this situation, refinery planning and scheduling becomes a very important tool as it can utilize all potentials to extend the economic margin to its maximum level. The refinery operations comprise activities spanning across multiple departments and requiring tight coordination among them. [18,28,41]

The refinery planning and scheduling problem is usually divided into three different sub-problems. The first sub-problem is associated with unloading crude oil at the refinery's front end from crude carriers or pipelines, its transport to storage and charging tanks and the charging schedule of crude blends into the crude distillation units (CDUs). The second sub-problem focuses on the procurement of crude blendstocks into intermediate products. The third sub-problem is related to planning and scheduling of pooling problem of intermediates into final products, inventory management and lifting of final products by means like pipelines. In addition, production systems are commonly designed without considering the required utility system. Only subsequently, the utility system is designed for the given production system. This traditional optimization method for these sub-systems is a sequential hierarchical approach and can be described as rather “master and slave” than entities of equal significance. [42-48]

In reality different refinery processes are tightly interconnected and function as coherent entities involving several cross-functional coordination across enterprise functions. Therefore, most of the traditional business decision support systems have been disjoint and thus incapable of utilizing the convoluted intricacy among them and attempting to solve each part in a sequential push or pull manner may result in infeasible or suboptimal solutions.[43,45,49-51] The means for achieving optimal solutions of the refinery problem is by horizontal and vertical integration of the refinery processes and following an enterprise-wide approach through coordinated management of operational and utility departments in the refinery enterprise.[22,40,50,52] Nevertheless, there are challenges associated with this integrated approach which arise from the difficulty of modeling the entire system and obtaining a solution with reasonable quality and solution times which makes the large scale integrated model computationally intensive. The integrated model leads to a mixed-integer nonlinear programming (MINLP) problem. This complex problem contains multilinear terms for the material balances, blending process and gas emission and also highly nonlinear terms related to product yield and quality constraints. These nonconvex constrains result in inconsistency between solution quality and time and overshadows the benefits of the integrated approach.[40,45,53-55]

The refining industry began using linear programming (LP) shortly after its invention and by early 1950s, major oil companies began using LP-based production planning and scheduling models. The integration across different echelons of refining enterprise has been an area of active interest both in academic and industrial settings ever since.[56]

One of the first contributions to consider integration in refinery supply chain is that of Charnes et al. [57] They conducted a study on programming interdependent activities in an integrated oil company notably on the blending of aviation gasolines. They employed linear programming techniques to model the blending operations of aviation fuels. Ten constraints with 22 variables were developed to represent the technological and policy restrictions which were applied to a net receipts functional for optimization with respect to three aviation gasolines and a premium motor fuel. They demonstrated that intelligent planning of production, transportation, manufacturing or marketing generally requires solution of blending problems as an initial or integral part of the whole process, as it is in blending that the final outputs are determined. Catchpole [58] investigated the supply problem of an integrated oil company comprising the allocation of crude oils to refineries, the calculation of refinery programs and the transportation of finished products to the market. His problem was not simply a linear programming problem if it was described fully to contain convex and concave nonlinearities, stochastic parameters, dynamic programming and size of the problem. To simplify and reduce the size of his model, he proposed a decomposition method by reducing the amount of detail in the model and by removing those parts of the problem where the answer seems reasonably clear. The resulting Linear Programming matrix contained some 260 equations and 285 variables, and the solution time averaged about 8 hours for a complete run. He concluded the most important feature from the mathematical viewpoint was the sheer size of the integrated problem and the solution of the integrated supply problem in detail would depend on developments in the fields of faster computers and computational algorithms. Jackson [59] examined two aspects in the design of integrated refineries for consistency with the basic design objective: reliable production consistent with low initial and operating costs. He presented an integral approach to optimization of energy consumption which first considers integration through mechanical, utility, and heat linkages, then suggests review of the operating problems resulting from integration. He demonstrated the advantage of the integrated approach over a typical series of sequential steps and utilized the technical and operating factors in determining the most suitable degree of integration for widely differing refining situations.

As an another example of successful application of mathematical programming in integrating activities across a refinery supply chain, Klingman et al. [61] proposed a model to address the short-term planning and operational issues associated with the supply, distribution, and marketing of refinery products. They developed an innovative optimization package named SDM (Supply Distribution Marketing) which integrates the company's key economic and physical supply, distribution and marketing characteristics over a short term (11 week) planning horizon. The system is used to support top management decisions concerning refinery run levels, where to sell products and what prices to charge (by location and line-of-business), how much product to hold in inventory, how much product to ship by each mode of transportation and the critical timing considerations associated with all of these decisions. A network modeling framework adopted to develop, implement, and use the integrated model of their business decision variables. They implemented this system at Citgo Petroleum Corporation and reported successful results including a reduction in product inventories, working capital costs and an addition to bottom line profits. They attributed the success of their system to factors such as improved communication between the supply, distribution, marketing, and refining groups; elimination of unnecessary terminals and added insights into pricing strategies.

Up to this point all proposed models were linear or linearized versions of the equations in its linear programing planning models where the model nonlinearities were relaxed. Unfortunately, plans from these planning LP's often had limited relevance to the blender's problems. Accurate modeling of nonlinear properties such as octane and boiling points was very important. The approximations and averages which were satisfactory for planning purposes were not acceptable to the blender. This left a gap between planning and scheduling, a serious management problem. Moreover, neither of the previous authors had taken the importance of blending operation into consideration. In an attempt to account for these blend nonlinearities and integrate blending operation with other refining activities to achieve the highest profit, Ramsey and Truesdale [62] introduced a new approach. They investigated the integration of the blending support system with the upstream functions of scheduling and planning in addition to using this system in a real-time, in relationship with the downstream functions of control and reporting. The objective was to look weeks or months into the future and, based on expected unit performance, crude availability, and product demands, and come up with a plan for operating the refining facility. The net result was to place production targets in the hands of the scheduler. Their proposed tool, Omega system, was a gasoline blending system utilizing a nonlinear programing algorithm, an on-line data base, and an interactive user interface. It used a successive linear programing optimizer whose speed and reliability were its principal problems.The system was also enhanced with a menu-driven user interface, and it has been implemented on personal computers as well as on mainframes. They implemented their model at Texaco Refining and Marketing Inc. refineries and claimed the positive contribution of their system to overall profitability of the refineries. However, a mere comparison of earnings before and after the implementation of Omega was not enough to draw a conclusion because too many other factors such as market demand, profit margins, and even changes in refining equipment would affect refinery performance. In a different approach with a different objective in integration of activities, Munasinghe [60] studied the integration of electricity and oil subsector investment planning and pricing within the framework of an energy master plan that determines energy policy, ranging from short-run supply/demand management to long- run planning with contradictory goals. He analyzed important interactions between and activities within different energy subsectors using shadow prices essentially within a partial equilibrium framework technique. He proposed a two stage strategy to drive energy pricing structures. First, the shadow-priced margined opportunity cost (MOC) of a given form of energy is determined. Next, demand-side effects including distortions in the prices of substitute fuels, are used to derive from the MOC, the strictly efficient energy price level. In the second stage of the pricing procedure, the efficient price further adjusted to yield a realistic pricing structure that meets social subsidy considerations, the need to change prices gradually and simplicity of price structure for metering and billing. He demonstrated with rising energy costs, changes in relative fuel price and substitution possibilities, the advantages of an integrated energy policy have become evident.

Beginning of the 21st century witnessed a spike in the literature in the context of integration of supply chain echelons. In particular, the context of integration among refinery sub-systems has enjoyed extensive attention from both industry and academia ever since. There was a clear need for modern decision support systems in an enterprise wide level where the process and business policy decisions could be integrated . To address these demands, Julka et al. [45] addressed a need for a decision support system to make decisions at the enterprise level by developing an agent based decision support system for refinery supply chain management where software agents imitate the sub-divisions of the refinery which is divided into three sub-processes of crude selection and purchase, crude delivery and storage, and crude refining . This agent-based supply chain modeling framework called PRISMS (The Petroleum Refinery Integrated Supply Chain Modeler and Simulator) was a modeling-simulation- scheme which provided an environment where all business processes could be emulated in an integrated manner. Various supply chain scenarios can be configured; simulated and analyzed. PRISMS could model a refinery with procurement, sales, logistics, storage and operations departments. Their system could be used to study the effects of internal policies of a refinery by comparing different business policies under a variety of business scenarios in order to identify the ones suitable for actual implementation in the enterprise. Their enterprise-wide model demonstrated a better ability to lower inventory levels and enhanced the refinery's inability to handle demand fluctuation by increasing the storage capacity in the tank farm. With ever increasing need to include further activities within an integrated decision support system, scheduling of product distribution was at the spotlight. In this direction, Chen [63] highlighted the importance of integrating production and distribution operations and planning and scheduling. He reviewed the integrated models that explicitly involve both production and distribution decisions at the tactical and operational levels and classified existing explicit production-distribution (EPD) models into five categories according to level of decisions, structure of production-distribution integration, and problem parameters. He suggested the following topics deserve more research: EPD models with stochastic demand, EPD models at the detailed scheduling level, Value of coordination , Mechanisms for coordination, Fast and robust solution algorithms, a more general model to address multiple products competing for limited production capacity and a nonlinear transportation cost structure, more general problems with a dynamic demand rate and eventually to consider vehicle routing decisions as part of the problem. Up to this point, the optimisation based formulations for short-term refinery scheduling in literature were few and those existing ones, did not incorporate the model complexity of the entire unloading, blending and distillation process. In addition, there was a difficulty in understanding the rationale underlying the solutions proposed by a “black box" mathematical programming model, in contrast to a simulation-based decision support approach. To address this problem, Chryssolouris et al. [64] addressed the scheduling of a refinery activities in addition to the arrangement of the temperature cut-points for each distillation unit. They described a simulation-based approach to the refinery operation, which is modelled based on the assumption that the refinery facility model, the operation constraints, quantities and crude oil volume fractions for each tank as well as crude oil types properties in addition to the quality and quantity range specifications of the end products are defined in advance. During the solution process, every node is simulated and for each node, the simulation mechanism takes the values of the decision variables of the node, utilizing a set of material balance and crude oil evaporation–temperature equations. Material balance is modelled by a set of differential equations assuming instantaneous uniform mixing in tanks and streams. The implemented system generates, simulates and evaluates alternative sets of actions and at the end, it proposes the best alternative found for the vessels unloading schedule, the crude oil transfer, blending and charging schedule, as well as the determination of the temperature cut points of each CDU. Their approach, may accelerate the scheduling process by increasing the accuracy of computations and allowing the investigation of what-if scenarios However, due to the entire process complexity and the stochastic disturbances in the production level, their model was not completely accurate and suggested taking advantage of mathematical programming techniques or rule based models to improve the performance of their approach. Grossmann [2] provided an overview of enterprise-wide optimization (EWO) as an emerging area that involves optimizing the operations of supply, production and distribution of a company to reduce costs and inventories. He noted a major focus in EWO is the optimal operation of production facilities, which often requires the use of nonlinear process models. He highlighted the integration of the information and the decision-making among the various functions as one of the key elements of EWO. He further emphasized on modern IT tools as emerging tools to develop deterministic and stochastic optimization models and algorithms to explore alternatives of the supply chain to obtain optimum economic performance and higher levels of customer satisfaction. Previous research in the field mostly assumed no limitations on refinery feedstock availability and mainly modeled refinery problem through continuous models where binary decision variables were not included. To rectify these issues, Al-Qahtani and Elkamel [52, 65] addressed the design and analysis of multisite integration and coordination strategies within a network of petroleum refineries and petrochemical complexes. Their objective was to develop a simultaneous methodology for designing a process integration network between petroleum refining and the petrochemical industry. The refinery and petrochemical systems were modeled as a mixed integer linear programming (MILP) problem that leads to an overall refinery and petrochemical process production levels and details blending levels at each refinery site. The objective function was a minimization of the annualized cost over a given time horizon. Expansion requirements to improve production flexibility and reliability in the refineries were also considered. Their study showed that the optimization of the downstream petrochemical industry has an impact on the multi refinery network integration and coordination strategies and emphasized the importance of developed methodology. However, all parameters were assumed to be known with certainty and did not account for the situation of fluctuating crude oil prices, changes in demand, and the direct effect this can have on the downstream petrochemical system underlines the importance of considering uncertainties. Therefore acknowledging the shortcomings of their deterministic models they concluded the importance of the consideration of uncertainties in the integration problem. Despite the popularity and the rationale of the integration as a concept so far, few authors had attempted to quantify and compare the effectiveness of the integration over solving the problem through a sequential hierarchical approach. The demonstrate this effectiveness, Guyonnet et al. [51] explored the merits of the integration of the refinery production planning with the crude oil uploading and product distribution problems. They considered a marine access refinery with only one set of tanks that are storage and charging tanks at the same time, and the crude distillation charging plan. Crude oil is transported by large tankers to the refinery's front end where crude oil is unloaded into crude storage tanks at a docking station. For the production planning, they assumed a linear fixed yield scheme for all refinery units without considering the nonlinearity of the processing units. For the product distribution, they neglected the product transportation from the refinery to distribution center which is mainly implemented through pipelines. Nevertheless, they modeled the product distribution from depots to the consumer markets which in turn they modeled through a truck transportation system without taking the potential routing problem into consideration. They presented a mixed integer nonlinear programming model (MINLP) where the mix in the storage tanks constraints the feed to the refinery. The schedule of parcel arrivals as well as production requirement and initial inventory level at the docking station are known a priori. They modeled this MINLP problem in GAMS [131] and used solver DICOPT [90] to solve it. They established that integrating the different divisions of the refinery supply chain achieves better results than solving each part in a sequential push or pull manner. Refineries develop purchasing plans that are based on market predictions for crude oil in order to maximize profits. When executing a plan, they are exposed to financial risks due to the fluctuations in crude oil prices during the period between purchase and payment. One way of lowering the financial risk related to crude oil purchases is to establish a portfolio of different types of contracts such as long-term, spot, and futures contracts. To account for these fluctuations through the contracts, Park et al. [66] developed an integrated model based on two-stage stochastic programming for operational planning and financial risk management of a refinery. They selected downside risk as the objective function to be minimized. Subsequently, they optimized the contract sizes and the operational plan according to their developed model and the price scenarios. They established that financial risk can be substantially minimized by diversifying suppliers with spot contracts and cross-hedging with future contracts and concluded their model is beneficial in aiding refineries with decision-making on operational and financial strategies. Traditionally, the management of industrial units such as refining industry was carried out in sequential steps: scheduling of the manufacturing unit first, subsequently estimating and designing the utility system to accommodate for this manufacturing unit. This master-slave treatment of the production facilities at the expense of utility system could lead to infeasible or suboptimal solutions. To address this problem, Agha et al. [67] investigated the integration of production and utility systems in process industries. They discussed the traditional management of industrial units in three sequential steps: scheduling of the production unit by minimizing inventory, estimating the utility needs of production unit and eventually operation planning of the utility system. They developed a multi period mixed integer linear programming (MILP) model to compare traditional and integrated approaches and indicated that the integrated approach results in significant reduction in energy costs while minimizing the emissions of harmful gases. As discussed earlier, crude-oil blending is a common practice to obtain qualified mixing oils for refinery processing at low costs. The blending component crudes are subject to inventory constraints, which in turn are dynamically affected by the refinery purchase plan including the crude-oil types, amounts, and delivery over a planned period of time. As the crude-oil price and availability constantly changes in a volatile market, the crude-oil blending and purchase planning should be coordinated and simultaneously optimized to maximize the potential profitability of a refinery plant. This becomes even more important when the uncertainty of crude-oil delivery time is also taken into account. In this direction, Zhang et al. [68] addressed the integration of crude oil blending subject to inventory constraints and purchase planning including the crude oil types, amounts, and delivery with delivery uncertainty consideration to account for the crude oil price and availability changes in a volatile market. They developed inventory-related flexibility indices to characterize the ability of a refinery for handling the uncertainty of crude-oil delivery delays. They modeled these simultaneous refining activities through a general MINLP model. Their research disclosed in-depth relations between the production flexibility and the plant profit. They demonstrated the efficacy of the developed methodology by industrial case studies. In general, it is very challenging for an oil refinery to make integrated decisions encompassing multiple functions based on a traditional Decision Support System (DSS), given the complexity and interactions of various decisions. To overcome this limitation, Hu et al. [69] proposed an integrated Decision Support System (DSS) by combining both business and engineering systems with an operator–computer interface. Under their proposed DSS, the decision maker would decide on the values of a subset of decision variables. These values, or the first-stage decision, are forwarded through the dashboard to the DSS. For the given set of first-stage decision variables, a multi-objective robust optimization problem, based on an integrated business and engineering simulation model, was solved to obtain the values for a set of second-stage decision variables. The business model was simulated using the agent-based software NetLogo [49]. The business model characterizes the crude oil and end-product markets by simulating oil refinery supply and the customer demand. In the case study, the engineering and business simulations are connected through an interface program used to run both simulations programmatically and exchange information between Netlogo and Aspen HYSYS[73]. They used a small case study to show the decision support role of dashboard and how it can be used to coordinate across various departments in decision making. It was observed that a maximum simulated profit can be achieved in the two case study scenarios. However, as the size of the business and engineering models grows, the proposed optimization based framework could have some computational difficulties and issues. With the environmental challenges facing the global industry in particular refineries, new CO_2 legislation forces the petroleum refining industry to review its operations and processes to cope with the new limitations of allowable CO_2 emissions. Simultaneously, petroleum refineries, face another challenge represented by clean fuel products (low sulfur content) regulations. In an attempt to provide operational solutions to these issues, Alhajri et al. [70] presented an integrated refinery model that simultaneously solves the refinery planning, hydrogen and CO_2 management problems to cope with the strict environmental regulations facing the refining industry. Their overall model was formulated as a mixed integer nonlinear program (MINLP) and was evaluated through different case studies. In the CO_2 management model, they considered three different mitigation alternatives for CO_2 emission reduction: Load balancing or shifting by adjustment of production throughput to reduce CO_2 emissions, Fuel switching, which reduces the CO_2 emissions by switching from one type of fuel to another cleaner one, Capture technology, which considers installation of a capture process to reach high levels of CO_2 reduction. They demonstrated results indicating that the integrated model leads to better profit margins and that successful CO_2 mitigation options to meet a given reduction target. Their obtained results also showed that the load shifting and fuel switching options can contribute up to a 23% reduction of CO_2 emissions. To achieve greater than 30% reductions, the results required a CO_2 capture technology must be employed in the petroleum refining industry.

They suggested that the load shifting and fuel switching options contributes mainly to this reduction. Beside CO_2 emissions, other air emissions such as NO_2, when exist in large amounts, could cause different types of serious diseases and illnesses. This prompted Al-Rowaili et al. [72] to discuss simultaneous profit maximization and maintaining a desired final products quality and minimum NO_2 emissions from the oil refinery. Their study aimed for the cost/profit analysis of an oil refinery with the inclusion of visbreaking unit for its high economic power and to identify strategies to reduce NO_2 emissions from oil refineries while maintaining profit at maximum possible level using mathematical programming approach. They proposed three methods for NO_2 reduction : balancing, fuel switching and use of technology for NO_2 reduction. Their proposed MINLP models were validated through a case study and represented a contribution in maximizing profits, maintaining good quality products and reducing NO_2 emissions. As discussed, rising energy prices and stricter limitations on greenhouse gas emissions have also led to greater attention on energy savings. The configuration of process units in a total refining site has a great impact on both material and energy requirements. The simultaneous optimization of materials and energy is highly important for an enterprise. Hence, Zhang et al. [22] discussed the simultaneous optimization of materials and energy balance in an oil refinery and proposed material and energy integration for a total refining site to minimize costs. They developed an MINLP model comprising production planning for materials, energy requirements of process units based on pinch analysis, operational planning and balance for utility systems. Their mathematical model was an MINLP problem with the nonlinear formulations including exponential terms. Through an industrial example, they conducted a comparison between the simultaneous and sequential optimization methods for materials and energy in a total refining site. Their study demonstrated some major conclusions: Firstly, simultaneous optimization of materials and energy can obtain higher profit than sequential optimization can. Secondly, the sequential optimization of materials and energy preferentially produces higher value products to maximize the material profit without considering the energy cost, while simultaneous optimization makes a careful trade-off between the material profit and energy cost in process units and utility systems. Finally, the quantity and level of steam produced or consumed in process units should be coordinated with the throughputs and product distributions of process units, as well as the configuration of the utility system, to achieve maximum total profit. They stated maximizing steam production in process units is not always effective from the view of the total site. When the material balances of the intermediate products between the two complex processes such as upstream refinery and downstream petrochemical plant are considered, the potential of increasing the overall margin can be explored. Zhao et al. [53] proposed an integrated optimization approach to couple the refinery and its down-stream ethylene plant. A mixed-integer nonlinear programming (MINLP) model was formulated to optimize the production planning of the processing units in the refinery and the ethylene plant simultaneously. Due to the model complexity, they applied a Lagrangian algorithm to decompose the integrated mathematical model into an MILP problem for the refinery and a small-scale MINLP problem for the ethylene plant. They investigated performance of the their approach on industrial case studies and illustrated the economic advantage in the enterprise-wide network in terms of improvement in overall profit over the sequential approach. The integration specifically addressed intermediate material transfer between processing units at each site. Their study drew two conclusions: Firstly, integrating the two networks can obtain higher profit than the original optimization that the two systems are modeled separately and optimized sequentially. The optimization of intermediate steams that correlates the upstream refinery with the down-steam ethylene plant has expanded the space for profit enhancement, which is especially critical for the overall products production because of the increasing price of raw material. Secondly, the original optimization of either refinery or the ethylene plant preferentially produces higher value products to maximize the material profit without considering the intermediate production utilization in other system, while the proposed optimization model presents a balance between the refining products and chemical products production. In addition to some sources of uncertainty and volatility discussed earlier such as oil sources scarcity, and price variability, the oil supply chain is facing other challenges due to emerging issues such as new alternative energy sources with high impact on demand and production and profit margins reduction. Additionally, the existence of large, complex and world wide spread businesses implies a complex system to be managed where distribution can be seen as one of the key areas that needs to be efficiently and effectively managed. Different types of distribution modes characterize the oil supply chain where the pipeline mode is one of the most complex to operate when having multiproduct characteristics. Relvas et al. [71] addressed the these challenges of the planning for a petroleum derivatives transportation system employing a multiproduct pipeline that connects a refinery to a storage tank farm. They developed two alternative MILP models with the aim of fulfilling costumers' demands while minimizing the medium flow rate. Their model integrates the inventory management in the final solution to represent the real world synergies between tank farm product needs and pipeline operation. The major strengths of their proposed approach are the possibility of obtaining medium term solutions for a complex problem faced by many companies in the oil sector, without conditioning the solution through decomposition approaches and avoiding the need to run the model several times so as to determine a number of feasible time intervals or number of pumping batches. However, their proposed models have to be tested under other system settings, to conclude on model robustness and also more operational details should be included in the present formulation, such as inventory management on tanks rather than using aggregated capacity. In addition, the model should be improved to address planned or unforeseen pipeline stoppages, interfaces or electricity costs and the settling period representation. Usually, in a refinery both oil acquisition and product selling are predefined by the organization. Therefore, a minimum and a maximum market for a product, and the volume of oil acquired are usually predefined in order to meet the organization expectations. The refineries must check the feasibility of this planning, and in case of adversities (lack of supply, broken equipment, etc.), it must match to the new reality. The volume of each oil type acquired is the most important information, since it will affect the entire refining system. To take these parameters into consideration, Sales et al. [74] presented the integration of optimization and simulation of refinery units to obtain a production planning to maximize profit, account for external loads, product pricing, blending and achieve global optimum solution in small computational times. Their refinery under study contains four units: Distillation (CDU), Delayed Coking (DCU), Hydrotreatment (HDT), and Fluid Catalytic Cracking (FCC). The distillation separates crude oil into eight intermediates whose external loads were added in the system. The objective function maximizes the profit of the refinery subject to 35 operational and capacity constraints. They utilized sensitivity analysis and the determination of break-even points (BEP) of external loads to bolster the refinery planning and the resultant profit. Their sensitivity analyses showed that any variation in the produced volumes of fuel oil export grade can strongly influence the refinery profit, and the production of petrochemical naphtha is bad at any produced volume. This type of analysis demonstrated that capacity bottlenecks or undesirable products for any refinery and any product is enabling the planners to look for unseen potential improvements and problems. Siwi et al. [75] developed a multi-objective multi-period MINLP model for optimal strategic planning of entire petroleum and petrochemical supply chain (PPSC) to support decision making for petroleum and petrochemical industries. Nonlinear behavior of the oil reservoir was considered for accurate prediction of crude production. The environmental impact based on Eco-indicator 99 was introduced as an objective function in addition to economic performance. They demonstrated the capability of their proposed model and solution approach through an industrial scale example and provided results illustrating the effect of considering environmental impact on the operation of PPSC. Utomo et el. [76] developed an optimization framework for simultaneous consideration of production and utility systems during production planning. Their model makes use of crude cocktail rather than a single crude in the production process. They demonstrated the solutions obtained by the integrated model with crude cocktail results in higher profit than that obtained by the single crude model and the sequential model. Leenders et al. [42] proposed a method for the optimal design of integrated batch production and utility systems , which covers decisions on the system structure, component sizing and scheduling of both production and utility system. Their method integrates superstructure MILP models of a utility and a production system. Through two case studies, they demonstrated that simultaneous design and scheduling of the integrated system is beneficial and shown to reduce cost and increase profit. In addition, their analysis indicates that their proposed method is even more beneficial for industry sectors with high share of energy costs. Assis et al. [77] contributed to the literature by developing a model for the management of crude oil supply at the operational level, incorporating elements of maritime inventory routing and crude oil scheduling .To tackle this problem, they proposed a discrete time MINLP formulation to be solved by an iterative

MILP-NLP decomposition, which relies on domain reduction, bivariate piecewise McCormick envelopes to yield the MILP relaxation, and a NLP solver to reach feasible solutions.

They suggested their strategy might not be effective for large scale problems and suggested two strategies to handle large instances: First, Lagrangian decomposition to decompose the large scale problem to smaller sub-problems. Second, Clustering strategy which consists in organizing groups of platforms and storage tanks in clusters, so that crudes are transferred from platforms to storage tanks that belong to the same cluster. Besides reducing the number of routes for vessels, clustering can be done in such a way to minimize the mixing of crudes in storage tanks. Their strategy was able to find small gap solutions on small and medium size instances and found good feasible solutions for the larger instance within a reasonable CPU time. Intuitively, one of the main goals of any process industry, which is to generate maximum revenues at low costs by maintaining high production levels in order to satisfy the demand for products. Integration of activities serves as an exceptional tool for achieving this is by following a plant-wide approach. One of the activities to be integrated within the refining industry and has not been discussed to this end is the maintenance tasks in the overall process system. Kopanos et al. [39] presented a rolling horizon optimization framework for the integrated planning of utility and production system under uncertainty. They proposed a linear MILP model for the integrated planning problem which follows a rolling horizon modeling representation in order to readily deal with various types of uncertainty, such as fluctuations on the demand for final products, unit breakdowns, variations of cost terms, or data inaccuracies. In brief, in the rolling horizon scheme, a planning problem is solved for a certain length of time horizon (i.e., prediction horizon), and then the solution for a part of that time horizon (i.e., control horizon) is executed. After each iteration, a new planning problem is solved by moving forward the time horizon by the length of the control horizon considered. The optimization goal is to minimize the total cost of the production and the utility system. They demonstrated through a couple of instances that their integrated approach can yield significantly better solutions over sequential approaches in terms of total costs, extra energy consumption, and cleaning and startup/shutdown operations. They associated the significant reduction in total costs to the enhanced energy efficiency of the entire system through the optimized consumption of energy . They also indicated that unnecessary purchases of resources can be avoided by their proposed approach. They concluded it is essential to consider condition-based maintenance policies for the equipment of a process plant to increase its overall energy efficiency, operability and stability. They claimed their integrated approach can result in a cleaner production which in turn could lead to more sustainable production practices.

All of the surveyed literature mentioned above are outstanding contributions to the field of integration in refinery supply chain management and have deepened our knowledge and understanding of interaction and interconnection among cohesive but apparently separate refinery sub-systems. However, there is still a need to broaden the scope of integration and include more refinery supply chain echelons within the integrated model even though at the expense of more computational intensity. Most of the literature surveyed so far do not include all major refinery sub-systems within their integrated model and therefore present a partial integration of refining enterprise activities. The other main issue is the highly nonlinear nature of the refinery processing units which needs to be accounted within the integrated model while most of the literature mentioned thus far do not consider the inherent nonlinearity of refinery processes within the refinery production model. Lastly, the corresponding MINLP model for the integrated refinery problem is nonlinear and nonconvex due to the presence of bilinear or quadratic, signomial, exponential or logarithmic terms in the material balance, blending, product yield and quality constraints, and consequently the standard methods for solving this integrated refinery problem may fail to converge to a feasible solution or lead to sub-optimal solutions. Therefore, standard optimization heuristics are not suitable if the global optimum is desired and most of the literature dealing with integrated models mentioned so far, do not guarantee the global optimality.

1.3. Uncertainty in the Oil Industry

The next topic investigated in this research is uncertainty. Real-world system designs encounter different types of uncertainties which are usually beyond the direct control of the designer:

(A) Type I variations: Changing environmental and operating conditions such as operating temperature, pressure, humidity, changing material properties.

(B) Type II variations: Production tolerances and actuator imprecision. To avoid expensive high precision machinery, the design parameters of a product is only realized to a certain degree of accuracy.[78-79]

(C) Model Errors: Uncertainties in the system output due to imprecision in the evaluation of the system output and the system performance. This kind of uncertainty includes measuring errors and all kinds of approximation errors due to the use of models instead of the real physical objects.

(D) Feasibility Uncertainties: Uncertainties concerning the fulfillment of constraints the design variables must obey.[78]

There are different possibilities to quantify the uncertainties classified under (A)–(D) mathematically. Basically, the uncertainties can be modeled deterministically, probabilistically, or possibilistically: (1) the deterministic type defines parameter domains in which the parameter uncertainties can vary, (2) the probabilistic type defines probability measures describing the likelihood by which a certain event occurs, and (3) the possibilistic type defines fuzzy measures describing the possibility or membership grade by which a certain event can be plausible or believable.[78,80]

In some disciplines, an epistemological classification perspective of uncertainties are used differentiating the uncertainties into objective and subjective ones. Objective uncertainties, also called aleatory [81] or random uncertainties, are of intrinsically irreducible stochastic nature. That is, these kinds of uncertainties are of physical nature, e.g., humidity, temperature, material parameters (stiffness, conductivity etc.). These uncertainties cannot be removed and due to the probabilistic nature, probability distributions are the adequate means for the mathematical description of these uncertainties.[78,82]

In contrast to the objective character of aleatory uncertainties, epistemic uncertainties reflect the lack of knowledge a designer has about the problem of interest. This kind of uncertainty is regarded as subjective, because it is due to a lack of information that could, in principle, be reduced by increased efforts. Epistemic uncertainties include uncertainties about the model used to describe the reality, its boundary and operation conditions, also referred to as model form errors, and also the errors introduced by the numerical solution methods used (e.g., discretization error, approximation error, convergence problems). Such uncertainties can be modeled by type (1) and (3) techniques.[78,83]

From a process operations point-of-view, uncertainties can be classified as external (exogenous) uncertainties and internal (endogenous) uncertainties. As the name suggests, external uncertainties are exerted by outside factors that impact the process. The decisions at each stage are independent of the decisions taken in previous periods. On the other hand, internal uncertainties arise from deficiencies in the complete knowledge of the process. The decisions at each stage depend on decisions taken in previous periods.[84-86]

Uncertainty in chemical processes can notably result from the following probable sources: [87,88]

(1) Model inadequacy comes from nonideal conditions of all modeling procedures, such as doubt in input variables and inadequate data. This type of uncertainty source exists because of an approximation of the reality and also referred to as structural uncertainty or model bias.

(2) Observation error or experimental uncertainty is a typical uncertainty source, especially when a calibration problem occurs.

(3) Parameter uncertainty exists because known parameters within the model can be considered as potential sources of uncertainty. For instance, material properties can be probable sources of parameter uncertainty in the chemical processing field.

(4) Algorithmic uncertainty comes from numerical approximations implemented in the computer model (discretization such as finite difference, finite element). This is also known as numerical or discrete uncertainty.

The oil industry is subject to uncertainties such as unpredictable product demand, unstable market prices, fluctuations in oil supply, operational breakdowns, variations of contract and cost terms or model and data inaccuracies. [39,84,89]

Uncertainty becomes an even more critical factor in the decision making processes as the span of the planning horizon expands and if not taken into account, could lead to unfeasible or suboptimal designs. To account for uncertainty in strategic planning for the process and notably oil industry, numerous modeling schemes have been reported in the literature. Among these methods, the most common approaches to deal with uncertainty have been two-stage stochastic programming [91], robust programming [92-94], and fuzzy possibilistic programming. [95-97]

One of the uncertain and unsolved problems in the actual oil products supply chain systems is how to organize efficient, reliable and cost effective transportation from the refineries to main consumer markets over the distance of several thousands of miles. Transportation network is crucial to the whole logistic process. Unreasonable design of transportation structure will not only greatly increase logistics fees , but also reduce the ability to adapt the possible risk and fluctuation of supply chain systems . Therefore, selecting transportation modes and the optimal construction of transportation structure are of great significance in supply chain systems construction . Meanwhile, depots in hub cities are faced with various problems, such as utilization inefficiency and weak regulating ability. The inappropriate design of depots capacity will dissatisfy the requirements for steady operation in the complex system, and even cause unexpected production shutdown. To address this type of uncertainty, Zhang et al.[91] studied the reliable design of oil products supply chain system with hub disruption through a stochastic linear programming approach. To account for uncertainties, they adopted Monte Carlo sampling to create random instances according to probability distribution of uncertain parameters in transportation process of oil products, the stochastic hub disruption and the demand uncertainty. They proposed a multi-scenario MILP model coupled with Monte Carlo sampling for the reliable design of oil products supply chain system. To consider the unavoidable depot faults in practice, they discussed allocation level and successful service probability for non-hub city. On the basis of above factors, their proposed model accounted for uncertain factors such as demand and depot failure probability. They adopted the scenario based robust optimization approach to solve out the most reasonable design which is applicable to each specified scenario. The objective function was the minimum total cost, including depreciation cost of initial investment, infrastructure investment and operation cost. Infrastructure investment refers to the depreciation cost of hub city infrastructure, pipeline, and depots. Under the constraints of transportation modes, allocation level, depot construction, their model was established and solved by the scenario based robust optimization approach. A real case was presented to illustrate the application of their proposed model. The results indicated that the total cost involving uncertainties is relatively higher than that without any uncertainties. The refineries may also fail to supply oil products to downstream depots under uncertain conditions, which will affect the infrastructure construction plan and transportation scheme of supply chain system. Although the robust optimization formulation can be used to model uncertainty in a wide variety of MILP problems, there are some limitations of the proposed approach. For instance, some of the probability distribution functions are only applicable to constraints that contain a single uncertain parameter (i.e., uniform, binomial, Poisson). This is due to limits in probability theory and not the proposed formulation. Also, the robust optimization formulation cannot address dependent uncertain parameters which are related through general nonlinear expressions, but it is applicable to linearly dependent uncertain parameters. In this line, Janak et al.[92] considered robust optimization methodology for the problem of scheduling under uncertainty where the uncertain problem parameters had a known probability distribution function. They used a min–max formulation and applied it to mixed-integer linear programming (MILP) problems to produce "robust counterparts" and solutions that are immune against data uncertainty. They accounted for uncertainty in the coefficients of both the objective function, as well as the coefficients and right-hand-side parameters of the inequality constraints.

Verderame and Floudas [93] investigated the operational planning of a large-scale multiproduct and multipurpose industrial batch plant with demand uncertainty due to the length of the time horizon. They also developed a robust operational planning model to address the objective of providing a reliable daily production profile which is immune to various forms of demand uncertainty. Recently, Dai et al.[94] proposed a data-driven robust optimization (DDRO) scheme for crude oil blending under uncertainty caused by oil properties. The information about property uncertainty during blending process was effectively extracted and the optimization robustness was improved using historical data of blending effect to construct the data-driven uncertainty set. A data-driven robust model was built on the basis of this set to optimize crude oil blending under property uncertainty. The uncertainty of sulfur content during the blending process was merely considered to simplify the introduction. They used a dual transformation to convert the problem into an LP model to solve the DDRO model. They extracted uncertainties of oil components from production data by recursive least squares method by utilizing the blending effect model. Then, they constructed the uncertainty set by combining principle component analysis and robust kernel density estimation according to the historical data of blending effects. Eventually, they developed a robust model for recipe optimization of crude oil blending by using the obtained uncertainty set. The demonstrated the applicability of the proposed DDRO model by a real-world production case study of crude oil blending system. Their results claimed that the proposed method increases the robustness of solutions and protects CDUs effectively by using uncertainty data. They concluded the sulfur content of mixed oil in the worst condition with this method is still in the safe range. They balanced the level of conservatism and robustness of the proposed DDRO model by robustness parameters. Robust optimization algorithms are useful when the probability distributions of the uncertain parameters are available. In the absence of these distributions, fuzzy logic programming schemes become handy. Liu and Sahinidis [95,96] presented application of fuzzy programming in process planning. They considered the long-range planning problem for a chemical process involving a network of chemical processes that are interconnected by raw materials, intermediates and products that may be purchased from and/or sold to different markets. The main decision problem was the selection of processes from among competing technologies and the subsequent timing of process expansions. Also important was to determine the optimal production levels for the installed processes. The decision maker is to maximize the net present value (NPV) of the project over a long range horizon consisting of a finite number of time periods during which prices and demands of chemicals, and investment and operating costs of the processes can vary. Using fuzzy programming techniques, the process planning problem with uncertain parameters and soft constraints was transformed into an MINLP problem by introducing a new variable indicating the degree of satisfaction of constraints and goals. Uncertainties in material availabilities and product demands, material costs, product prices, and process yields were considered. A global optimization algorithm based on the branch-and-bound algorithm was adopted to solve this MINLP problem. For this nonconvex minimization problem, this algorithm was used in order to develop lower and upper bounds of the optimal objective function value. As the algorithm progressed , these techniques yield increasingly tighter lower and upper bounds of the subproblems solved in the course of the branch-and-bound search. Through illustrative examples they demonstrated the usefulness of their models. They claimed their solutions obtained from the fuzzy models were capable of handling a larger range of the uncertain parameters than the deterministic solution.

Fuzzy programming by using fuzzy logic represents the truth of the uncertainty values. Although the choice of parameter values in fuzzy logic is often quite subjective and depends on the user's preference, it reduces the computational burden significantly and is suitable for the uncertainty that lacks information. For instance, when parameters such as conversion rate or capital cost for integration are hard to obtain due to the immaturity of the technologies such as biorefineries. As an example of such instances, Tong et al.[97] addressed the optimal design of an advanced hydrocarbon biofuel supply chain integrated with existing petroleum refineries under various types of uncertainties. They proposed a multiperiod mixed-integer linear programming model to take account of main characters of advanced hydrocarbon biofuel supply chain, such as integration with petroleum refineries, "drop in" fuels blending with crude derivatives, and use of pipelines to distribute products. They considered biomass availability, product demand, conversion rate and corresponding cost for insertion points in the petroleum refinery as the fuzzy numbers in their model. Possibility, necessity and credibility measures were introduced and applied in the possibilistic programming. Their computational results demonstrated that the model size increases slightly as there are uncertain parameters in the objective function. In their possibility model, the capital cost and production costs tend to be lower, which results in more production in the petroleum refineries. However, in the necessity model, the cost is relatively high and it tends to reduce production in the petroleum refineries. Their credibility model is a tradeoff between their possibility model and necessity model.

Despite the popularity of uncertainty quantification and assessment for the oil refining industry in the academic research, to the best of our knowledge few to none have focused on the strategic enterprise-wide planning of an integrated oil supply including all major refinery supply chain echelons. The other issue is the operating variables or the process severity within the refinery units and inherent nonlinearity of the refinery processing units which needs to be accounted within the stochastic planning model as any uncertainty for instance in demand data will affect all refinery sub-subsystem processes who are interconnected and should be adjusted upon realization of the uncertain parameters. The other main issue is that the integrated stochastic refinery planning model is a nonconvex MINLP, and if the global optimum is required, most of the literature dealing with uncertainty in oil refining industry do not warrant the global optimality.

As discussed earlier, the corresponding MINLP model for the integrated refinery problem is nonlinear and nonconvex due to the presence of bilinear or quadratic relationships in the material balance, blending and product yield correlations and highly nonlinear terms such as signomial, exponential or logarithmic terms in the product quality constraints. To obtain the global optimal solutions for the enterprise-wide refinery problem, while accounting for the highly nonlinear nature of the processing units and the uncertainties in the final product demand and crude oil and final product market prices, these nonlinearity and nonconvexity must be handled through a global optimization strategy.

Most global optimization approaches for solving bilinear programs rely on the convex McCormick envelopes [98], which provide a relaxation of the original problem. The quality of the relaxation is highly dependent on the lower and upper bounds of the variables involved in the bilinear terms, improving as their domain is partitioned. This can be done iteratively, as in piecewise McCormick envelopes [99-102] or simultaneously, using spatial branch and bound frameworks [103-105] or univariate parameterization techniques [106,107].

Multiparametric disaggregation technique (MDT) [108-111] and its variant normalized multiparametric disaggregation technique (NMDT) [112-113] is a univariate parameterization technique adopted in this research which handles bilinear terms by discretizing one of the variables of the bilinear term to a specified accuracy level and will be discussed in detail in the relevant chapter. To linearize highly nonlinear terms, an aggregation scheme referred to as lumped variable linearization (LVL) technique [114-115] has been utilized in this study. In LVL, all variables within a nonlinear term in a constraint are aggregated into one lumped variable LV and the entire statement is linearized and is initialized by assigning initial values to every variable congregated within the lumped variable. This technique will also be discussed in detail in the relevant chapter(Specify the chapter).

Despite all the described complexity associated with the enterprise-wide integrated refinery planning, this study presents a novel integrated optimization approach with a multi-period mixed-integer nonlinear programming (MINLP) model for the oil refinery network to handle inherent nonlinearity of refinery processing units, integration of operations in a broad range of refinery supply chain associated with crude unloading, procurement, final product pooling and blending, inventory management, distribution by pipeline, utility system and environmental impacts, accounting for the uncertainties in the final product demand and crude oil and final product market prices and finally obtaining global optimal solutions for the enterprise-wide integrated refinery problem.

To Summarize, in this research, techno-economic studies of refinery operations have been presented to enhance the profit margin in the refinery supply chain system. Three problems have been addressed: First the nonlinear nature of refinery processing units have been accounted for and the results of the nonlinear refinery model are evaluated versus a linear fixed yield input-output model of the refinery. This will assist with optimizing product yield and final property values to meet the market demand and specifications and extend the profit margin. For the CDU, a nonlinear data-based swing-cut (SW) model and another nonlinear model based on the Geddes fractionation index (FI) have been adopted. The remaining refinery units are modeled by empirical nonlinear correlations within a refinery wide production planning problem and all are presented in Chapter 2.Second, this nonlinear production planning model is integrated with other refinery supply chain echelons such as crude unloading, product blending, utility and product distribution by pipeline. The integration of refinery sub-problems will aid a more coordinated decision making process across refinery supply chain and in turn will contribute more to optimal refinery operations and higher profit margins. The deterministic version of this integrated refinery planning problem has been investigated and compared with a sequential model of the refinery where the refinery sub-problem models are solved in a sequential manner. To solve the complex integrated refinery model which leads to a nonconvex MINLP model, an aggregation/disaggregation global optimization framework has been proposed. The aggregation scheme utilizes Lumped Variable Linearization technique (LVL) and the disaggregation scheme uses Normalized Multiparametric Disaggregation Technique (NMDT) to linearize highly nonlinear terms and bilinear terms respectively. This second problem with its proposed solution methodology and global optimization framework is outlined in Chapter 3. In the third problem, uncertainty in price and demand parameters in refining industry has been investigated. Accounting for uncertainty will help with more realistic understanding of the refinery operational outcomes in case of volatility and perturbations in demand and price parameters. This stochastic version of this integrated refinery planning problem where product demands and crude oil and product prices are subject to uncertainties, have been modeled through three uncertainty appraisal methods. These three methodologies include robust optimization algorithm , fuzzy possibilistic programming and two-stage stochastic programming with financial risk management and the results of the stochastic integrated refinery modeled by these three methods have been investigated and presented in Chapter 4. The numerical results and discussion for all three problems are presented in Chapter 5. The remainder of this treatise contains conclusions, future work, data tables and appendices.

Chapter 2

EMPIRICAL NONLINEAR MODELS OF REFINERY UNITS

2.1. Preface

In this chapter, a novel production planning strategy for refinery wide optimization is established. Two novelties are introduced: From a managerial perspective, it gives an effective tool to refinery planner to adjust the temperature distribution within the distillation unit and the process severity within the other refinery units to obtain desired cut point temperatures and maximum yield and desired property of final products which in turn results in a higher profit for a certain amount of crude feedstock. In addition, it provides a tool for a refinery planner to make advance decisions on the amount of the crude oil to be purchased to address a forecast demand in the upcoming months while meeting the demand requirements.

Three objectives are pursued in this chapter: First, a data-based nonlinear model and another nonlinear model based on Geddes fractionation index (FI) for CDU and empirical nonlinear correlations for the remaining refinery units are applied to a refinery wide production optimization including the following processes: Crude Distillation Unit (CDU), Fluid Catalytic Cracking (FCC), Catalytic Reforming (CRU), Hydrocracking (HC), Hydrotreating (HT), Hydrodesulfurization (HDS), Visbreaking (VB) and Delayed Coking (DC). The improvements in the overall profit of the refinery via the nonlinear models have been compared with a linear input-output model through thirteen case studies and substantiate the outstanding advantage of the nonlinear model utilizing a CDU model based on fractionation index (FI) over the linear input-output model and data-based nonlinear model. Second, the global optimal solutions of the refinery production problem by simply using BARON as a global optimizer are obtained. Lastly, comprehensive yield and product quality data for all intermediate and final products are calculated. The rest of this chapter is organized as follows: the problem statement is outlined in the next section and the overall refinery material balance is presented in section 3. Subsequently, the nonlinear mathematical models for the refinery units including product yield and quality equations are described in section 4. The product quality constraints in blending units are delineated in section 5. Section 6 defines the total profit objective function. Section 7 describes a linear input-output model as a reference of comparison to demonstrate the effectiveness of the current nonlinear unit models. The numerical results and discussion are presented in chapter 6.

2.2. Problem Statement

Figure 2.1 demonstrates a simplified representation of the refinery processes in this study. For simplicity, refinery gas, fuel gas and LPG are not presented in the outlet streams of the units as the focus of this study has only been on the four major final products. The set *fpr = {G,JF,DF,FO}* is the set of major final products where G,JF,DF and FO represent gasoline, jet fuel, diesel fuel and fuel oil respectively. The set *U = {CDU, CRU, FCC, HC, HT,HDS,VB, DC, BU, ctank, ptank} i*s the set of refinery units where CDU, CRU, FCC, HC, HT,HDS,VB and DC represent crude distillation unit, catalytic reforming, fluid catalytic cracking, hydrocracking, hydrotreating, hydrodesulfurization, visbreaking and delayed coking units respectively and are the operating units of the refinery. The crude distillation unit comprises both atmospheric and vacuum distillation sections. From the set of operating units, there is only one unit for each category except for HT and HDS: HT includes two separate hydrotreaters HT1 and HT2 for the straight run light naphtha and middle distillate respectively. HDS includes three separate

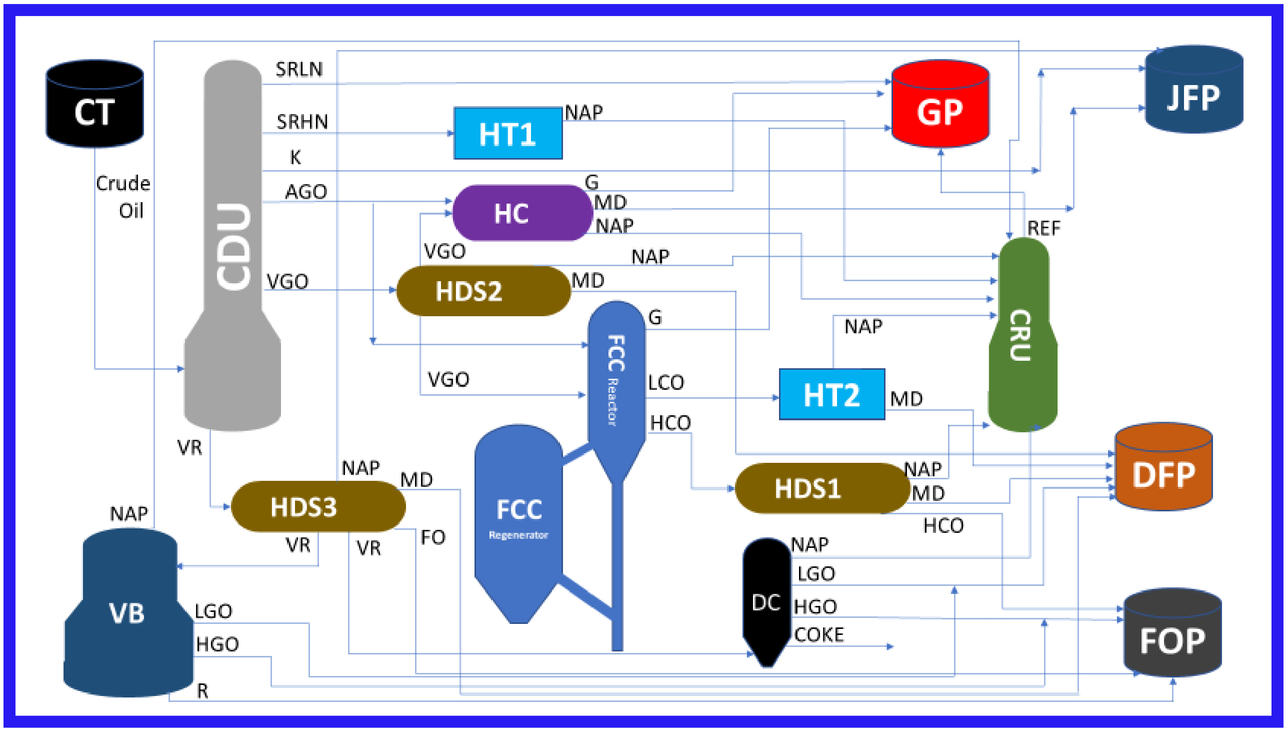

Figure 2.1. Simplified Schematic Diagram of the Refinery in this Study

hydrodesulfurizers HDS1, HDS2 and HDS3 for heavy cycle oil, vacuum gas oil and vacuum residue respectively.

The remaining refinery unit sets *BU*, *ctank* and *ptank* represent blending units, crude tanks and final product tanks. *BU* in turn includes the set of product pools *{GP,JFP,DFP,FOP}* which in turn stand for Gasoline, jet fuel, diesel fuel and fuel oil pools. There is assumed to be only one crude storage and charging tank to CDU and the set *ptank* also represents *{GT,JFT,DFT, FOT}* which demonstrate gasoline, jet fuel, diesel fuel and fuel oil final product tanks. As discussed further in the following section, the empirical units merged with material balance equations, will calculate the final product yields and properties for each unit. For the operation of the entire refinery under study, the deterministic product demand and unit selection for the processes and operation mode has been used. With these assumption and simplifications, this refinery problem could be stated with the following knowns and remaining decision variables:

Given:

1-The horizon is only one stream day

2-Type of the crude oil used which is Alaskan crude in this study

3-Unit operations, their numbers and maximum capacity, and limits on their inlet and outlet streams

4-Final products and their demand data

5-Prices for the final products, Alaskan crude and intermediate products like ethanol

6-The operational costs for the units are neglected as the main idea of the current study is a comparative study of global maximum profit by the nonlinear refinery model through calculating yield and product quality and linear input-output model (fixed yield and property)

To be determined:

1-Amount of the crude to be purchased to meet the product demand

2-Yield and properties of all intermediate and final products

3-The blending recipe will be obtained by meeting the final product demand and quality requirements in the blending units

The major assumptions made in this problem:

1-The uncertainty in the demand and price data for the final product or the price and availability for the crude or any other types of operational uncertainty is neglected for this study and all data are deterministic.

2-The mixing in all blending units is perfect and shrinkage and volume change does not occur for the purpose of this study.

3- As the study has been conducted for a short horizon of one stream day, the effect of the inventories have not been taken into account for the purpose of this study.

The objective function is the overall profit of the refinery which will be calculated by simply subtracting the crude oil and purchased intermediate product costs from the revenue made by the final product sales. In the following sections, the overall material balance and the nonlinear unit models are discussed.

2.3.Overall Refinery Material Balance

2.3.1. Material Balance for Operating Units

All refinery operational units have at least 5 equations for their material balance constraints. Equation 2.1 constrains the inlet flow rate to each unit. Equations 2.2 and 2.3 calculate the outlet flowrate of each product from the unit using the volumetric or weight yield value obtained from the nonlinear unit models. Equation 2.4 enforces conservation of mass under an assumption of no shrinkage and volume change and constant density in all processes. Equation 2.5 enforces the maximum inlet capacity for each unit and uses the refinery throughput, that is, the CDU inlet flow rate as the upper bound for the feedstock flowrate of each unit. Equation 2.6 sets $A_m(u, c, u')$ the amount of product c flowing from unit u to unit u' and is equal to the outlet flowrate of the product c from unit u for all refinery products excluding AGO from CDU, VGO from HDS2 and VR from HDS3 where the product outlet stream is split into more than one downstream units. $pathu(u, c, u')$ is a set that verifies the product c is on that flow path from unit u to unit u'. For CDU rather than having (4) constraint as the upper bound, the sum of all final product demands are used as the lower bound as shown in equation 2.7.

$$F_{in}(f, u) = \sum_{u'} \sum_{c} A_m(u', c, u) \;\; \forall\, u' \in U, c \in C \qquad (2.1)$$

$$F_{out}(u, c) = 0.01 \times Y(c, u) \times F_{in}(f, u) \;\; \forall\, u \in U, c \in C \qquad (2.2)$$

$$F_{out}(u, c) = \frac{[0.01 \times Y_w(c, u) \times F_{in}(f, u) \times SG(f, u)]}{SG(c, u)} \qquad \forall\, u \in U, c \in C \qquad (2.3)$$

$$F_{in}(f, u) = \textstyle\sum_c F_{out}(u, c) \;\; \forall\, u \in U, c \in upr \qquad (2.4)$$

$$F_{in}(f, u) \leq F_{in}(f, CDU) \; \forall\, u \in U \qquad (2.5)$$

$$A_m(u, c, u') = F_{out}(u, c) \quad \forall\, u, \in U, (c, u') \in pathu \qquad (2.6)$$

$$F_{in}(f, CDU) \geq \textstyle\sum_{fpr} Demand\;(fpr) \qquad (2.7)$$

2.3.2. Material Balance for Blending Units

For product pools four sets of previous equations for the operating units will apply as well, that is, equations (2.1,3-5). Nevertheless the product pools will require two extra constraints as follow: equation 2.8 enforces $Demand\ (fpr)$, the demand of final product fpr as the lower bound for $A_m(BU, fpr, ptank)$ which is the amount of final product fpr flowing from blending unit BU to final product tank $ptank$. Equation 2.9 enforces $Capx\ (ptank)$, the maximum capacity of the final product tank $ptank$ as the upper bound for $A_m(BU, fpr, ptank)$ the amount of final product fpr flowing from blending unit BU to final product tank $ptank$:

$$A_m(BU, fpr, ptank) \geq \ Demand\ (fpr) \qquad (2.8)$$

$$A_m(BU, fpr, ptank) \leq \ Capx\ (ptank) \qquad (2.9)$$

2.4.Mathematical Model

HPI petroleum refining process correlations[116] present empirical correlations for predicting product yields and properties for the following processes: Fluid Catalytic Cracking (FCC), Catalytic Reforming (CRU), Hydrocracking (HC), Hydrotreating (HT), Hydrodesulfurization (HDS), Visbreaking (VB) and Delayed Coking (DC). The objective of these correlations is simply for techno-economic studies to estimate yields and properties for petroleum refining process units.

While the operating conditions have not been accounted explicitly in the derivation of most of these correlations, Nevertheless, the user specifies the severity level or degree of conversion and the yields represent mid-life or average run conditions. Thus, the process conditions vary from case to case over a narrow range defined by the operating severity, and the effect of operating conditions required for a specific performance can be accounted for implicitly via the adjustments for feedstock quality. [116]

2.4.1.Fluid Catalytic Cracking (FCC) Model

The FCC process can be characterized by the feed properties as input variables as follows:

Conversion Level, *C* (LV.PCT.) , Feed Specific Gravity, SG_f (60°F/60°F), Feed API Gravity, API_f, Feed Volumetric Average Boiling Point, $VABP_f$ (°F), Feed Aniline Point, AP_f (°F), Feed Sulfur Content, S_f (WT.PCT.) and Feed Watson Characterization Factor, K_f .

The operating variables in the FCC unit are: Reactor and regenerator pressure, Reactor temperature, Weight hourly space velocity, WHSV (h^{-1}), Catalyst Activity and Catalyst-to-oil ratio. The product streams from the FCC unit are defined by the set *fccpr = {C3/400, GASO,LCO,HCO,COK}*.Total mathematical model for the FCC unit comprises 45 correlations which for brevity just some of them are outlined as follows. [116]

Equation 2.10 defines *feed quality parameter.* Equations (2.11-14) determine yield (LV PCT.), API gravity, research octane number (clear?) and Reid vapor pressure (psia) for the FCC gasoline.

$$FQP = 75.0 - 0.065\left(VABP_f\right) - 0.9\left(S_f\right) + 0.6\left(AP_f\right) - 0.26\left(AP_f/SG_f\right) \quad (2.10)$$

$$GASOV = [GASO/C_3PROD][C_3/400\ YIELD] \quad (2.11)$$

$$API_G = 66.84 - [15.5\,(C/100) + 8.33\,(C/100)^2 - 31.2(FQP/100) + 35.6\,(FQP/100)^2] \quad (2.12)$$

$$RONCL = 0.00139(C)(FQP) - 0.0384(C) - 0.187(FQP) + 101.3 \quad (2.13)$$

$$RVP = -23.8 + 2.5\left(K_f\right) + 0.3\left(S_f\right) \quad (2.14)$$

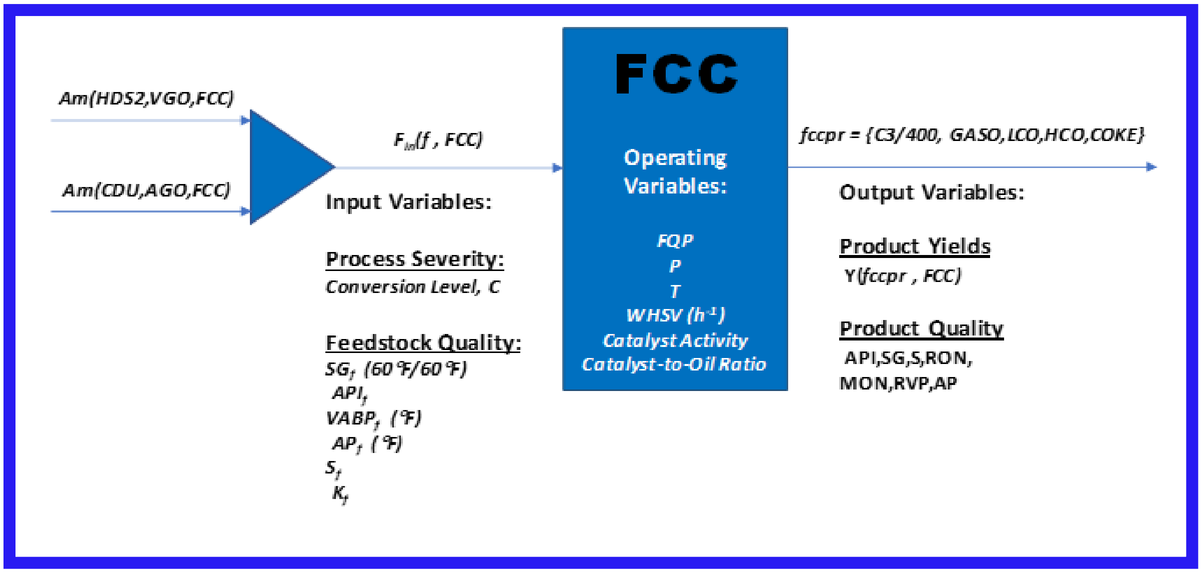

Figure 2.2. Schematic Diagram of the Mathematical Model in FCC

2.4.2.Catalytic Reforming (CRU) Model

The process correlation for catalytic reforming estimates the product yields and reformate properties for reforming full-boiling range naphthas. The yields represent catalytic reformers employing platinum-rhenium catalyst. Average reactor pressure, a key design parameter, may vary from 100 to 500 psig and here a typical operating pressure of 200 psig and a weight-hourly space velocity of 2.0 is considered. The correlation provides adjustments for operating pressure. The two most important governing factors for the yield are: (1) the feedstock quality represented by the N2A content: Naphthene content plus 2 times the aromatic content of feedstock and (2) the operating severity as measured by the clear research octane number of the C_5^+ reformate. [116] The product streams from the CRU unit are defined by the set *crupr = { FG, LPG,REF}*.Total mathematical model for the CRU unit comprises 19 correlations, some of which are presented here Are the others in the appendix?. Equations (2.15-17) compute pressure corrected yield (vol. pct.), motor octane number (clear) and Reid vapor pressure (psia) of C_{5^+} Reformate.

$$\text{REFORMATE} = (\text{REFBASE}) + \big(2.0 - 0.01\ (\text{P})\big)\big[\text{EXP}\big(1.4245 - 13.225(\text{N2A}) + 12.0\ (\text{N2A})(\text{RON})\big)\big] \quad (2.15)$$

$$MONCL = 11.38 + 77.42\ (RON) \quad (2.16)$$

$$RVP = [3.044112 - 0.013476\ (N2A) + 2.452896\ (N2A)(N2A) - 4.798783\ (RON) - 2.607458\ (N2A)(RON) + 2.782781\ (RON)(RON)]/[1.0 + 1.275414\ (N2A) + 0.567611\ (N2A)(N2A) - 2.209418\ (RON) - 1.779277\ (RON)(N2A) + 1.374308\ (RON)(RON)] \quad (2.17)$$

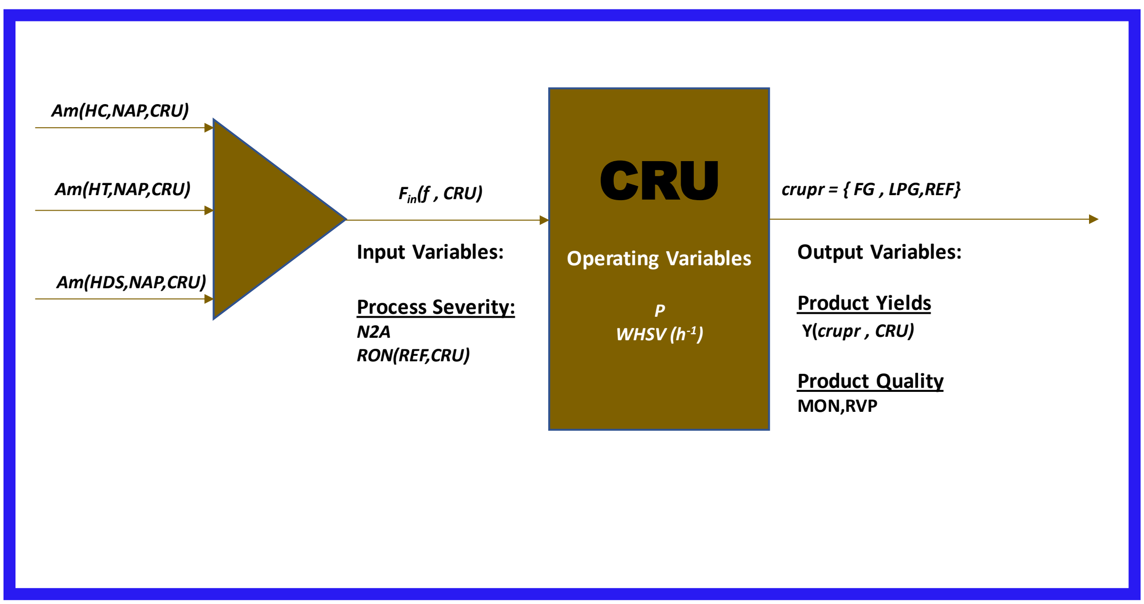

Figure 2.3. Schematic Diagram of the Mathematical Model in CRU

2.4.3.Hydrocracking (HC) Model

The product distribution in gas oil hydrocracking is a function of operating severity and feedstock quality. The HPI gas oil hydrocracking correlation uses the light gasoline (C_5/180° F) yield as a measure of the conversion achieved during hydrocracking. The other product yields are correlated with the light gasoline yield. There are correlations for 3 modes of operations: maximum gasoline production, maximum jet fuel /kerosene production or maximum diesel fuel production, which for the purpose of this study the correlations for the maximum jet fuel /kerosene production have been used. [116]

The product streams from the HC unit are defined by the set *hcpr = {RG , NAP, G, MD}*.Total mathematical model for the HC unit for all operational modes comprises a total of 107 correlations for product yields, Naphtha yield and property in each operation mode, property correlations for Gasoline, Kerosene/Jet Fuel and Diesel products within those operation modes. Some of the major correlations from maximum Kerosene/Jet Fuel production are presented here. Equation 2.18 provides yield (WT. PCT.) for light gasoline. Equations 2.19-21 compute yield (WT. PCT.), Smoke Point (mm) and Luminometer Number of kerosene. Research octane number (clear) and motor octane number (clear) of naphtha are determined by Equations 2.22-23.

$$LG = (HC/100.0)\left[0.15\left(API_f\right) + 2.4\left(K_f\right) - 17.29\right] \quad (2.18)$$

$$KERO = HC - RG - C_4\,LPG - LG - HN \quad (2.19)$$

$$SP_K = 17.8\,(K_K) - 185.0 \quad (2.20)$$

$$LN_K = -12.03 + 3.009\,(SP_K) - 0.0104\,(SP_K)^2 \quad (2.21)$$

$$RONCL = -19.3\left(K_f\right) + 288.3 \quad (2.22)$$

$$MONCL = 0.91\,(RONCL) + 5.4 \quad (2.23)$$

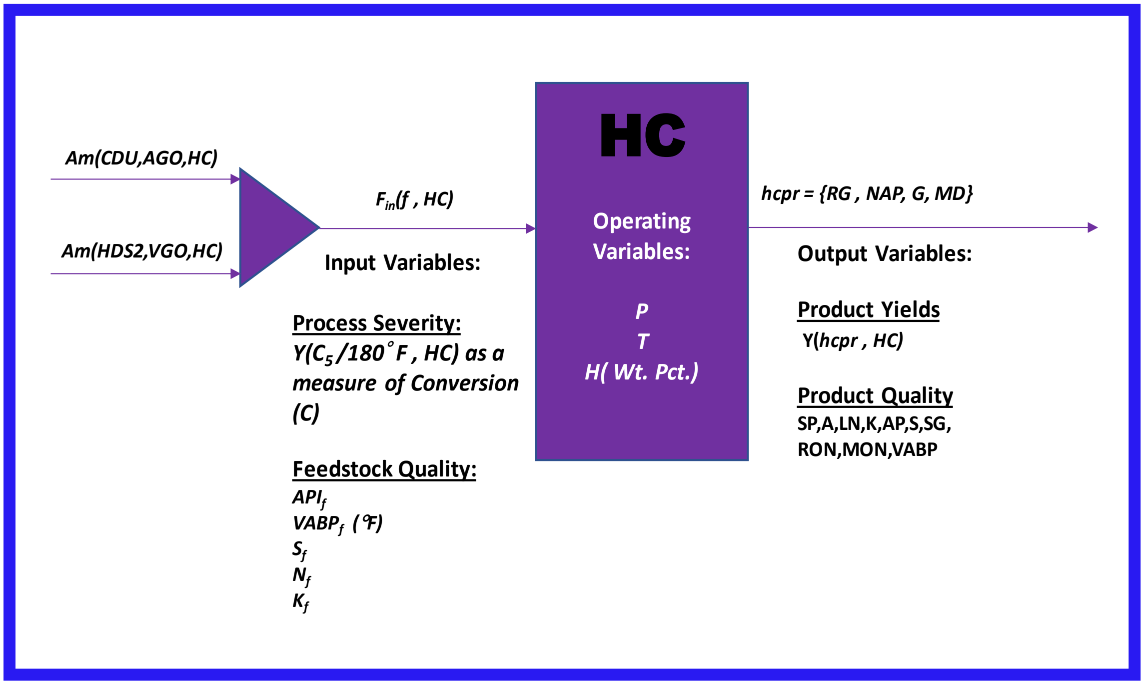

Figure 2.4. Schematic Diagram of the Mathematical Model in HC

2.4.4. Hydrotreating (HT) Model

The refining industry hydrotreats a wide range of petroleum stocks for different purposes. Naphtha hydrotreating aims at removing sulfur, nitrogen, oxygen and metals that would otherwise poison the valuable catalysts used in downstream catalytic reforming processes. For straight-run naphthas, hydrotreatment does not significantly change the quality of the naphtha other than removing the sulfur, nitrogen and trace metal contaminants. However, unsaturated stocks like naphthas coming from visbreaker or coker units do undergo considerable changes due to the saturation of olefinic molecules. For middle distillates like light cycle oil from catalytic cracking, hydrotreating is performed to enhance their quality by removing sulfur and trace contaminants, carbon residue and olefin content. It improves their cetane index and burning characteristics, color and storage stability and resistance to sludging. The operating variables of the catalytic hydrotreating process include pressure, temperature, catalyst loading, hydrocarbon feed rate and hydrogen concentration. The effect of operating conditions required for different feedstocks are accounted for implicitly via the adjustments for feedstock quality.[116]

The correlations presented here are to estimate the product yields and properties in commercial hydrotreating operations. Total mathematical model for the naphtha and middle distillate HT unit includes a total of 37 correlations which some of the correlations are presented here. Equations 2.24-28 compute aromatic saturation factor (ASF), paraffins content (LV. PCT.), naphthenes content (LV. PCT.), aromatics Content (LV. PCT.) and research octane number (clear) of hydrotreater naphtha. Whereas Equations 2.29-31 calculate yield (WT. PCT.), cetane index and pour point (°F) for middle distillate in hydrotreater.

$$ASF = 0.011 + 76.0\,(N_f)^2 + 0.039\,(S_f) \quad (2.24)$$

$$P_n = P_f + 0.85\,(O_f) + 0.10\,(ASF)(A_f) \quad (2.25)$$

$$CP_n = CP_f + 0.15\,(O_f) + 0.90\,(ASF)(A_f) \quad (2.26)$$

$$A_n = A_f - (ASF)(A_f) \quad (2.27)$$

$$RON_n = RON_f - 0.33\,(O_f) + 1.5 - 0.31\,(ASF)(A_f) \quad (2.28)$$

$$MD = 100.0 + H - H_2S - NH_3 - RG - HN \quad (2.29)$$

$$CI = -420.34 + 0.016\,(API)^2 + 0.192\,(API)(Log_{10}\,VABP) \\ +65.01\,(Log_{10}\,VABP)^2 - 0.0001809\,(VABP)^2 \quad (2.30)$$

$$PP_d = PP_f + [40.0\,(B_f)/(PP_f + 100.0)] - [10.0\,(11.9 - K_f)(FCC)] \quad (2.31)$$

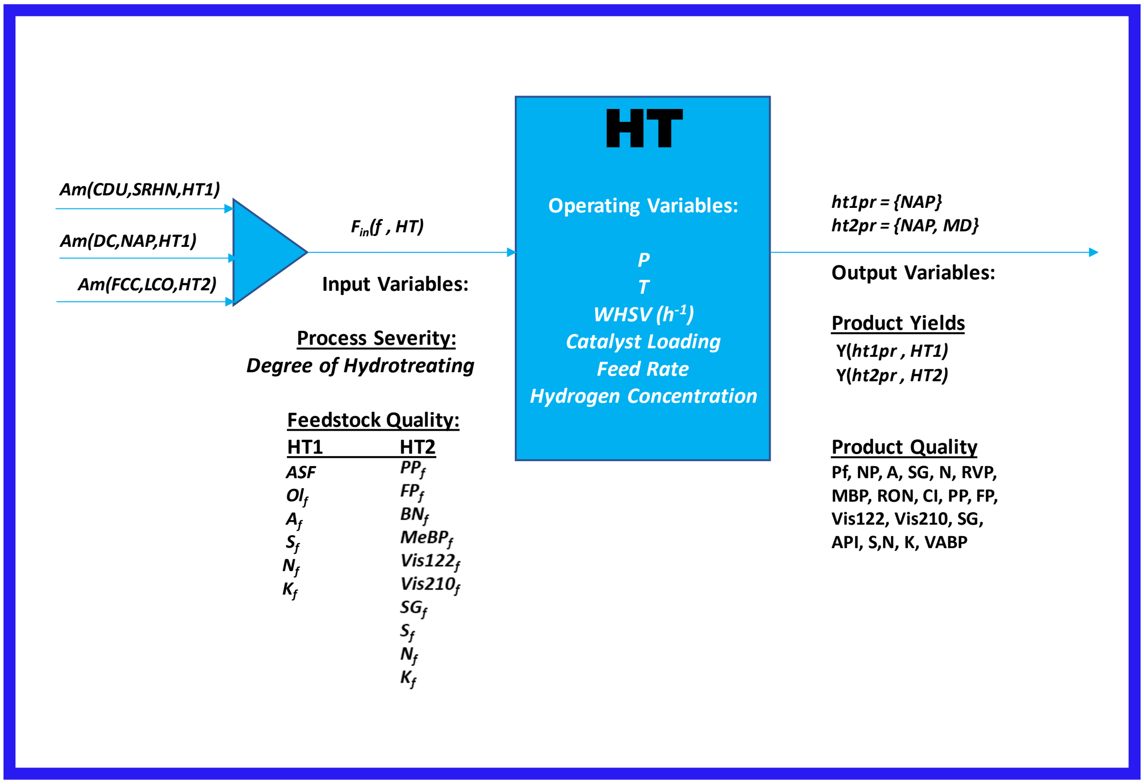

Figure 2.5. Schematic Diagram of the Mathematical Model in HT

2.4.5. Hydrodesulfurization (HDS) Model

One of the most frequently encountered reactions in hydrogen treating is desulfurization. Although sulfur removal is usually the main objective, catalytic hydrodesulfurization is also used to eliminate nitrogen, oxygen and other contaminants. In commercial practice, refineries usually operate their hydrodesulfurization units to treat stocks like heavy cycle oil from cat cracker, vacuum gas oil and vacuum residue from vacuum distillation units. Heavy cycle oil and vacuum gas oil are hydrodesulfurized for two reasons: (1) to produce low-sulfur blendstocks for fuels and (2) to improve the cracking characteristics of catalytic cracking feedstocks. This process removes sulfur, nitrogen, metal contaminants, carbon residue constituents and saturates and polyaromatics from the feedstocks and thereby resulting in improved conversion and gasoline yields. Residue hydrodesulfurization is increasingly important as pollution regulations regarding sulfur emissions have become more strict. In addition to producing low sulfur fuel oils, residue HDS units have also been used to produce low sulfur feedstock for delayed coking process.[116]

Table 1 shows the operating severity in terms of degree of desulfurization for the refining process in this study. The correlations presented here are to estimate the product yields and

Table 2.1. Operating Severity for Refinery Processes [116]

Chargestock	Approximate TBP Boiling Range, °C (°F)	Severity
Naphtha	C_5/190 (C_5/375)	1 ppm sulfur in product
Middle Distillate	190/343 (375/650)	95% desulfurization
Heavy Gas Oil	343/566 (650/1050)	90% desulfurization
Atmospheric Residue	343+(650+)	85% desulfurization
Vacuum Residue	566+(1050+)	80% desulfurization

properties in commercial hydrodesulfurization operations. Total mathematical model for heavy cycle oil, vacuum gas oil and vacuum residue HDS units includes a total of 55 correlations which some of the correlations are presented here. Equation 2.32 calculates viscosity-gravity constant for the feed. Equations 2.33-36 determine viscosity-gravity constant, viscosity at 210 °F (SSU), yield (WT. PCT.) and pour point (°F) for heavy gas oil (HGO). Equations 2.37-41 compute yield (WT. PCT.), sulfur content (WT. PCT.), viscosity-gravity constant, viscosity at 210 °F (SSU) and metals content (PPM WT.) in Residual Fuel Oil.

$$VGC_f = \frac{SG_f - (0.1244)\,Log_{10}(SUS210_f - 31.0)}{0.9255 - (0.0979)\,Log_{10}(SUS210_f - 31.0)} - 0.0839 \quad (2.32)$$

$$VGC_{hgo} = VGC_f - 0.89\left(SG_f - SG_{hgo}\right) \quad (2.33)$$

$$Log_{10}\left(SUS210_{hgo} - 31.0\right) = \frac{(0.9255)\,VGC_{hgo} - SG_{hgo} + 0.0776}{(0.0979)\,VGC_{hgo} - 0.1162} \quad (2.34)$$

$$HGO = 100.0 + H - H_2S - NH_3 - HN - MD \quad (2.35)$$

$$PP_{hgo} = PP_f - \left[9.0\left(11.9 - K_f\right)(FCC)\right] \quad (2.36)$$

$$FO = 100.0 + H - H_2S - NH_3 - RG - HN - MD \quad (2.37)$$

$$S_r = [(20.0)\,S_f - (S_n)(HN) - (S_d)(MD)]/FO \quad (2.38)$$

$$VGC_r = VGC_f + 0.56\left(SG_r - SG_f\right) \quad (2.39)$$

$$Log_{10}(SUS210_r - 31.0) = \frac{0.9255\,(VGC_r) - SG_r + 0.0776}{(0.0979)\,VGC_r - 0.1162} \quad (2.40)$$

$$M_r = 16.0(M_f/FO) \quad (2.41)$$

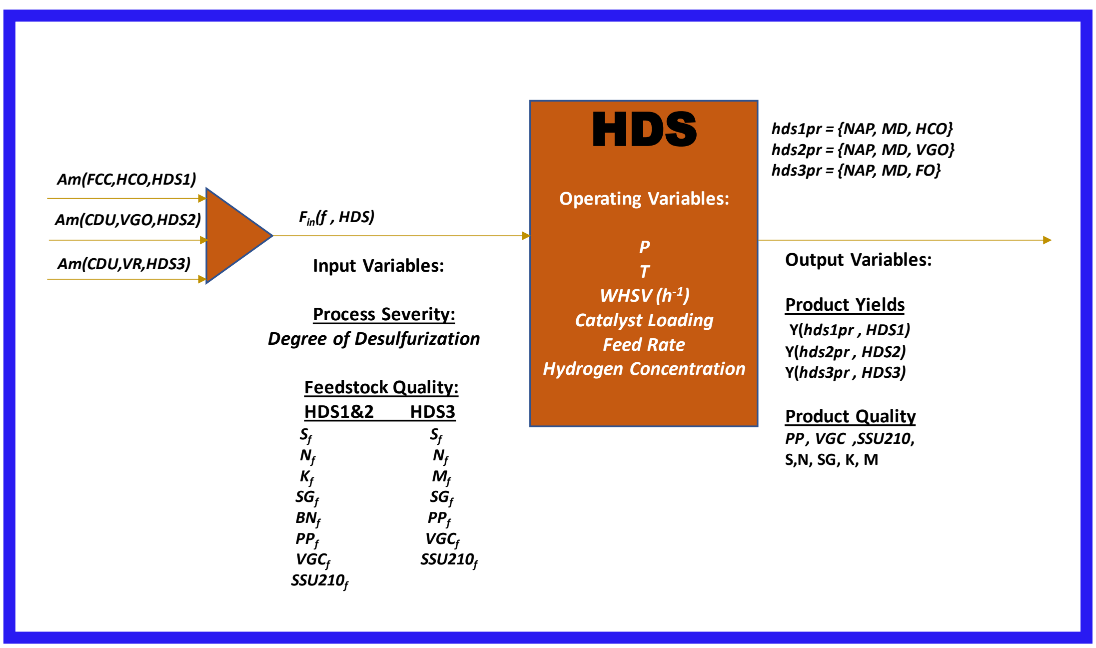

Figure 2.6. Schematic Diagram of the Mathematical Model in HDS

2.4.6. Visbreaking (VB) Model

Visbreaking is a special application of the thermal cracking process used to convert heavy, high viscosity petroleum stocks into lower viscosity stocks suitable for use as heavy fuel oil. The primary purpose for visbreaking residual stocks is to reduce their viscosity and pour point. The visbreaking correlations are used to predict yields and product properties from visbreaking oil stocks at the maximum severity. The yield from these correlations are consistent with fuel products which will not undergo phase separation and severe viscosity increase during storage and will not lead to large scale deposits and coking in the furnace tubes. The yield equations use the normal pentane insoluble (NC5) content of the visbreaker chargestock as the correlation parameter. The sediment content of the chargestock appears to affect the thermal stability of the visbroken fuel. Two sets of correlation equations presented: one for low sediment contents (0.02 pct. and lower) and one for high sediments contents (greater than 0.02 pct.).[116]

The product streams from the VB unit are defined by the set *vbpr = {FG, LPG, NAP, LGO, HGO,R}*. Total mathematical model for visbreaking unit includes a total of 20 correlations. Some of the correlations are outlined here. All equations are based on a sediment less than or equal to 0.02 (wt %). Equation 2.42 computes yield (LV %) for Visbreaker naphtha (C_5/400 °F). Equations 2.43-47 determine yield (LV Pct.), specific gravity, pour point (°F), viscosity blending number and viscosity at 210 °F (CS) for the Visbreaker vacuum residue (900 °F +)

$$VN = 12.29 - 0.071\left(NC5_f\right) \quad (2.42)$$

$$VTB = 59.64 - 0.183\ (NC5_f) \quad (2.43)$$

$$SG_{vtb} = SG_f\left(\frac{VTB\ Weight\ Yield}{VTB\ Volume\ Yield}\right) \quad (2.44)$$

$$PP_{vtb} = PP_f + 10.0 \quad (2.45)$$

$$VBN_{vtb} = [(VFO)\left(VBN_{vfo}\right) - (0.0366)(LGO) - 0.2104\ (HGO)]/VTB \quad (2.46)$$

$$\ln(CS210_{vtb}) = (6.9078\ VBN_{vtb})/(1.0 - VBN_{vtb}) \quad (2.47)$$

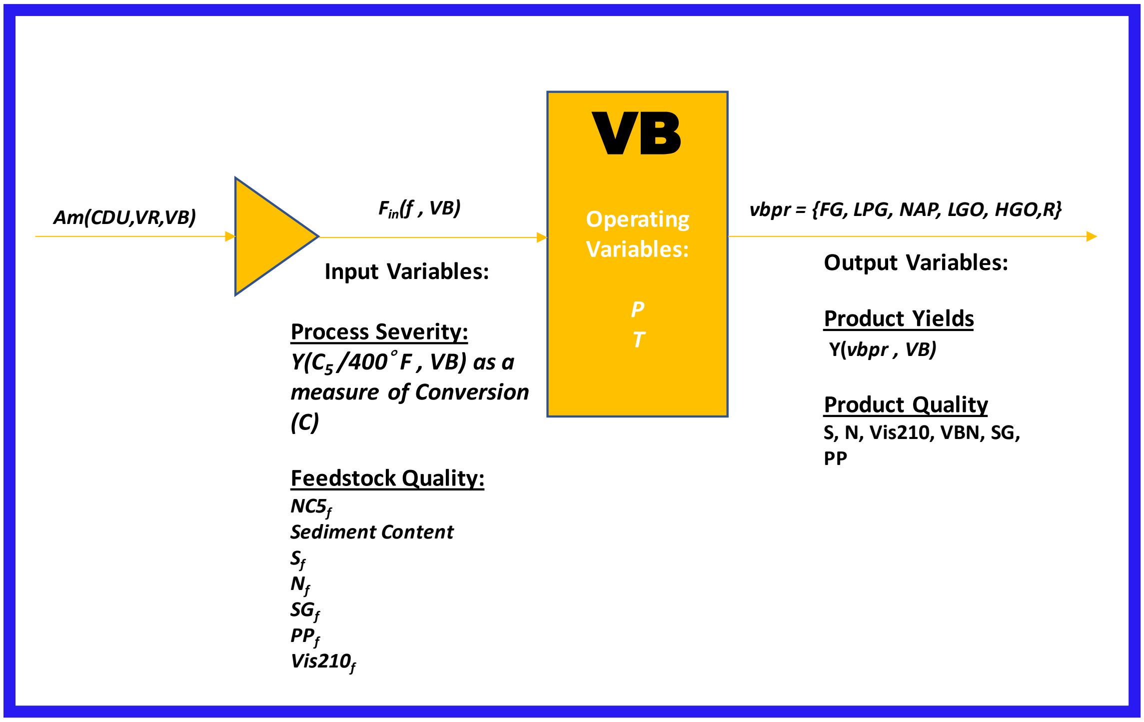

Figure 2.7. Schematic Diagram of the Mathematical Model in VB

2.4.7.Delayed Coking (DC) Model

Delayed coking was introduced as a refining process in the early 1930's. In early refineries severe thermal cracking of residual stocks resulted in unwanted coke deposits in the heaters. Gradually refiners learned to design the heaters so that the residual feedstock could be heated above the coking temperature without significant coke formation in the heaters. The Delayed Coking Correlations uses the Conradson carbon residue (CCR) of the feedstock as the correlating parameter for estimating yields for conventional delayed coking operations.[116]

The product streams from the DC unit are defined by the set *dcpr = { RG, LPG, NAP, LGO, HGO,COKE}*. Total mathematical model for delayed coking unit includes a total of 15 correlations which some of the correlations are presented here. Equation 2.48 determines yield (wt. pct.) for the Coker naphtha (C_5/400°F). Equations 2.49-51 calculate yield (wt. pct.),sulfur and nitrogen content for the coke product.

$$NAP = 11.38 + 0.335\,(CCR_f) \quad (2.48)$$

$$COKE = 1.6\,(CCR_f) \quad (2.49)$$

$$S_{coke} = [100.0\,(S_f) - 23.52\,(S_f) - 0.14\,(S_f)(NAP) - 0.45\,(S_f)(LGO) - 0.82\,(S_f)(HGO)]/COKE$$

(2.50)

$$N_{coke} = [100.0\,(N_f) - 0.01\,(N_f)(NAP) - 0.24\,(N_f)(LGO) - 0.63\,(N_f)(HGO)]/COKE$$

(2.51)

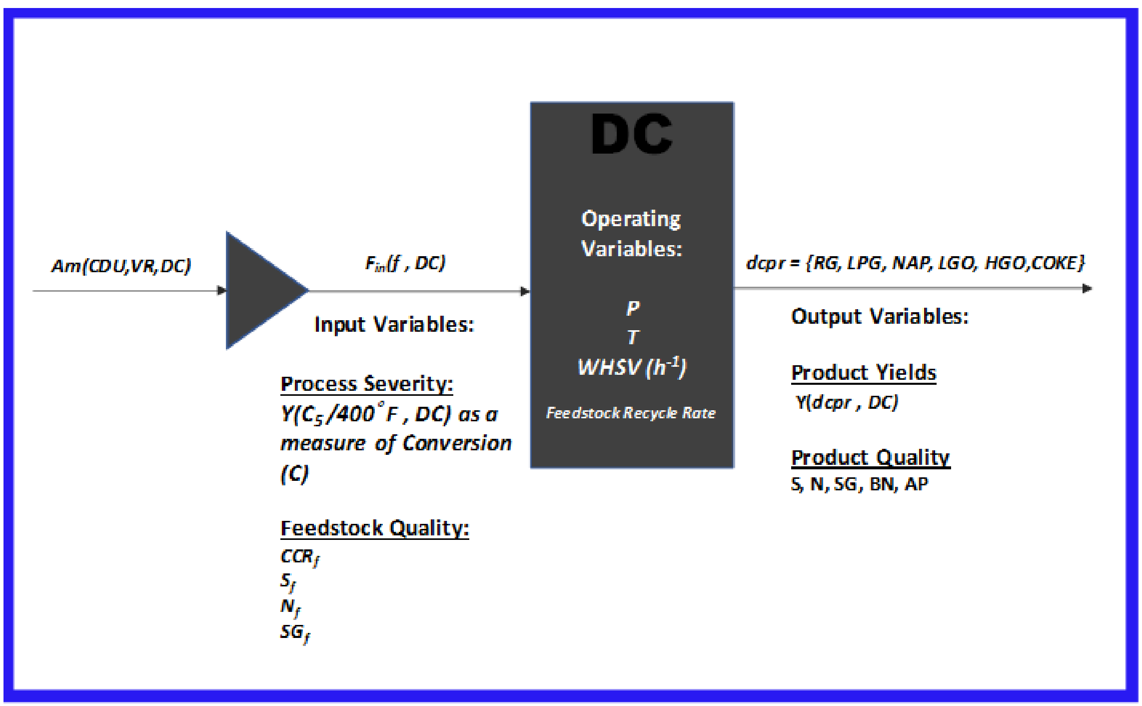

Figure 2.8. Schematic Diagram of the Mathematical Model in DC

2.4.8. Crude Distillation Unit (CDU) Model

2.4.8. 1. Swing-cut Data-Based Model

The data based CDU model is adopted from Alhajri et al.[31] . The key attribute for characterizing the hydrocarbons composing crude oil in this study is the True Boiling Point (TBP) curve. Table 2 shows the cuts produced in the CDU for the TBP data for typical crude oil fractions.

Table 2.2.Boiling Range Data for Typical Crude Oil Fractions [31]

Fraction	TBP-Boiling Range (°F)
SRLN	90-220
SRHN	180-380
Kerosene	330-520
Diesel	420-630
VGO	610-1050
Residue	950^{+}

The mathematical model for the CDU is expressed by the operating variable of the CDU unit which is the cut-point temperature for fraction (*s*), $x = TE_{CDU}$. Also, the products stream for the CDU unit are fractions *s* ($s \in S_{\mathrm{CDU}}$ = *LPG*, *SRLN*, *SRHN*, *Kero*, *Diesel*, *VGO*, *and Rsd*). The CDU model is described as follows:

Equation 2.52 represents the cuts as a polynomial function in $TE_{\mathrm{CDU},s}$, which is equivalent to the End-Point Temperatures (EP). The upper and a lower bounds for the $TE_{\mathrm{CDU},s}$ of all fractions *s* from the CDU is referred to as the swing cut. The coefficients of the polynomial of the CDU equation are listed in Table 3. The residual cut volume percent is expressed by equation 2.53. Since the last cut is the residue of the crude, it is assumed that the accumulative vaporized percent will be 100%. Each product volumetric flow rate is calculated by subtracting its accumulated volume percent vaporized from the previous cut volume and multiply the result with crude feed to the CDU as described by equation 2.54. Key properties of the CDU products e.g. API gravity, Sulfur and nitrogen percent are expressed by equation 2.56 as polynomial functions in each product mid-volume percent vaporized. The mid-volume for a product is determined by equation 2.55 and calculated by averaging the accumulative current cut volume percent with the previous cut volume percent vaporized.

$$Cut_S = \sum_{k=0}^{4} a_k \left(TE_{CDU,s}\right)^k \quad \forall\, s \in S_{CDU} - \{Rsd\} \qquad (2.52)$$

$$Cut_{s=Rsd} = 100 \quad (2.53)$$

$$V_{CDU,S} = F_{CDU} \times \left(\frac{Cut_s - Cut_{s-1}}{100}\right) \forall\, s \;\; S_{CDU} \qquad (2.54)$$

$$MidV_{CDU,S} = \left(\frac{Cut_s + Cut_{s-1}}{2}\right) \forall\, s \;\; S_{CDU} \qquad (2.55)$$

$$PV_{CDU,S,P} = \sum_{k=0}^{4} a_k \left(MidV_s\right)^k \quad \forall\, s \in S_{CDU}, p \in P_s \qquad (2.56)$$

Table 2.3. CDU model equations coefficients [31]

Parameter a_k	**Cut% (Vol.) Equation (52)**	**API Equation (56)**	**SUL% Equation (56)**	**N% Equation (56)**
a_0	4.040637061	81.84796736	0.050579083	–0.000882902
a_1	–0.047271899	–3.778147973	–0.02036269	0.000304355
a_2	0.000324992	0.113288448	0.001849373	–2.2968E–05
a_3	–2.84324E–07	–0.0015436414	–3.25656E–05	4.58852E–07
a_4	8.15312E–11	7.19024E–06	2.0301E–07	6.76957E–09

2.4.8.2. Geddes Fractionation Index (FI) Based Model

The fractionation index (FI) is a quantitative criterion for sharpness of fractionation with complex mixtures by a fractionator. [35] The index is the equivalent number of theoretical plates, operating at total reflux, which would affect the same component separation as the fractionator. The FI model is a more accurate nonlinear model for the complex crude distillation unit (CDU) than the fixed yield or the swing cuts models and optimizes the crude cuts quantities and temperature while being independent from crude type, characteristics of the CDU, and readily calculated.[19]

The nonlinear FI model for the CDU in this work has been adopted from Alattas et al.[1.] It starts with a mass balance around each unit *j* and component *i*. Every unit yields the top product $PD_{j,i}$ feeding the next unit and the bottom product $PB_{j,i}$ which is the product crude cut. There is also a summation equation for each type of stream over its set of constituent components *i*'s as shown by equation 2.57. Equation 2.58 implies that the top product of each unit *j* is also the feed to next downstream unit *j+1.* A summation equation over all components *i* for each unit is also used in the FI model as demonstrated by equations 2.59, 2.60 and 2.61. The component distribution at each unit *j* is based on the light key LK_j and heavy key HK_j components for each unit based on the initial and end boiling points relative to each cut. The components lighter than the light key are only obtained in the top product stream, while the ones heavier than the heavy key are only obtained in the bottom product stream as shown in equations 2.62 and 2.63.

The splits of the distributed components are calculated using the FI parameters. For each unit, there are two FI values, one for the rectifying section and another for the stripping section. The rectifying FI (*FIr*) is used if the temperature is greater than the component boiling temperature; otherwise, the stripping FI (*FIs*) is used. Equations 64 and 65 represent this fact and the FI choice. $Y_{i,j}$ is a binary variable which is equal to one if the component is in the stripping section and zero otherwise, $\gamma_{i,j}$ is a placeholder for the FI value, $T_{b,i}$ is the component boiling point, and T_j is the cut point temperature. Notice that at $Y_{i,j} = 0$ (false) that $\gamma_{i,j} = FIr_j$ and $T_{b,i} \leq T_j$ while at $Y_{i,j} = 1$ (true) that $\gamma_{i,j} = FIs_j$ and $T_{b,i} \geq T_j$. The exact representation of this disjunction is considered with linear mixed-integer constraints using convex hull as in equation 2.64 and big M formulation as in equations 2.65 and 2.66 .Since the components are listed in the order of increasing boiling point, equation 2.67 is also included. The reference components have the composition ratio of 1 and a boiling point equal to the cut point temperature of the fractionation unit or crude cut, T_j. This reduces the FI equation to equation 2.68. This equation is combined with the component mass balances (equations 2.57-63) to yield the equation for the component flow rate in the bottom product stream as represented by equation 2.69 noting the relationship between the relative volatility with the equilibrium constant, $K_{j,i}$, of the subject component (equation 2.70) . The equilibrium constant is calculated by equation 2.71. The vapor pressure can be calculated by Antoine equation for the major cuts and by an equation of state proposed by Twu et al.[117] for the pseudocomponents as represented in equations 2.72 and 2.73.

The separation temperature is the arithmetic average of the initial and end boiling points relevant to each cut as shown in equation 2.74. Moreover, the temperature decreases along the CDU column from bottom to top, which is expressed in equation 2.75.

$$F_{j,i} = PD_{j,i} + PB_{j,i} = PD_{j,total}x_{PD,j,i} + PB_{j,total}x_{PB,j,i} \quad (2.57)$$

$$F_{j+1,i} = PD_{j,i} = PD_{j,total}x_{PD,j,i} \quad (2.58)$$

$$F_{j,total} = \sum_i F_{j,i} \quad (2.59)$$

$$PD_{j,total} = \sum_i PD_{j,i} \quad (2.60)$$

$$PB_{j,total} = \sum_i PB_{j,i} \quad (2.61)$$

$$PD_{j,i} = F_{j,i} \ , \ PB_{j,i} = 0 \quad i < LK_j \ (2.62)$$

$$PB_{j,i} = F_{j,i} \ , \ PD_{j,i} = 0 \quad i > HK_j \ (2.63)$$

$$\gamma_{i,j} = FIr_j * \left(1 - Y_{i,j}\right) + FIs_j * Y_{i,j} \quad \forall j, \ LK_j \le i \le HK_j \qquad (2.64)$$

$$T_{b,i} + M_L * Y_{i,j} \le T_j \quad \forall j, \ LK_j \le i \le HK_j \quad (2.65)$$

$$T_j \le T_{b,i} + M_U * (1 - Y_{i,j}) \quad \forall j, \ LK_j \le i \le HK_j \quad (2.66)$$

$$Y_{i,j} \le Y_{i+1,j} \quad \forall j, \ LK_j \le i \le HK_j \quad (2.67)$$

$$\frac{y_{j,i}}{x_{j,i}} = \alpha_{j,io}^{FI}\,(T_j) \quad (2.68)$$

$$PB_{j,i} = \frac{F_{j,i}}{\frac{PD_{j,total}}{PB_{j,total}} K_{j,i}^{\gamma_{i,j}} + 1} \quad \forall j, \ LK_j \le i \le HK_j \ (2.69)$$

$$\alpha_{j,io} \frac{K_{j,i}}{K_{j,o}} = \frac{Pv_i(T_j)}{Pv_o(T_j)} \quad (2.70)$$

$$K_{j,i} = \frac{Pv_{j,i}(T_j)}{P} \qquad \forall j, i \qquad (2.71)$$

$$Pv_{j,i} = \exp\left(\left(PVA_i - \frac{PVB_i}{T_j + PVC_i - 273.15}\right) * 2.303\right) \quad \forall j, i \in HC \quad (2.72)$$

$$Pv_{j,i} = Pc_i * \exp([-5.96346 * (1 - Tr_{j,i}) + 1.17639 * (1 - Tr_{j,i})^{1.5} - 0.559607 * (1 - Tr_{j,i})^3 - 1.319 * (1 - Tr_{j,i})^6]/Tr_{j,i} + \omega_i * ([-4.78522 * (1 - Tr_{j,i}) + 0.413999 * (1 - Tr_{j,i})^{1.5} - 8.91239 * (1 - Tr_{j,i})^3 - 4.98662 * (1 - Tr_{j,i})^6]/Tr_{j,i}$$

$$\forall j, i \in PsC \quad (2.73)$$

$$T_j = \frac{TE_j + TI_j}{2} \qquad \forall j, i \qquad (2.74)$$

$$T_j \geq T_{j+1} \quad \forall j \qquad (2.75)$$

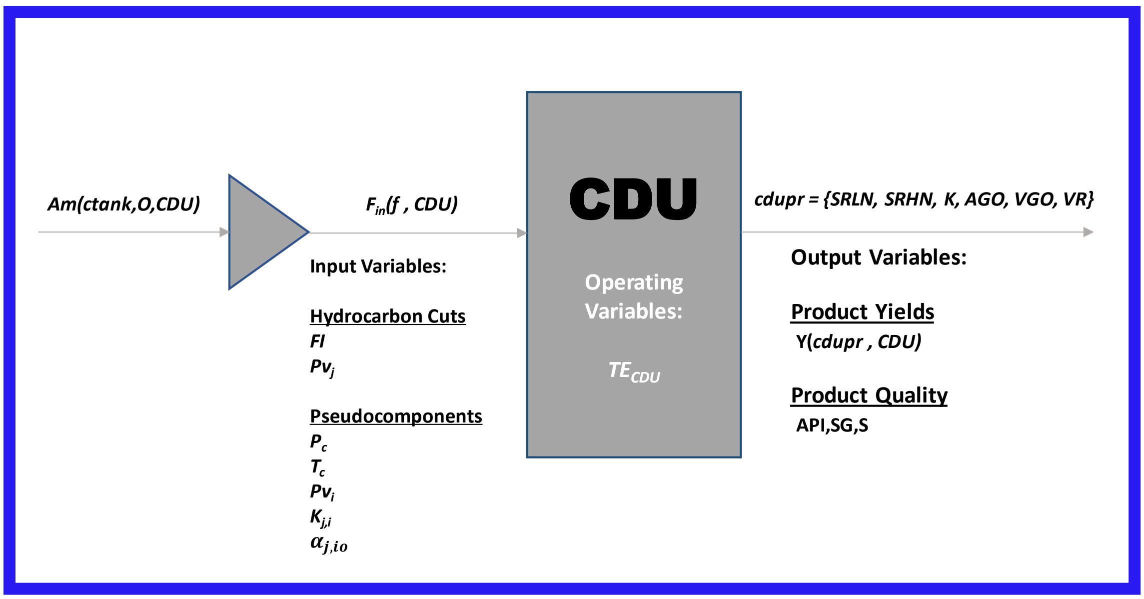

Figure 2.9. Schematic Diagram of the Mathematical Model in CDU

2.5.Product Quality Constraints in Blending Units

The final Product quality from the blending units must meet the requirements enforced by the customers and environmental regulations. In this section the constraints to meet the product quality are discussed.

2.5.1. Gasoline Pool (GP)

The blending in the gasoline pool is assumed based on the octane blending method. For simplicity, there are only two sets of requirements for the final gasoline product: (1)The volume fraction of oxygenate ethanol in the final gasoline product should not exceed 0.097 as defined by equation76, (2) Posted Octane Number required for the final Gasoline Product should be a minimum of 87 as defined by equation 2.77. The posted octane number can be calculated by equation 2.78.

$$vol\_frac(EtOH, GP) \leq 0.097 \quad (2.76)$$

$$PON(G, GP) \leq 87 \quad (2.77)$$

$$PON(G, GP) = [\sum_{c} RON(c, GP) \times vol\_frac(c, GP) + \sum_{c} MON(c, GP) \times vol\_frac(c, GP)]/2$$

$$\forall c \in fgp \quad (2.78)$$

2.5.2. Jet Fuel Pool (JFP)

The blending in the jet fuel pool is based on meeting three product quality requirements as follows: (1) the smoke point of the final jet fuel product should be a minimum of 19 mm and is calculated based on linear blending rule as defined by equation 79, (2) the maximum sulfur content for the final jet fuel Product should not exceed 0.3 (wt%) as defined by equation 80, *(*3) the freezing point of final jet fuel product in Fahrenheit is calculated based on nonlinear correlations adopted from Chevron and Albahri et al.[118] and linear blending indices rules as defined by equations 2.81-83, and *(*4) the maximum freezing point temperature of the final jet fuel Product should not exceed -40 *(*°F*)* as defined by equation 2.84.

$$SP(JF, JFP) \geq 19 \quad (2.79)$$

$$S(JF, JFP) \leq 0.3 \quad (2.80)$$

$$FPBI(c,u) = 55.16793 \times (1.0368976)^{FP(c,u)} \quad (2.81)$$

$$FBPI(JF,JFP) = \sum_{c} [\, vol\_frac(c,JFP) \times \; FPBI(c,u) \,] \;\; \forall c \in pathu(u,c,JFP) \quad (2.82)$$

$$FP(JF,JFP) = -111.1628 + 27.68212 \times \ln\big(FPBI(JF,JFP)\big) \quad (2.83)$$

$$FP(JF,JFP) \leq -40 \quad (2.84)$$

2.5.3. Diesel Fuel Pool (DFP)

The blending in the diesel fuel pool is based on meeting four product quality requirements as follow: *(*1) The viscosity at 122 (°F) in centistokes (cSt) for the final diesel fuel product is calculated by Refutas method adopted from Maples[119] and Chevron and Albahri et al.[118] and linear blending indices rules as expressed by equations 2.85-87, *(*2) The lower and upper bound for the viscosity of final diesel fuel product in centistokes (cSt) at 122 (°F) are expressed by equations 2.88-89, (3) the cetane index of the final diesel fuel product should be a minimum of 40 and is calculated based on linear blending indices as expressed by equation 2.90, and (4) The maximum sulfur content for the final diesel fuel Product should not exceed 0.35 (wt%) as expressed by equation 2.91.

$$VBI122(c,u) = 10.975 + 14.535 \times \ln\,[\ln\{(Vis122(c,u) + 0.8\}] \quad (2.85)$$

$$VBI122(DF,DFP) = \sum_{c} [\, vol\_frac(c,DFP) \times \; VBI122(c,u) \,] \;\; \forall c \in pathu(u,c,DFP) \quad (2.86)$$

$$\log[Vis122(DF,DFP)] = \frac{[-0.315 + 1.796 \times VBI122(DF,DFP)]}{[1 - 1.264 \times VBI122(DF,DFP) + 0.45 \times (VBI122(DF,DFP))^2]} \quad (2.87)$$

$$Vis122(DF,DFP) \geq 1.9 \quad (2.88)$$

$$Vis122(DF,DFP) \leq 4.1 \quad (2.89)$$

$$CI(DF,DFP) \geq 40 \quad (2.90)$$

$$S(DF, DFP) \leq 0.35 \qquad (2.91)$$

2.5.4.Fuel Oil Pool (FOP)

The blending in the diesel fuel pool is also based on meeting four product quality criteria as follow: *(*1)The viscosity at 210 (°F) in centistokes (cSt) for the final fuel oil product is calculated by the methods adopted from Chevron and Albahri et al. [118] and linear blending indices rules as described by equations 2.92-94, *(*2) the lower and upper bound for the viscosity of final fuel oil product at 210 (°F) in centistokes (cSt) are described by equations 2.95-96, (3) the maximum sulfur content for the final fuel oil Product should not exceed 0.5 (wt%) as described by equation 2.97, (4) the pour point of the final fuel oil product should not exceed 65°F as described by equation 2.98, *(*5) pour point in Fahrenheit (°F) for the final fuel oil product is calculated by the methods adopted from Hu and Burns [42] and linear blending indices rules are described by equations 99-101.

$$VBI210(c,u) = \frac{[0.183 + 0.458 \times \log(Vis210(c,u))]}{[1.105 + 0.305 \times \log(Vis210(c,u))]} \quad (2.92)$$

$$VBI210(FO,FOP) = \sum_{c} [\, vol\_frac(c,FOP) \times \; VBI210(c,u) \,] \quad \forall c \; \in pathu(u,c,FOP) \quad (2.93)$$

$$\log[Vis210(FO,FOP)] = \frac{[-0.315 + 1.796 \times VBI210(FO,FOP)]}{[1 - 1.264 \times VBI210(FO,FOP) + 0.45 \times (VBI210(FO,FOP))^2]} \quad (2.94)$$

$$Vis210(FO,FOP) \geq 5.0 \qquad (2.95)$$

$$Vis210(FO,FOP) \leq 8.9 \qquad (2.96)$$

$$S(FO,FOP) \leq 0.50 \qquad (2.97)$$

$$PP(FO,FOP) \leq 65.0 \quad (2.98)$$

$$PPBI(c,u) = 3262000 \times \left(\frac{PP(c,u) + 460]}{1000}\right)^{12.5} \quad (2.99)$$

$$PPBI(FO,FOP) = \sum_{c} [\, vol\_frac(c,FOP) \times \; PPBI(c,u) \,] \quad \forall c \in pathu(u,c,FOP) \quad (2.100)$$

$$PP(FO,FOP) = 1000 \times \left(\frac{PPBI(FO,FOP)]}{3262000}\right)^{0.08} - 460 \quad (2.101)$$

2.6.Objective Function

For simplicity, the refinery operating costs have been assumed based on the total refinery throughputs and as all models have the same throughput as their inputs and the focus of this research is a comparative study between nonlinear and input-output planning models and later on two nonlinear models with different CDU models, the operating costs have been neglected and the simple profit function is calculated merely by subtracting the purchase costs of crude oil and intermediate products like ethanol from the revenue from sales of all final products:

$$Profit = \sum_{u,c,u'} Am(u,c,u') * Prices(c) - Am(ctank,o,CDU) * Prices(o) \quad (2.102)$$
$$- Am(EtOHT,EtOH,GP) * Prices(EtOH) \quad \forall\, u \in bu, c \in fpr, u' \in stank$$

2.7.Linear Input-Output Model

To compare and quantify the effectiveness of the nonlinear refinery model, a linear fixed yield and product quality model or input-output model scheme has been adopted from Guyonnet et al.[51] as a reference. For yield equations, the conversion of mass in unit *u* is represented using percent yields that do not depend on the feed properties and the amount of products is equal to the total inlet flow multiplied by a constant, the percent yield of that unit for the specific crude

($yield_{u,c}$).Equation 2.103 demonstrates this definition. The linear product properties can be accomplished in following way: Product c with properties q leaving unit u (PO_{ucq}) is calculated as the sum of the flow fraction times the properties of each flow in the same way as linear blending equations as described by equation 2.104. This equation is nonlinear but is linearized by using the bounds on this property as product quality is within certain specifications. Equation 2.105 describes these bounds. Substitution of $PO_{u,c,q}$ as defined in 2.104 and multiplication by the denominator of 2.104 will linearize the expression.[51]

$$F_{out}(u,c) = F_{in}(f,u) \times Yield_{u,c} \quad \forall u \in U, c \in upr \quad (2.103)$$

$$PO_{u,c,q} = \frac{\sum_{u' \in U} \sum_{c' \in C} A_m(u',c',u) \times pro(u',c',q)}{\sum_{u' \in U} \sum_{c' \in C} A_m(u',c',u)} \quad (2.104)$$

$$\forall u \in U, \forall c \in upr,, \forall q \in QO_{u,c}$$

$$pn_{c,q} \leq PO_{u,c,q} \leq px_{c,q} \quad (2.105)$$

$$\forall u \in U, \forall c \in upr,, \forall q \in QO_{u,c}$$

2.8. Refinery Case Studies

A total of 13 different refinery case studies have been created: The first 3 case studies with various product demands and throughputs are used to verify the effectiveness of the nonlinear refinery model utilizing the data-based CDU model (DBNLM) over the linear input-output model (IOM) with fixed yield and property for the products and the impact of introducing process nonlinearity on the total profit improvement. The numerical results and discussion are presented in chapter 5.

Chapter 3

DETERMINISTIC INTEGRATED REFINERY MODEL

3.1. Preface

This chapter presents a novel integrated optimization approach with a multi-period mixed-integer nonlinear programming (MINLP) model for the oil refinery network. The proposed model considers operations in a broad range of refinery supply chain integrating decisions associated to crude unloading, procurement while accounting for the highly nonlinear nature of the processing units, final product pooling and blending, inventory management, distribution by pipeline, utility system and environmental impacts. The main feature of this chapter is the development of a aggregation/disaggregation scheme based on lumped variable linearization (LVL) and normalized multiparametric disaggregation technique (NMDT) [106-113] through a two-level optimization algorithm and obtaining ε-global optimal solutions for the integrated refinery problem. The proposed model can be used as a deterministic decision-support tool for enterprise wide integrated production planning of an oil refinery. Further, in this study, broad comparisons are drawn between the solutions of the proposed integrated approach and the sequential approach in terms of the economic and operational objectives to illustrate the potential and trade-offs involved in the integrated model. A motivating example has demonstrated the advantages of the proposed approach over its sequential counterpart and showed that the proposed integrated approach gains improvement in overall profit margin and can provide significantly better solutions in terms of optimal utility units operation, energy consumption, startup/shutdown operations, pipeline utilization, batch contamination, delayed or lost consumer demand and so on.

3.2.Problem Statement

Figure 3.1 illustrates a simplified representation of the refinery supply chain in this study. The focus of this study is a coastal refinery system consisting of crude carrier vessels , docking stations to unload crude at the refinery's front end, storage tanks for storing crude oil before transferring to charging tanks where blending operation is carried out for subsequent transfer to crude distillation units (CDU).

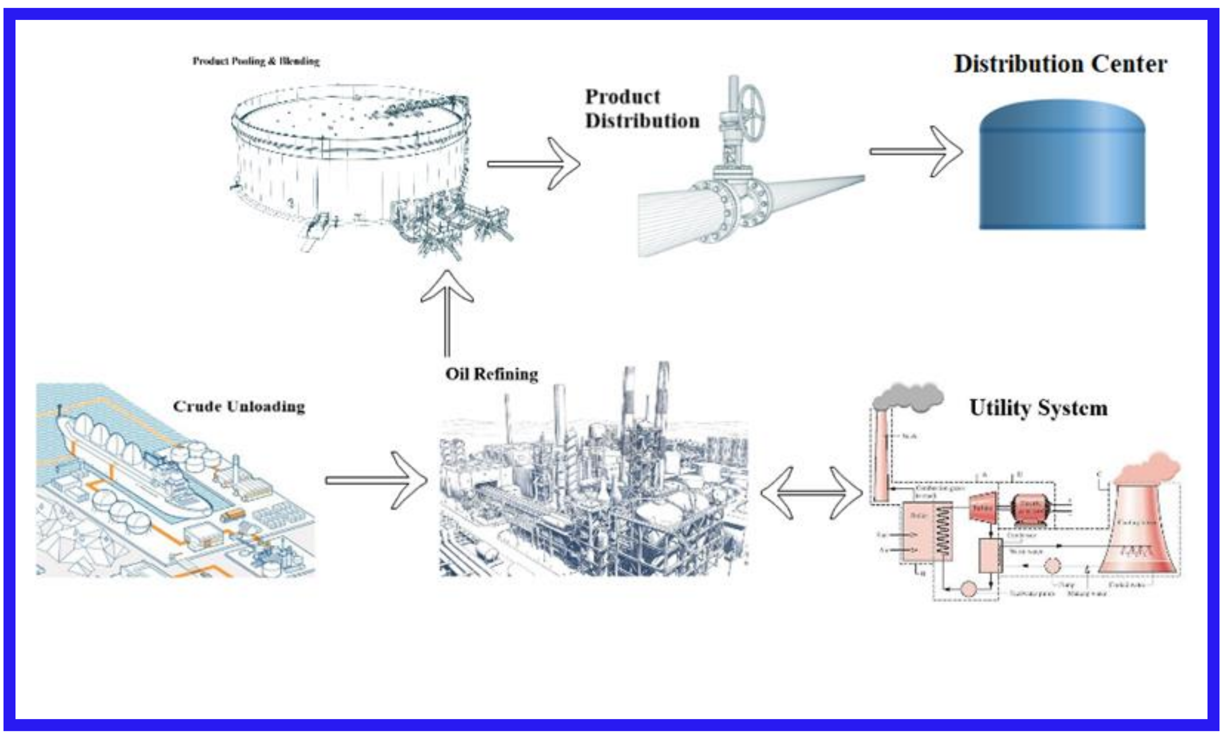

Figure 3.1. Simplified Representation of the Refinery Supply Chain in this Study.

For the crude unloading sub-system, all the transport operations are achieved in interconnected departments by means of a pipe network. The design objective for the unloading sub-system is to minimize the overall cost of operation by minimizing demurrage or sea waiting time for each vessel prior to the unloading process, duration of unloading for vessels, inventory levels for vessels, storage and charging tanks at each time interval, CDU charging rates to minimize harmful flow fluctuations to CDUs or shutdown, time and sequence of charging of crude blends into each CDU to minimize changeover cost (CC) and time and sequence of crude transfer from storage to charging tanks to minimize tank switchover costs (CS). [120]

Following the transfer of crude blendstocks to CDUs the fractionation is carried out to produce intermediate products which subsequently are transformed through further processing in the other operating units. The refinery production system in this study consists of a set of refinery units such as crude distillation unit (CDU), catalytic reforming (CRU), fluid catalytic cracking (FCC), hydrocracking (HC), hydrotreating (HT), hydrodesulfurization (HDS), Visbreaking (VB) and delayed coking (DC) units. The refinery produces a set of three major final products where gasoline (G) and diesel fuel (DF) fulfill the customers' demands and fuel gas (FG) is utilized internally to operate the utility system. The design objective for the production sub-system is to maximize the overall profit which is calculated by subtracting the operating costs plus crude oil and purchased intermediate product costs from the revenue made by the final products sales. [55]

For the final product blending and pooling problem, a pq-formulation has been formulated where different streams of the intermediate products from the processing units are mixed together to produce final products gasoline and diesel fuel which must satisfy certain requirements on the qualities of attributes. For the pooling problem two gasoline and diesel fuel pools and five product quality requirements are considered: The gasoline product must meet a certain research octane number (RON) and motor octane number (MON) and the diesel fuel product should satisfy a certain cetane index (CI), sulfur content and viscosity at 122 °F.

For the distribution of the final products from the refinery end to the distribution center (DC) a unidirectional multiproduct pipeline system is considered. Different batches of final products that is, gasoline and diesel fuel are pumped into the pipeline and discharged successively at DC. The most important decision for the pipeline distribution system is to determine the batch sequencing and scheduling of injection and discharging of different product batches. Each product is stored in its own dedicated product storage tank at the refinery end and the DC who must meet the daily demands of customers. The design objective for the pipeline distribution is both operationally and economically oriented. The objective function comprises minimizing the difference between the total discharged volume and the total demands of customers, maximizing the minimum inventory among all of the products that is, the inventory level of the product with the lowest final inventory level on the last day of the time horizon, minimizing the underutilized pipeline capacity during the entire time horizon, minimizing the total violated peak electricity hours, minimizing the volume of contaminated interfaces between two subsequent injected batches and finally minimizing the loss or delays in supplying the customer demand by the due dates. [121]

On the account of the utility demands estimation, the criterion in the design for the utility system is to satisfy specific power and different grades of steam (LP,MP,HP) demands for the refinery processing units while minimizing the operational costs comprising of fuel cost, extra electricity purchase cost and penalty cost incurred by the emission of harmful gases such as greenhouse gas (GHG) and sulfur oxides (SO_x). The utility system in this study encompasses fuel gas repository, boilers to produce HP steam (high pressure), steam turbines for electricity generation, let-down valves for reducing pressure and mixing equipment for mixing steams of same grade. [67]

The major assumptions made in this problem:

(1)The uncertainty in the demand and price data for all commodities or any operational uncertainty is neglected and the entire model is deterministic.

(2)The mixing in all blending units is perfect and shrinkage and volume change does not occur in the tanks.

(3) The pipeline is full at the beginning of the scheduling horizon and the batch sizes for injection and discharging are identical.

(4) There is a mandatory settling period an newly discharged batch from pipeline that enters the product storage tank at the DC.

(5) During the peak electricity hours the cost of electricity energy is higher than the regular hours

(6) Steam temperatures and pressures are constant at the inlet and exit of the boilers resulting the enthalpy difference to be a parameter.

With the aforementioned definitions and assumptions , the integrated refinery problem could be outlined with the following knowns and decision variables to be determined:

Given:

(1) The time horizon is 90 streams day (2) The number of crude carrier vessels, their crude type and content (3) Crude vessels arrival and departure day (4) initial inventory levels (5) inventory costs for storage and charging tanks, changeover, switchover and shutdown costs for CDUs (6) Operation mode, units, their numbers and maximum capacity, and limits on their inlet and outlet streams.(7) Demand data for the final products (8) Prices for the final products, crudes and intermediates (8) the contaminated volume of interface between two consecutive batch of different products

To be determined:

(1) Type and amount of crudes to purchase to meet the final product demands (2) The target blending recipe will be resulted from the final product demand and property requirements in the pooling problem (3) Yield and quality for all intermediate and final products.(4) Batch sequencing for pipeline operations (5) amount of fuel gas to operate utility system (6) amount of electricity and steam grades to produce to meet the demand of refinery processing units. The framework based on the objectives and constrains mentioned above is the underlying foundation for modeling the integrated refinery problem and overall objective function in this study. The following section will briefly describe the mathematical models for each refinery sub-systems.

3.3.Mathematical Model

3.3.1.Crude Unloading, Blending and Inventory Management Model

Crude oil unloading and processing is a well explored problem for which a numerous models have been proposed. In this study, a crude oil unloading and processing model has been adopted from Hamisu et al.[120] Figure 3.2 represents a typical configuration of crude oil unloading process.

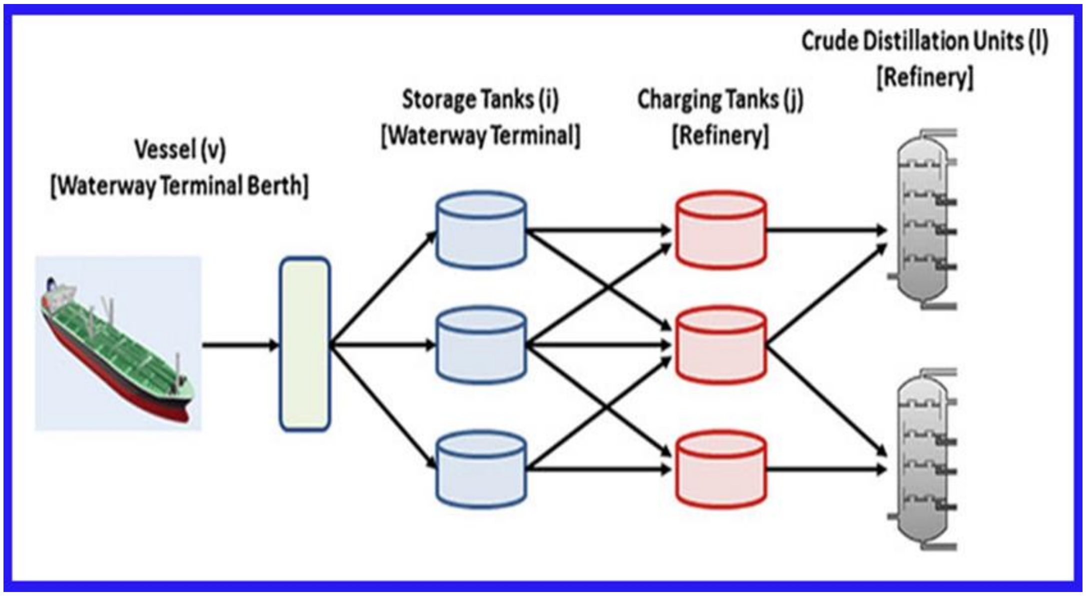

Figure 3.2. Typical Configuration of Crude Oil Unloading Process

A coastal refinery is considered with one docking station where the crude vessels unload their content; segregated storage tanks for storing crude oil before transfer to charging tanks; charging tanks where blending operation is carried out for subsequent transfer to CDUs according to the CDUs crude blend quality demands. These transfer operations are achieved in different units/facilities interconnected by means of a pipe network. The unloading model is characterized by 50 correlations representing operating rules, hydraulic capacities and property specification for the key component notably sulfur in this case which for brevity just the objective function and the variables involved in the integration constraints are outlined in this chapter. A brief representation of the unloading mathematical model is represented in Appendix A and for a detailed account the reader is referred to Hamisu et al.[120]

The objective function for crude unloading, blending and inventory management is the operating cost function to be minimized, which includes unloading and sea waiting costs for the crude vessels, the storage and charging tanks inventory costs, changeover cost and the penalties for shutdown and tank-tank switch over:

$$COPR_{UNL} = CUNL_v \sum_{v=1}^{NV} (TL_v - TF_v) + CSEA_v \sum_{v=1}^{NV} (TF_v - TARR_v)$$

$$+ CINST_i \sum_{i=1}^{NST} \sum_{t=1}^{NSCH} (\frac{VS_{i,t} - VS_{i,t-1}}{2}) + CINBT_j \sum_{j=1}^{NBT} \sum_{t=1}^{NSCH} (\frac{VB_{j,t} - VB_{j,t-1}}{2})$$

$$+ \sum_{t=1}^{NSCH} \sum_{j=1}^{NBT} \sum_{l=1}^{NCDU} (CC \times Z_{j,l,t}) + \sum_{t=1}^{NSCH} \sum_{l=1}^{NCDU} (CS \times XD_{l,t})$$

$$+ \sum_{t=1}^{NSCH} \sum_{i=1}^{NST} \sum_{j=1}^{NBT} (CSSU \times \alpha_{i,t})$$

(3.1)

3.3.2.Crude Procuring and Production Planning Model

The refinery production model for the purpose of this study is a modified version of the production planning model adopted from Siamizade.[55] Figure 3.3 demonstrates a schematic representation of the refinery processing units in this study. The refinery under study comprises a crude distillation unit (CDU) for crude fractionation and the following units for further processing of the intermediate streams: Fluid Catalytic Cracking (FCC), Catalytic Reforming (CRU), Hydrocracking (HC), Hydrotreating (HT), Hydrodesulfurization (HDS), Visbreaking (VB) and Delayed Coking (DC). Crude distillation unit comprises both atmospheric and vacuum distillation sections. From set of the operating units, there are only one unit for each category except for HT: HT includes two separate hydrotreaters HT1 for straight run light naphtha and HT2 for coker naphtha and middle distillate respectively. HDS includes only a unit for residue hydrodesulfurization. For crude distillation unit (CDU) a nonlinear model based on Geddes fractionation index (FI)[1,35] and for the remaining of the refinery processes, HPI petroleum refining process correlations[116] are utilized. These empirical correlations predict product yields and properties for the processing units for techno-economic studies. Refinery processing units in this study are represented by a total of 317 correlations. The correlations for the objective function, research octane number (RON) and motor octane number (MON) for the gasoline product and cetane index (CI), sulfur content and viscosity at 122 °F for the diesel fuel product are represented here. A detail account of remaining nonlinear correlations of refinery processing units may be found in Siamizade[55] and Baird[116] . Equation 3.2 defines the research octane number (RON) for the final gasoline product according to linear blending index rule:

$$RON(G,GP) = \sum_{c}[RON(c,GP) \times vol\_frac(c,GP)] \qquad \forall\, c \in fgp \qquad (3.2)$$

Equation3 presents required motor octane number (MON) (Baird[54]) *:*

$$MON(G,GP) = 0.778 \times RON(G,GP) + 9.5 \qquad (3.3)$$

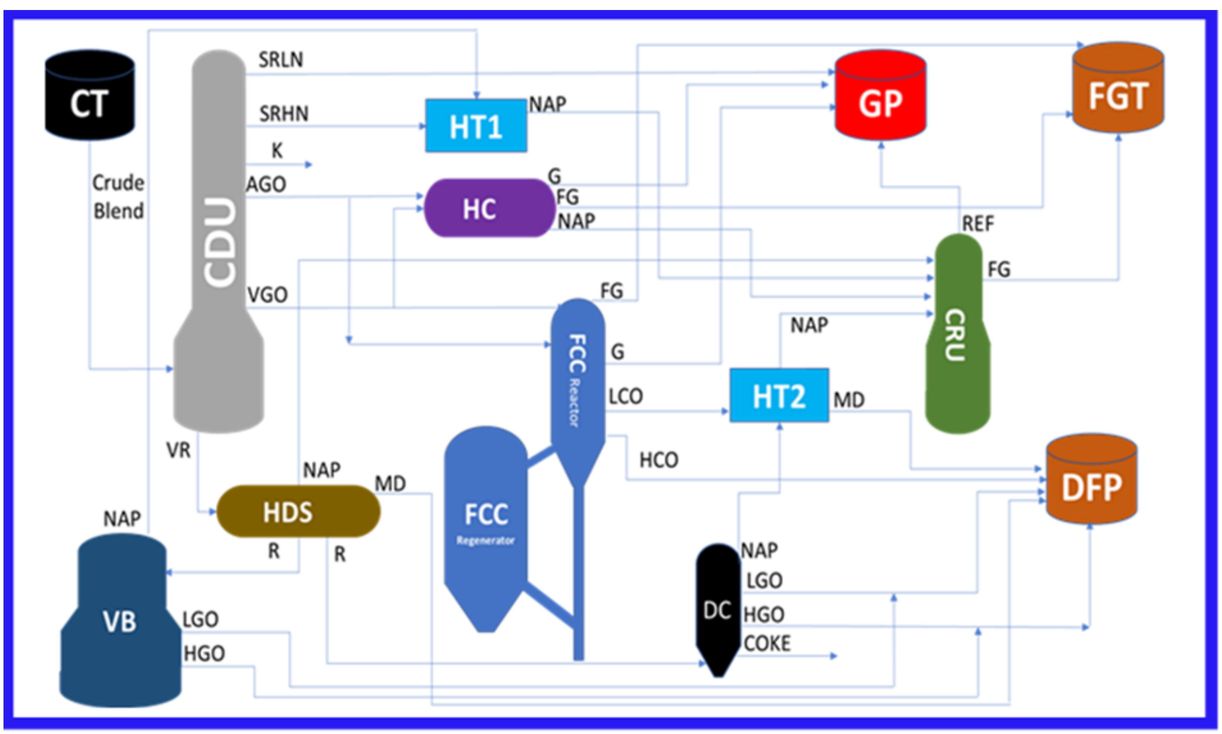

Figure 3.3. Schematic Representation of the Refinery Processing Units in this Study

Where c is the set of all commodities flowing to the gasoline pool GP as the components of the final gasoline product.

The viscosity at 122 °F for the diesel fuel product *expressed by* equation 3.4 and calculated by a method presented by Chevron and Albahri et al. [118]

$$\log[Vis122(DF,DFP)] = \frac{[-0.315 + 1.796 \times VBI122(DF,DFP)]}{[1 - 1.264 \times VBI122(DF,DFP) + 0.45 \times (VBI122(DF,DFP))^2]} \quad (3.4)$$

Equation 3.5 is an approximate correlation for the cetane index (CI) of diesel fuel product (Baird [116]):

$$CI(DF,DFP) = -420.34 + 0.016\,(API)^2 + 0.192\,(API)(Log_{10}\,VABP) + 65.01\,(Log_{10}\,VABP)^2 - 0.0001809\,(VABP)^2 \quad (3.5)$$

Where API is the API gravity (60 °F) and $VABP$ is the volumetric average boiling point (°F) of the diesel fuel product. The sulfur content (S) for the diesel fuel product could be approximated by equation 3.6 presented by Riazi et al.[122]

$$S(DF,DFP) = 177.4482 - 170.9463\left(n - {}^{d}/_{2}\right) + 0.2258\,M(n - 1.475) + 4.054\,SG \quad (3.6)$$

Where n is the refractive index at 20 °C , d is the density at 20 °C and 1 atm, M is the molecular weight and SG is the specific gravity at 15.5 °C of the diesel fuel product. Lastly, the objective function for the refinery production is the overall profit to be calculated by subtracting the operating costs of processing units and crude oil and purchased intermediate product costs from the revenue made by the final product sales:

$$REV_{PROD} = \sum_{bu,fpr,ptank,t}[Am(bu,fpr,ptank,t) * Prices(fpr,t)] - \sum_{u,t}[Fin(f,u,t) * OC(u,t)] - \sum_{ctank,o,t}[Am(ctank,o,CDU,t) * Prices(o,t)] - \sum_{t}[Am(EtOHT,EtOH,GP,t) * Prices(EtOH,t)] \quad (3.7)$$

3.3.3.Final Product Pooling Problem

The pooling problem is a nonlinear network flow problem that models the operation of the final product blending within the refinery where intermediate streams from the processing units are blended to produce final products. The problem then calls for finding the optimal flows in the network so as to minimize the cost of the pooling operations. Nonlinearities arise in attribute balances around pools since the pool attribute qualities as well as the inflows and outflows are all variables. The main challenge in finding optimal solutions to pooling problems is that the nonlinearities result in many local optima. [105] As shown in Figure 3.4, the pooling problem may be defined as a network flow problem over three sets of nodes: supply, transshipment, and demand nodes. Supply nodes represent the raw material components that flow to final product destinations (demand nodes) either directly or indirectly through pools (transshipment nodes). The unit costs as well as attributes, such as component concentrations of raw materials and final products are given. [105]

The pooling problem topology for the purpose of this study comprises 12 components, 2 product pools, 3 final product blends and 5 attributes as the target qualities for the final products. The first 3 components of 12 supplies are fuel gas from FCC, CRU and HC that will all blend in the fuel gas tank (FGT) to produce the final product fuel gas for the utility department. The next five components include SRLN from CDU, gasoline from FCC, reformate from CRU, gasoline from HC, and ethanol which will all blend in the gasoline pool (GP) to produce the final product gasoline. The last four of the supply components, middle distillate (MD) streams from HDS and HT2 and light gas oil (LGO) from VB and DC will all blend in the diesel fuel pool (DFP) to produce the final product diesel fuel. The set *path={ CDU.SRLN.GP, FCC.G.GP, FCC.FG.FGT,*

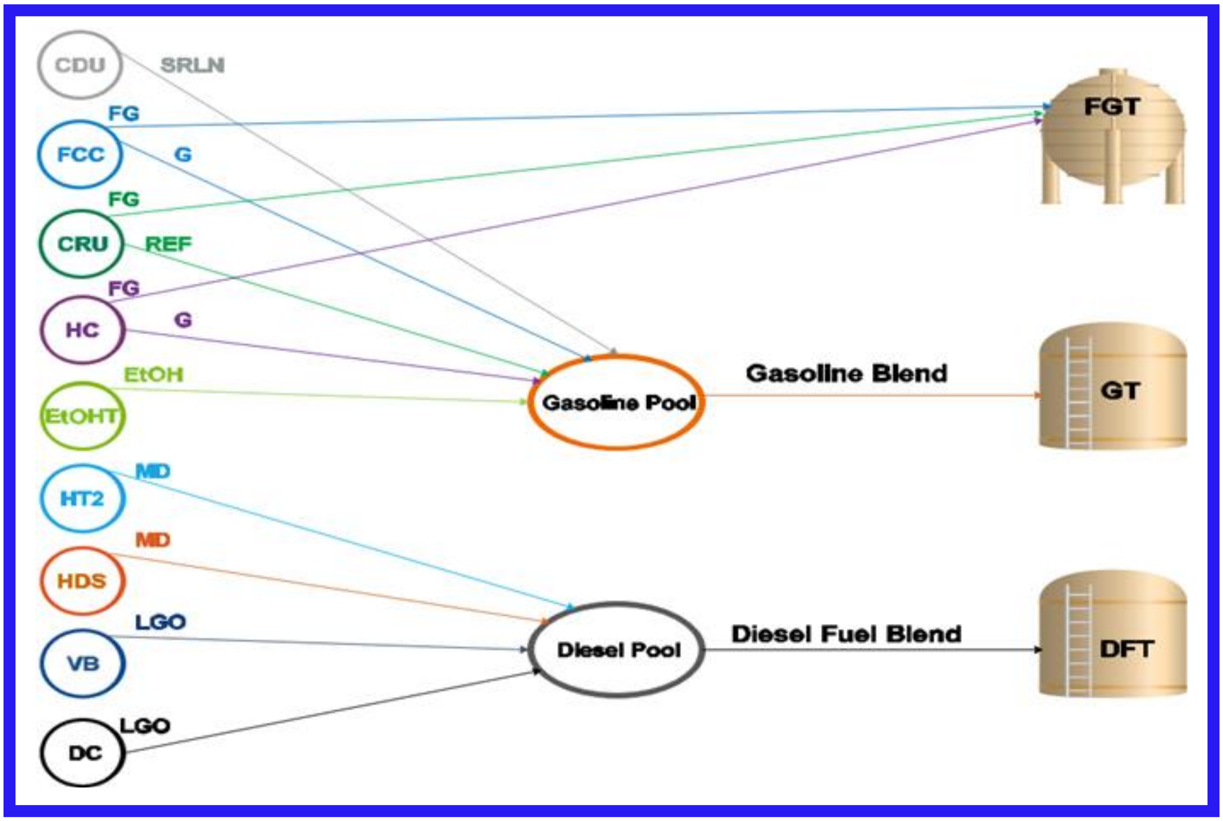

Figure 3.4. Schematic Diagram of the Product Pooling Problem in this Study.

CRU.REF.GP, *CRU.FG.FGT*, *HC.G.GP*, *HC.FG.FGT*, *EtOHT.EtOH.GP*, *HDS.MD.DFP*, *HT2.MD.DFP*, *VB.LGO.DFP*, *DC.LGO.DFP}* summarizes the potential connection and path of these streams. From the five attributes RON (research octane number) and MON (motor octane number) are to be within the specific quality domains for the gasoline product and CI (cetane index), S (sulfur content) and Vis122 (viscosity at 122 °F, cSt) to be met for the diesel fuel product. The set *qual={RON, MON, CI, S, Vis122}* also represents these qualities. For the final product pooling problem in this study a pq-formulation has been applied. For a detailed account of the pooling problem and pq-formulation in particular the interested reader is referred to Tawarmalani and Sahinidis. [105] The final product pooling problem model in this study is solved as a component of the refiner production planning model and its objective is to produce final products whose outlet flowrate and terminal qualities meets the customer demand and specifications for the relative products. Therefore, its costs have been accounted for as the operating costs within the production planning objective function. However, the constraints for the pooling problem are presented as follows:

3.3.3.1.Flow Constraints

1.The amount of product *pro* coming from product pooling *pool* at time period *t*, that is $yy(pool, pro, t)$, should be within the bounds of the product demand and the pool capacity:

$$yy(pool, pro, t) \geq demand(pro, t) \qquad (3.8)$$

$$yy(pool, pro, t) \leq psize(pool) \qquad (3.9)$$

2. The sum of fractions $q(comp, pool, t)$ of the amount of product *pro* from product pooling *pool* at time period t which is contributed by component *comp* coming to *pool*, should be equal to one:

$$\sum_{comp} q(comp, pool, t) = 1 \qquad (3.10)$$

$$\forall\, comp, pool \ \ \backslash ubq(comp, pool) > 0$$

The conditional $ubq(comp, pool) > 0$ states that there is a connection between component *comp* and product pooling *pool*.

3. The sum of all fractions $q(comp, pool, t)$ of the amount of product *pro* from product pooling *pool* at time period t which is contributed by components *comp* coming to *pool*, should be equal to its total amount $yy(pool, pro, t)$:

$$\sum_{comp}[q(comp,pool,t) * \ yy(pool,pro,t)] = yy(pool,pro,t) \qquad (3.11)$$

$$\forall\ comp,pool\ \ \backslash ubq(comp,pool) > 0$$

$$\forall\ pool,pro\ \ \backslash uby(pool,pro) > 0$$

The conditional $uby(pool,pro) > 0$ also states that there is a connection between product pooling *pool* and product *pro*.

3.3.3.2. Quality Constraints

1.The quantity of the property $qual$ of the product *pro* from all components $comp$ and all product pooling *pool*, should be within the specific lower and upper bounds:

$$\sum_{pool}\sum_{comp}[cqual(comp,qual) * q(comp,pool,t) * \ yy(pool,pro,t)]$$

$$\geq \sum_{pool}[pqlbd(pro,qual) * \ yy(pool,pro,t)] \qquad (3.12)$$

$$\forall\ comp,pool\ \ \backslash ubq(comp,pool) > 0$$

$$\forall\ pool,pro\ \ \backslash uby(pool,pro) > 0$$

$pqlbd(pro,qual)$ represents the lower bound value for quality *qual* of product *pro*.

$$\sum_{pool}\sum_{comp}[cqual(comp,qual) * q(comp,pool,t) * \ yy(pool,pro,t)]$$

$$\leq \sum_{pool}[pqubd(pro,qual) * \ yy(pool,pro,t)] \qquad (3.13)$$

$$\forall\ comp,pool\ \ \backslash ubq(comp,pool) > 0$$

$$\forall\, pool, pro \quad \backslash uby(pool, pro) > 0$$

$pqubd(pro, qual)$ represents the upper bound value for quality *qual* of product *pro*.

3.4. Final Product Distribution by Pipeline

Regarding the large volume of the petroleum products transported by pipeline across the globe, in this study a multiproduct pipeline for the purpose of final product distribution to depot has been considered. Petroleum products distribution by pipeline is also a widely explored problem for which variety of models have been presented. In this study, a multiproduct pipeline distribution model has been adopted from Moradi & MirHassani. [121] Figure 3.5. demonstrates a real-world pipeline network.

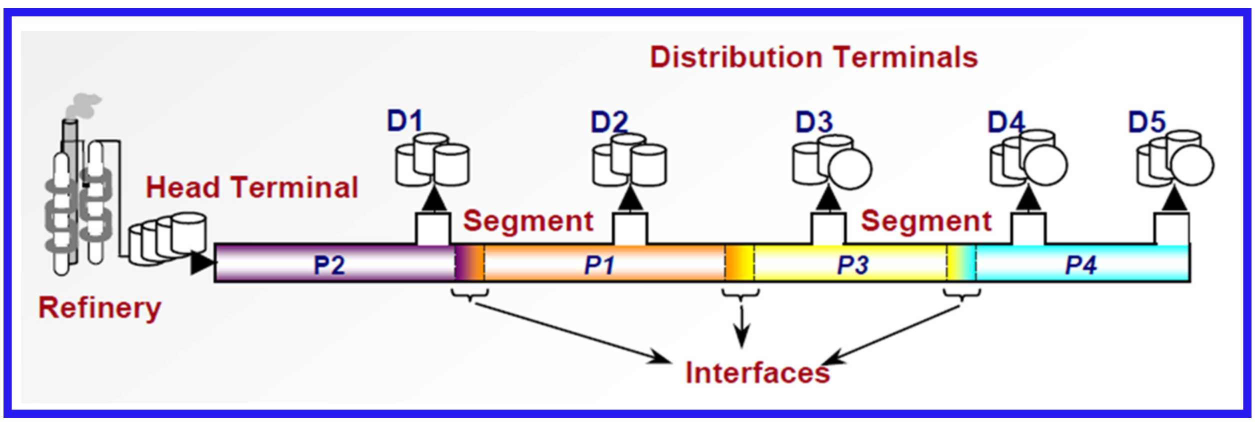

Figure 3.5. A Real-world pipeline network

The final products distribution by the multiproduct pipeline model is characterized by 43 correlations representing product allocation to the batches, Lot-sizing, inventory management at the refinery and the distribution center, calculation of contaminated interface volume between consecutive batches of different products, discharging time of bathes at the DC, peak electricity hours and the initial conditions of the pipeline at the beginning of the scheduling horizon. A brief representation of the mathematical model for the product distribution by pipeline is represented in Appendix B and a detail account is referred to Moradi and MirHassani. [121]

The objective function for the pipeline distribution is a multi-criteria function both operationally and economically motivated and is generated by normalizing the objective function terms (Moradi & MirHassani. [121]):

(a) The difference between the total discharged volume and the total demands of customers is minimized:

$$minZ_1 = \frac{diff}{\sum_{t \in T} \sum_{p \in P} Dem_{t,p}} \quad (3.14)$$

(b) The minimum inventory level among all of the products on the last day of the scheduling horizon ($minid$) is maximized. A minmax strategy is utilized to maximize the inventory level of the product with the lowest final inventory level:

$$\max\,(Z_2 = minid) \quad (3.15)$$

$$minid \leq \frac{inv_{|T|,p}^{total}}{inv_p^{max}} \qquad \forall\, p \in P \quad (3.16)$$

(c) The underutilized pipeline capacity within the entire hours of the scheduling horizon is minimized:

$$minZ_3 = \frac{1}{|T|} \sum_{t \in T} \left(\frac{dd_t - T_{|I|,t}^{dis}}{dd_t}\right) \qquad (3.17)$$

(d) The total violated peak electricity hours is minimized:

$$minZ_4 = \frac{1}{|T|} \sum_{t \in T} \left(\frac{ph_t}{peak_t}\right) \qquad (3.18)$$

(e) The total volume of contaminated interfaces occurring between two consecutive injection of different products is minimized:

$$minZ_5 = \frac{1}{|I||T|max_{p,q}(waste_{p,q})} \sum_{i \in I} \sum_{t \in T} inf_{i,t} \qquad (3.19)$$

(f) The back-order or demand loss resulting from the delays in meeting the customer demands by the due dates is minimized:

$$minZ_6 = \frac{1}{|P||T|B_{max}} \sum_{p \in P} \sum_{t \in T} B_{p,t} \qquad (3.20)$$

Thus, the overall pipeline objective function is as follows.

$$COPR_{PD} = w_1 Z_1 + w_2 Z_2 + w_3 Z_3 + w_4 Z_4 + w_5 Z_5 + w_6 Z_6 \qquad (3.21)$$

The first three terms of the objective function are operational and the remaining three are economical. w_l is the weight of the objective *l* indicating the significance and priority of this criteria in the objective function. For the purpose of this study all w_l are equal to 1 and all terms of the objective function are of the same priority.

3.5. Refinery Utility System

The industrial sector is reliant on utility supply of electricity, steam, hot water and other utilities to support its manufacturing processes. Plant machinery such as mixers, let-down valves, boilers, compressors, and condensers, are used for this purpose. Nowadays, high-energy intensive industries are inclined to produce all of their own needed utilities and particularly electricity. Such industrial processes are referred to as combined heat and power (CHP) or auto-production. CHP is an integrated technology as it simultaneously enhances the process energy efficiency while minimizing carbon footprint and greenhouse gas emissions.[123] For the refining industry with onsite utility systems, CHP is a popular technology. In this study, a utility system model has been adopted from Agha et al.[67] The objective of this section is to describe this utility system model that will be integrated with the refinery production process.

While only fuel gas is produced internally by the refinery and considered, the model allows utilizing more than one fuel type for the utility system. Figure 3.6 represents a simplified representation of this system which is a slightly modified version adopted from Agha et al. [67]

The utility system model is characterized by 29 correlations representing fuel gas storage model, boiler model including associating fuel consumption with steam generation, boiler shutdown and restart constraints, harmful gas emission constraints, returned electricity for boiler consumption and steam return constraints, turbine and mixer models. A brief representation of the mathematical model for the utility system is presented in Appendix C and a detailed account is available in Agha et al.[67]

The criterion used for the CHP based utility model objective function is the minimization of operational costs comprising of fuel cost, electricity purchase cost and penalty cost incurred due to the emission of harmful gases.

$$COPR_{UTIL} = \sum_{t}^{T} \sum_{j \in BOIL} \sum_{i \in FUEL} cf_i * (I_{t,j,i} + SI_{t,j,i}) + \sum_{t}^{T} ELP_t * CEL$$

$$+ \sum_{t}^{T} \sum_{j \in BOIL} XSOX_{t,j} * CSOX + \sum_{t}^{T} \sum_{j \in BOIL} XGHG_{t,j} * CGHG \qquad (3.22)$$

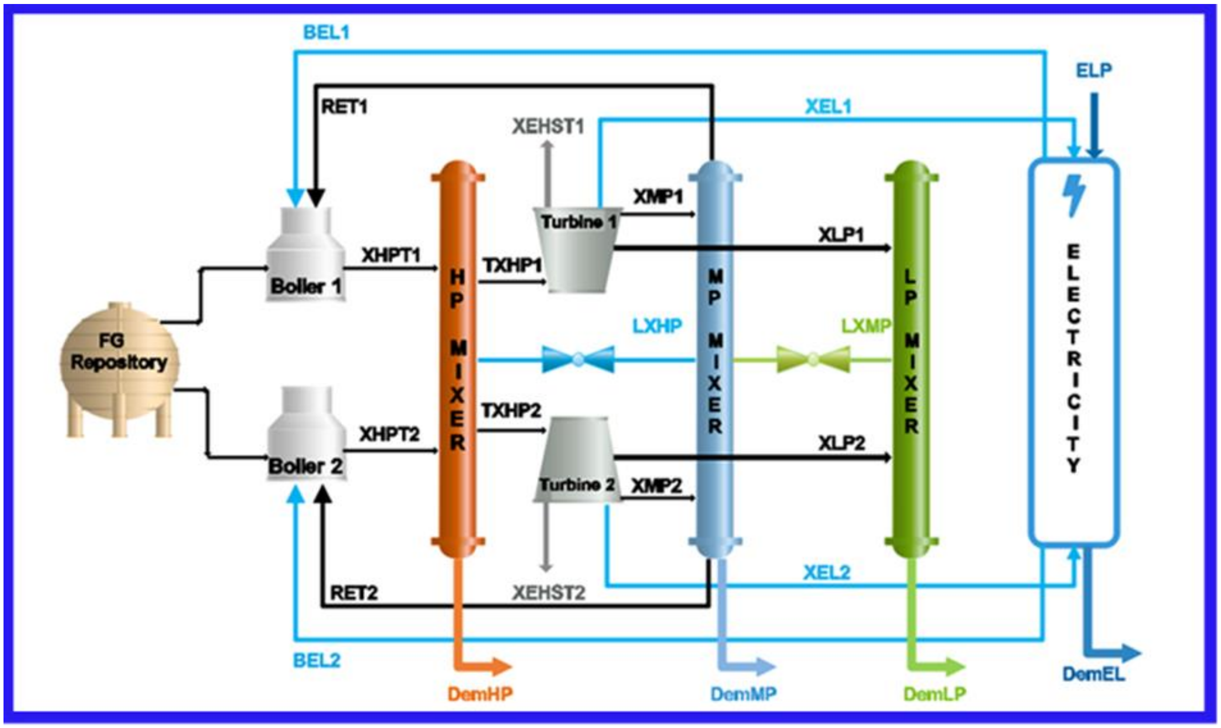

Figure 3.6. Simplified Representation of the CHP based Utility System in this Study [67]

3.6. Integration Constraints

To achieve the integration across the refinery departments, the inputs and outputs of every sub-system should be correlated through the integration constraints:

1.Unloading to production constraints:

The amount of the crude blend coming out of the blending tank at time period t in the unloading model should be equal to the same amount going to the CDU at time period t in the production model:

$$\sum_{l=1}^{NCDU} \sum_{j=1}^{NBT} FBC_{j,l,t} = Am('CT','CB','CDU',t) \qquad \forall t = 1, \dots, NSCH \qquad (3.23)$$

2.Production to product pooling problem constraints:

In every time period, the amount of all the components $comp$ entering the product pooling $pool$ in the pooling problem, should be equal to the amount of all the commodities *c* coming from all units *u* entering the respective blending unit *bu* (gasoline or diesel pool) in the production model providing that these commodities and units are in the path of the respective blending unit :

$$\sum_{comp} [q(comp, pool, t) * \ yy(pool, pro, t)] = \sum_{u} \sum_{c} Am(u, c, bu, t) \qquad (3.24)$$

$$\forall bu \in \{GP, DFP\}, pool \in \{1,2\}, pro \in \{1,2\}$$

$$\backslash ubq(comp, pool) > 0 \ \ and \ \ \backslash uby(pool, pro) > 0 \ \ and \ \ path(u, c, bu)$$

3.Pooling problem to pipeline distribution constraints:

In every time period, the amount of the respective product pro coming from the product pooling $pool$ in the pooling problem should be equal to the amount of the respective product P produced in the refinery side of the pipeline distribution model:

$$yy(pool, pro, t) = prate_{t,P} \qquad (3.25)$$

$$\forall t = 1, \dots, NSCH, , pool \in \{1,2\}, pro \in \{1,2\}, P \in \{P1, P2\} \quad \backslash uby(pool, pro) > 0$$

$prate_{t,P}$ terms appear in equations (99-100) of the pipeline distribution model.

4.*Production to utility system constraints:*

In every time period, the total amount of the fuel gas coming from all the respective units and entering the fuel gas tank in the production /pooling model should be equal to the amount of the utility fuel entering the fuel repository in the utility model:

$$\sum_{u} Am\,(u, 'FG', 'FGT', t) = PRF_{t,i} \qquad \forall t = 1, \dots, NSCH \qquad (3.26)$$

5. Overall integrated model objective function:

The overall objective function for the integrated refinery model is the net revenues from the production/pooling model minus the operating costs incurred by crude unloading, pipeline distribution and utility system:

$$Profit = REV_{PROD} - COPR_{UNL} - COPR_{PD} - COPR_{UTIL} \quad (3.27)$$

3.7.Proposed Solution Methodology

The integrated refinery problem $(\boldsymbol{P})$ considered in this study, can be represented as a nonconvex, mixed-integer nonlinear constrained problem (MINLP) with the following generic form as outlined by Castro et al.[112]:

$$\max f_0(x,y) \quad (3.28)$$

$$\text{subject to} \quad f_q(x,y) \le 0 \quad \forall q \in Q \setminus \{0\}$$

$$f_q(x,y) = \sum_{(i,j)\in BL} a_{ijq}\, x_i\, x_j + B_q(x) + C_q(y) + d_q \quad \forall q \in Q$$

$$0 \le x^L \le x \le x^U$$

$$x \in R^m, y \in \{0,1\}^r \quad (\boldsymbol{i},\boldsymbol{j}) \quad (\boldsymbol{P})$$

Where vector $\boldsymbol{x}$ denotes continuous non-negative variables and $\boldsymbol{y}$ is a vector of binary variables. Set *BL* represents an (i,j)-index set that represents the bilinear $x_i x_j$ terms in the problem.

$B_q(x)$ is nonlinear in x and $C_q(y)$ includes binary variables. Set Q accounts for all functions f_q, the objective function f_0 and all the constraints, a_{ijq} and d_q are scalars.

As discussed earlier, this MINLP model for the integrated refinery problem is nonlinear and nonconvex due to the bilinear or quadratic terms in some of the material balance and blending correlations and highly nonlinear terms due to the presence of signomial, exponential or logarithmic terms in the yield and quality constraints. To handle this nonlinearity and nonconvexity, a bi-level optimization strategy is devised .To linearize highly nonlinear terms, a lumped variable linearization (LVL) technique has been utilized in this study. In LVL, all variables x_i within a nonlinear term NLT in a constraint are aggregated into one lumped variable LV and the entire statement is linearized. Prior to running the model, an initial value from the industrial data adopted from HPI manual [116] is assigned to every variable $(x_i.l)$ and the overall calculated value is assigned to the initial value of the linearized lumped variable in the model $(LV.l)$. Equation29 represents this concept in a mathematical definition:

$$NLT = f(x_i) \xrightarrow{\textbf{\textit{Apply LVL}}} LV \xrightarrow{\textbf{\textit{Assign Initial Values}}} LV.l = f(x_i.l) \qquad (3.29)$$

To handle the bilinear or quadratic terms, normalized multiparametric disaggregation technique (NMDT) [106-113] has been utilized which is adopted from Castro[112] and explained shortly in the following paragraphs. A summarized context of implementing normalized multiparametric disaggregation technique is outlined in Appendix D and a detail scope is referred to Kolodziej et al.[106.110], Castro et al.[109,111-112], Andrade et al.[113] and Teles et al.[107,108]

Assuming a nonconvex bilinear term $w_{i,j} = x_i x_j$, multiparametric disaggregation operates by discretizing x_j over a set of powers , $l \in \{p, \ldots, P\}$,where $P = \lfloor \log_{10} x_j^U \rfloor$ and p is a user defined value for a desirable accuracy level. [106,108,111] The radix based relations for P are on a radix 10 discretization basis for the purpose of our study. Normalized version of multiparametric disaggregation technique discretizes $\lambda_j \in [0, 1]$, an auxiliary variable that is used to represent x_j as a linear combination of its lower x_j^L and upper x_j^U bounds:

$$x_j = x_j^L + \lambda_j\left(x_j^U - x_j^L\right) \quad \forall\, j \qquad (3.30)$$

Figure 3.7. depicts the continuous representation of variable λ_j achieved by discretizing the domain up to a certain level p and adding a bounded variable Δλj.

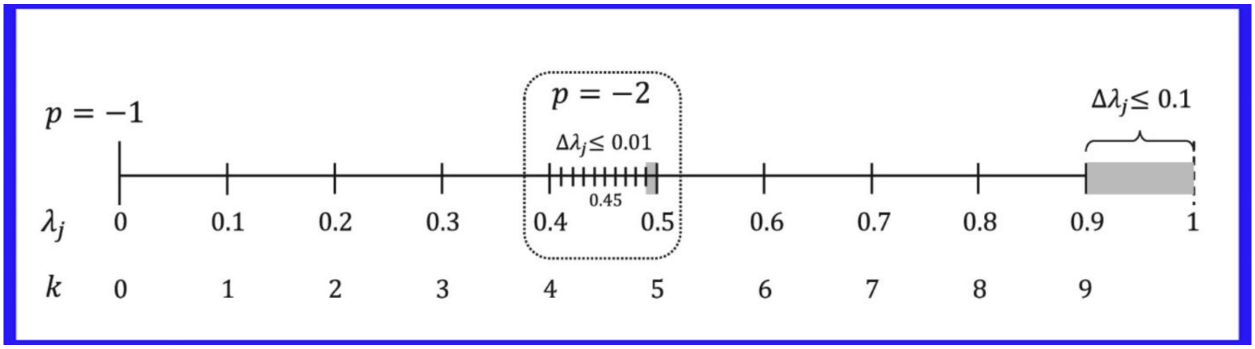

Figure 3.7. The continuous representation of variable λ_j by discretizing the domain up to a certain level p and adding a bounded variable Δλj [112]

The implementation of the normalized multiparametric disaggregation technique (NMDT) leads to the exact representation of bilinear terms $w_{ij} = x_i x_j$ through a set of mixed integer linear constraints resulting a relaxed optimization problem (PR) that is a relaxation of (P) (Castro et al.[111,112]) :

$$\max \quad f_0'(x, y) \tag{3.31}$$

$$subject\ to \qquad f_q'(x, y) \leq 0 \qquad \forall q \in Q \setminus \{0\}$$

$$f_q'(x, y) = \sum_{(i.j) \in BL} a_{ijq}\, w_{ij} + B_q(lv) + C_q(y) + d_q \qquad \forall q \in Q$$

$$\left.\begin{array}{c} x_j = x_j^L + \lambda_j\left(x_j^U - x_j^L\right) \\ \lambda_j = \sum_{l=p}^{-1} \sum_{k=0}^{9} 10^l . k . z_{jkl} \; + \; \Delta\lambda_j \\ 0 \leq \Delta\lambda_j \leq 10^p \end{array}\right\} \quad \forall j \in \{j | (i, j) \in BL\}$$

$$\left.\begin{array}{c} w_{ij} = x_i x_j^L + v_{ij}\left(x_j^U - x_j^L\right) \\ v_{ij} = \sum_{l=p}^{-1} \sum_{k=0}^{9} 10^l . k . \hat{x}_{ijkl} + \Delta v_{ij} \\ x_i^L . \Delta\lambda_j \le \Delta v_{ij} \le x_i^U . \Delta\lambda_j \\ \Delta v_{ij} \le (x_i - x^L) . 10^p + x_i^L . \Delta\lambda_j \\ \Delta v_{ij} \ge (x_i - x^U) . 10^p + x_i^U . \Delta\lambda_j \end{array}\right\} \quad \forall (i,j) \in BL$$

$$x_i = \sum_{k=0}^{9} \hat{x}_{ijkl} \qquad \forall (i,j) \in BL, l \in \{p, \dots, -1\}$$

$$\sum_{k=0}^{9} z_{jkl} = 1 \qquad \forall j \in \{j | (i,j) \in BL\}, l \in \{p, \dots, -1\}$$

$$z_{jkl} x_i^L \le \hat{x}_{ijkl} \le z_{jkl} x_i^U \qquad \forall\, (i,j), \;\; k \in \{0, \dots, 9\}, l \in \{p, \dots, -1\}$$

$$0 \le x^L \le x \le x^U$$

$$x \in R^m, w_{ij}, \lambda_j, v_{ij}, \hat{x}_{ijkl}, \Delta\lambda_j, \Delta v_{ij} \in R$$

$$y \in \{0,1\}^r, z_{jkl} \in \{0,1\} \qquad (\boldsymbol{PR})$$

This leads to a mixed integer linear program (MILP) of the integrated refinery problem. By this manner, upon running the model, an upper bound value for the problem (P) is calculated and the binary variables are relaxed by assigning them their initial value from the previous run. In the next step, a nonlinear problem (NLP) is solved using a commercial global solver BARON to $\varepsilon = 10^{-6}$ optimality criteria and global optimal solution for the integrated refinery problem is obtained in a reasonable solution time. Figure 3.5 illustrates the flowchart for the proposed solution algorithm.

3.8. Deterministic Integrated Refinery Case Study

The mathematical framework based on the crude unloading, blending and inventory management, crude procuring and production planning, final product pooling problem, final product distribution by pipeline, utility system, the overall objective function of the integrated problem and specific constraints for the solution strategy are used to develop the entire integrated refinery planning model. The numerical results and discussion is presented in chapter 5.

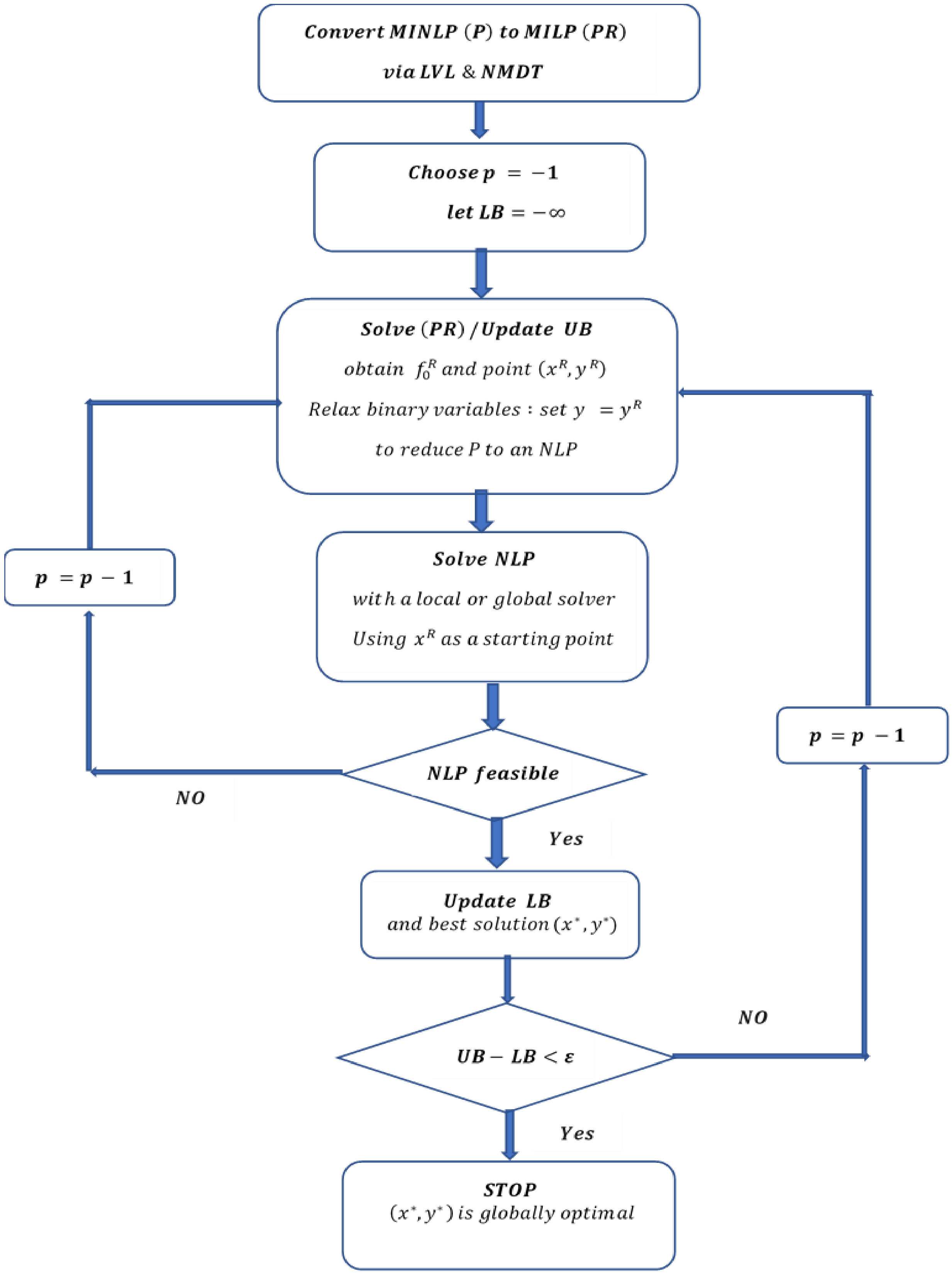

Figure 3.8. Algorithmic Flowchart for the Proposed Solution Methodology.

Chapter 4

STOCHASTIC INTEGRATED REFINERY MODEL

4.1. Preface

In this chapter, the stochastic integrated refinery model is employed for the strategic enterprise-wide planning of the integrated refinery where the uncertainties in the final product demand and crude oil and final product market prices are accounted for. The uncertainties are handled through three modeling schemes: (1) a robust optimization algorithm with a known probability distribution function for the uncertain parameters (2) a fuzzy possibilistic programming approach, where possibility and necessity measures are adopted to reflect the decision makers' risk preference (3) a risk aversion two-stage stochastic model coupled with Monte Carlo sampling with 100 independent realizations of uncertain demand and price data while managing the financial risk through imposing a penalty for risk by inclusion of the downside risk metric in the objective function. These methodologies are applied to an industrial case study, considering operations in a broad range of refinery supply chain integrating decisions such as crude unloading, crude procurement while accounting for the highly nonlinear nature of processing units, final product pooling and blending, inventory management, scheduling of product distribution by pipeline, utility system and environmental impacts. The planning horizon extends over a span of 7 years period. Further, in this study, broad comparisons are drawn between the solutions of three methodologies in handling uncertainty in terms of economic and operational objectives to illustrate the potential and trade-offs involved with these different methodologies. The results indicate significant economical and operational differences between the outcomes of three methodologies while highlighting an obvious advantage of the robust optimization scheme depending on the decision maker's risk attitude.

The proposed strategy can be used as an effective decision-support tool for enterprise wide integrated production planning of an oil refinery in presence of uncertainty. These decisions range from adjusting the temperature distribution within the distillation unit to the process severity within the other refinery units to obtain desired cut point temperatures and maximum yield and desired property of final products which in turn results in a higher profit for a certain amount of crude feedstock. In addition, it provides a tool for refinery planner to make mitigating decisions on utility units operation, energy consumption, startup/shutdown operations, pipeline utilization, batch sequencing within pipeline and mitigate delayed or lost consumer demands and so on.

To meet these objectives, the rest of this chapter is organized as follows: The problem statement is presented in the next section. The mathematical model for three methodologies in uncertainty treatment are outlined in section 3. The computational study results and discussion are presented in chapter 6.

4.2.Problem Statement

The focus of this study is the strategic planning for an integrated oil refinery with uncertainty in product demand and price data for both crude oil and final products. For an accurate and realistic modeling outcome both of these uncertainties need to be explicitly modeled within the planning strategy. The integrated refinery under study is identical to the system discussed in chapter 3 under the deterministic model.

Uncertainty in demand and price data appear in the coefficients of the objective function as uncertain price data, as well as the coefficients and right-hand-side parameters of the inequality constraints as uncertain demand data.
The corresponding stochastic integrated refinery planning model is similarly a nonconvex mixed integer nonlinear programming model (MINLP) and nonlinearity and nonconvexity within the model will be treated by the same an aggregation /disaggregation solution methodology based on lumped variable linearization (LVL) and normalized multiparametric disaggregation (NMDT) techniques.

The stochastic integrated refinery problem will be formulated based on the same knowns and unknowns for the deterministic model with the exception that the planning horizon is 7 years and demand and price data are stochastic. The framework based on the objectives and constrains from the integrated refinery sub-systems, the methodologies to model uncertainty, and the heuristic to handle the nonlinearity and nonconvexity within the model is the underlying foundation for modeling and solving the stochastic integrated refinery problem in this study.

4.3.Mathematical Model

A stochastic multiperiod mixed integer-nonlinear programming (MINLP) model for the strategic enterprise-wide planning of an integrated refinery is developed while accounting for the uncertainties in the final product demand and crude oil and final product market prices. The constraints and variables in the models of refinery sub-systems are identical to the deterministic integrated refinery model with the exception of the following. The overall objective function for the integrated refinery model is the revenues from the final products' sales minus the costs of purchasing crude oils and intermediates within the production/pooling model-where the uncertainty in price data will be manifested- minus the investment costs for capacity expansion and operating costs incurred by crude unloading, utility system and pipeline distribution-where the uncertainty in the right-hand-side parameters of demand data will be handled.

In addition, as discussed earlier, to model uncertainty through three methodologies the respective constraints and variables of the robust optimization scheme, fuzzy programming and two-stage stochastic programming with financial risk management are incorporated in the model.

A brief account of the refinery models are outlined in appendices A-F in supporting materials. For a comprehensive description of these models the interested reader is encouraged to refer to Siamizade[55] and Siamizade and Trafalis[114,115].

4.3.1.Constraints with Uncertain Parameters

As discussed earlier, uncertainty in price data is manifested in the coefficients of the production objective function and uncertainty in demand data are appeared as the coefficients and right-hand-side parameters of the product inventory and discharge constraints in the pipeline model. In the light of this clarification, the production objective function can be expanded as follows to display where the uncertain price parameters are correlated:

$$Profit = \sum_{u,c,u'} [Am(bu, fpr, stank) * Prices(fpr) - Fin(c, u) * OC(u) - Am(ctank, o, CDU) * Prices(o) - Am(EtOHT, EtOH, GP) * Prices(EtOH)] \quad (4.1)$$

For demand data, the total inventory level of product p on DC end at the end of day t ($inv_{t,p}^{total}$) correlates to the inventory from the previous day, sum of all batches discharged from the pipeline during day *t* ($\sum_i W_{i,t,p}$), backorders from the same day ($B_{t,p}$) and previous day ($B_{t-1,p}$), and the demand on day *t* ($Dem_{t,p}$).Thus, for the first day, we have:

$$inv_{t,p}^{total} - Initv_p - \sum_{i \in I} W_{i,t,p} - B_{t,p} \geq Dem_{t,p} \quad \forall\, t \in T, t = 1, p \in P \quad (4.2)$$

And for other days, we have:

$$inv_{t,p}^{total} - inv_{t-1,p}^{total} - \sum_{i \in I} W_{i,t,p} + B_{t-1,p} - B_{t,p} \geq Dem_{t,p} \quad \forall\, t \in T, t > 1, p \in P \quad (4.3)$$

In the following sections, we will elaborate the 3 different methodologies mentioned earlier to model these uncertainties.

4.3.2. Robust Optimization Framework

Robust design can be regarded as an optimization approach which accounts for uncertainties by constructing robust counterparts F of the original objective function. By applying the robust counterpart methodology, the solution of the problem can be immune against the perturbations of the uncertain parameters.[78]

Similar to the generic form of the stochastic mixed-integer linear programming problem considered by Janak and Floudas [92], the stochastic mixed-integer nonlinear programming problem (MINLP) of the integrated refinery can be represented as follows:

$$\textbf{max} \quad f_0(x, y) \quad (4.4)$$

$$\textbf{s.t.} \quad f_l(x, y) = A_l(x) + B_l(y) + \sum_{(i,j) \in BL} c_{ijl}\, x_i x_j + d_l \leq 0 \quad \forall l \in L \subset Q$$

$$f_u(x, y) = A_u(x) + B_u(y) \leq p \quad \forall u \in U \subset Q$$

$$0 \leq x^L \leq x \leq x^U$$

$$x \in R^m, y \in \{0,1\}^k \quad (\boldsymbol{P})$$

where $\boldsymbol{x}$ is a vector of continuous non-negative variables and $\boldsymbol{y}$ are binary variables. BL is an (i,j)-index set that defines the bilinear $x_i x_j$ terms present in the problem. $A_q(x)$ is nonlinear in x and $B_q(y)$ includes binary variables. Set Q is the set of all constraints: set L includes all functions f_l with bilinear and highly nonlinear terms, set U includes all functions f_u and the objective function f_0 which contains the uncertain parameters and c_{ijl} and d_l are scalars. Supposing that the uncertainty arises from both the coefficients and the right-hand-side parameters of the inequality constraints, namely, a_{um}, b_{uk} and p_u where u is the index of the uncertain inequality, m is the index of the continuous terms, and k is the index of the binary terms. Thus, we are concerned about the feasibility of the following inequality:

$$\sum_m \tilde{a}_{um} x_m + \sum_m \tilde{b}_{uk} y_k \leq \tilde{p}_u \qquad (4.5)$$

Where a_{um} , b_{uk} and p_u are the nominal values of the uncertain parameters and $\tilde{a}_{um}, \tilde{b}_{uk}$ and $\tilde{p}_u$ are the "true" values of the uncertain parameters and (~) sign denotes the uncertain parameters. Let's assume that for inequality constraint u , the true values of the uncertain parameters are obtained from their nominal values by random perturbations

$$\tilde{a}_{um} = (1 + \epsilon\xi_{um})a_{um}$$

$$\tilde{b}_{uk} = (1 + \epsilon\xi_{uk})b_{uk} \qquad (4.6)$$

$$\tilde{p}_u = (1 + \epsilon\xi_u)p_u$$

where ξ_{um}, ξ_{uk} and ξ_u are independent random variables and $\epsilon > 0$ is a given (relative) uncertainty level.

In this situation, a solution (x, y) is called robust if it satisfies the following (i) *(x, y)* is feasible for the nominal problem, and (ii) for every inequality u , the probability of violation of the uncertain inequality in Equation (4.5) (i.e., the left-hand-side exceeds the right-hand-side) is at most κ, here $\delta > 0$ is a given feasibility tolerance and is introduced to allow a small amount of infeasibility in the uncertain inequality, and κ > 0 is a given reliability level. Thus, κ represents the probability of violation of constraint u where κ = 0% indicates that there is no chance of constraint violation, yielding the most conservative solution. [92]

$$Pr\left\{\sum_{m} \tilde{a}_{um}\, x_m + \sum_{m} \tilde{b}_{uk}\, y_k > \tilde{p}_u + \delta \max[1, |p_u|]\right\} \leq \kappa \qquad (4.7)$$

This robust optimization methodology was first introduced for linear programming problems with uncertain linear coefficients by Ben-Tal and Nemirovski [124] and was extended in Lin et al.[125] and Janak et al.[92] to consider uncertainty in MILP problems. Thus, in this work, our objective is to extend this robust optimization framework to MINLP problems to generate "robust counterpart" problem whose solution is "reliable" and immune against uncertainty that can be described by a known probability distribution.

If the probability distributions of the random variables ξ_{um}, ξ_{uk} and ξ_u in the uncertain parameters are known, it is possible to obtain a more accurate estimation of the probability measures involved. Suppose that the distributions of the random variables ξ_{um}, ξ_{uk} and ξ_u in equation (4.6) are all standardized normal distributions with known mean and standard deviation. Then, given an uncertainty level (ϵ), an infeasibility tolerance (δ), and a reliability level (κ), the following will be the (ϵ, δ, κ)-robust counterpart ($RC[\epsilon, \delta, \kappa]$) of the original uncertain MINLP problem (p) from (4):

$$\mathbf{max} \qquad f_0(x,y) \qquad\qquad (4.8)$$

$$\mathbf{s.t.}$$

$$f_l(x,y) = A_l(x) + B_l(y) + \sum_{(i,j)\in BL} c_{ijl}\, x_i x_j + d_l \le 0 \quad \forall l \in L \subset Q$$

$$f_u(x,y) = A_u(x) + B_u(y) \le p \qquad \forall u \in U \subset Q$$

$$\sum_m a_{um}\, x_m + \sum_k b_{uk}\, y_k + \epsilon\lambda \sqrt{\sum_{m\in M_u} a_{um}^2\, x_{um}^2 + \sum_{k\in K_u} b_{uk}^2\, y_k + p_u^2}$$

$$\le p_u + \delta \max\,[1, |p_u| \qquad \forall u$$

$$0 \le x^L \le x \le x^U$$

$$x \in R^m, y \in \{0,1\}^k$$

where M_u and K_u define the sets of uncertain parameters a_{um} and b_{uk}, respectively, for constraint u, $\lambda = F_n^{-1}(1-\kappa)$ and F_n^{-1} is the inverse distribution function of a random variable with standardized normal distribution. Thus, λ and κ are related as follows:

$$\kappa = 1 - F_n(\lambda) \qquad (4.9)$$

$$\kappa = 1 - \Pr(\xi \le \lambda)$$

$$\kappa = 1 - \int_{-\infty}^{\lambda} \frac{1}{\sqrt{2\pi}} \exp\left(\frac{-\xi^2}{2}\right) d\xi$$

where ξ is a random variable with standardized normal distribution. For proof and more detail, theorem 2 from Janak et al.[92] is recommended.

In light of these definitions, the constraints containing the uncertain parameters of price and demand data in equations (1-3) can be rewritten as follows to create the robust counterpart of the integrated refinery problem:

$$Profit \quad \leq$$

$$\sum_{u,c,u'}[Prices(fpr)\, Am(bu,fpr,stank) - Prices(o)Am(ctank,o,CDU) -$$

$$Prices(EtOH)Am(EtOHT,EtOH,GP) - Fin(c,u) * OC(u)] \ +\delta -$$

$$\epsilon\lambda\sqrt{\sum_{u,c,u'} Prices(fpr)^2\, Am(bu,fpr,stank)^2 - \sum_{u,c,u'} Prices(o)^2\, Am(ctank,o,CDU)^2 - \sum_{u,c,u'} Prices(EtOH)^2\, Am(EtOHT,EtOH,GP)^2}$$

$$(4.10)$$

Where the *Prices* are the nominal or the deterministic values of the price data.Thus for demand data for the first day, we have:

$$inv_{t,p}^{total} - \ Initv_p - \sum_{i\in I} W_{i,t,p} - B_{t,p} \ \geq Dem_{t,p}\,(1 + \ \epsilon\lambda - \delta\,) \quad \forall\, t \in T, t = 1, p \in P \ \ (4.11)$$

And for other days, we have:

$$inv_{t,p}^{total} - \ inv_{t-1,p}^{total} - \sum_{i\in I} W_{i,t,p} + B_{t-1,p} - B_{t,p} \ \geq Dem_{t,p}\,(1 + \ \epsilon\lambda - \delta\,)$$

$$\forall\, t \in T, t > 1, p \in P \quad (4.12)$$

Where the $Dem_{t,p}$ are the nominal or the deterministic values of the demand data for product *p* in time period *t*.

4.3.3. Fuzzy Possibilistic Programming Approach

Whenever the statistical data and probability distribution are unreliable or even unavailable for the uncertain parameters, fuzzy set and possibility theory may provide an alternative which is simpler and less data demanding than the probability theory to deal with supply chain uncertainties [97]. Fuzzy programming assumes that uncertain parameters in a mathematical model are fuzzy numbers defined on a fuzzy set associated with a membership function. The concept of fuzzy set, was first introduced by Bellman and Zadeh.[126]

Therefore, in this section, we utilize fuzzy set and fuzzy membership concept to describe these uncertainties. Tong et al.[97] describe the fuzzy possibility and necessity measures as follows: Assume μ_A is the membership function for a fuzzy member α in fuzzy set A. Possibility and necessity measures of the event that α is in another fuzzy set B are defined as follows (Bellman and Zadeh [126]; Inuiguchi [127]):

$$\Pi_A(B) = \sup_r min\big(\mu_A(r), \mu_B(r)\big) \quad (4.13)$$

$$\mathrm{N}_A(B) = \inf_r max\big(1 - \mu_A(r), \mu_B(r)\big) \quad (4.14)$$

where μ_B is the membership function for fuzzy set B, and $\Pi_A(B)$ determines the extent it is possible for the possibilistic variable α -restricted by the possibility distribution μ_A – to be in the fuzzy set B. Furthermore, $\mathrm{N}_A(B)$ determines the extent it is certain that the α is in fuzzy set B. Then the relationship between possibility and necessity is described as follows:

$$\Pi_A(B) = 1 - \mathrm{N}_A(B) \quad (4.15)$$

Now, let's assume $B = (-\infty, g]$, i.e. B is a crisp set of real numbers not greater than g. It is further assumed that α has a triangle membership function, where $[\alpha^p \;\; \alpha^m \;\; \alpha^o]$ represents the most pessimistic, most possible and most optimistic value of fuzzy number α. Figure 4.1 reconstructed from Tong et al.[97], is a helpful graphical representation to perceive the concept of possibility and necessity degree of $\alpha \leq g$.

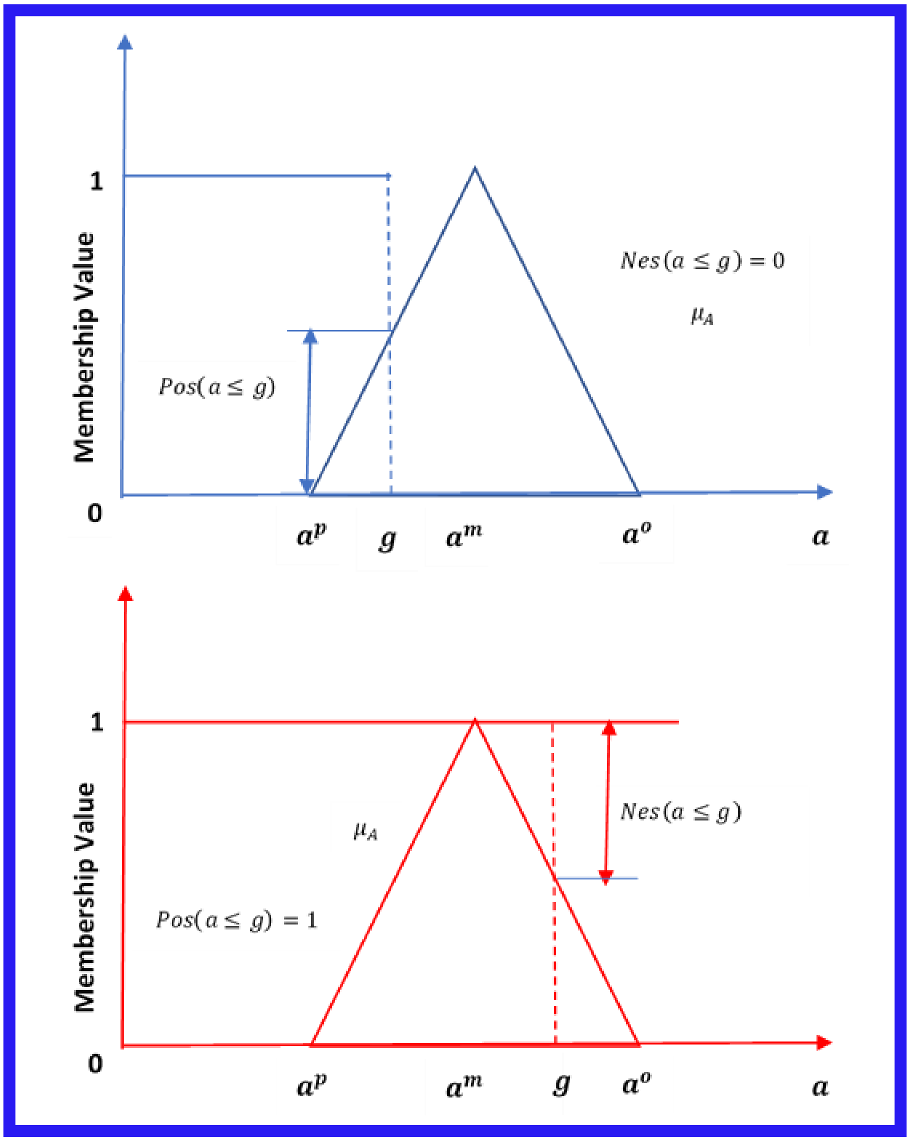

Figure 4.1. Possibility and necessity degree of $(a \leq g)$.[97]

Then we can easily obtain the interpretations for possibility and necessity in equations 4.16 and 17:

$$Pos(\alpha \le g) = \Pi_A\big((-\infty, g]\big) = \sup \{\mu_A(r) | r \le g\} \qquad (4.16)$$

$$= \begin{cases} 0 & g \le \alpha^p \\ \dfrac{g - \alpha^p}{\alpha^m - \alpha^p} & \alpha^p \le g \le \alpha^m \\ 1 & g \ge \alpha^m \end{cases}$$

$$Nes(\alpha \le g) = \mathrm{N}_A\big((-\infty, g]\big) = 1 - \sup \{\mu_A(r) | r > g\} \qquad (4.17)$$

$$= \begin{cases} 0 & g \le \alpha^m \\ \dfrac{g - \alpha^m}{\alpha^o - \alpha^m} & \alpha^m \le g \le \alpha^o \\ 1 & g \ge \alpha^o \end{cases}$$

By definition, we can conclude that if the attitude of the decision maker is optimistic, possibility measure is a good choice, while in the pessimistic sense necessity gives the measurement of the worst case of that event.

Similar to Tong et al.[97], we define a least possibility or necessity measure or confidence level θ at which the fuzzy constraints will hold. For the profit function (1) with fuzzy price parameters on it, we can reformulate it into equation (18), while maximizing C such that the possibility or necessity, for the objective value being greater than C is no less than the confidence level θ:

$$\mathbf{max} \qquad C$$

$$\mathbf{s.t.} \quad Pos/\,Nes\big(\widetilde{f_0}(x,y) \ge C\big) \quad \ge \theta \quad (4.18)$$

Similarly, for the constraints (2-3) where we have fuzzy uncertainties for demand data ,

we can simply use the following constraints:

$$\frac{Pos}{Nes\big(f_u(x,y) \ge \widetilde{Dem}\big)} \ge \theta \quad (4.19)$$

where C is the referenced profit and θ is the confidence level for the possibility or necessity of total profit being greater than C. The selection of these criteria is based on the decision maker's level of risk aversion and personal preference.

Equations (18,19) can be reformulated into linear representations. Consider the situation in which the possibility measure for α is less than or equal to g, we then use the following reformulations from Tong et al.[97] and according to equation (16,17):

$$Pos(\alpha \leq g) \geq \theta \Rightarrow g \geq \alpha^p + \theta.(\alpha^m - \alpha^p) \qquad (4.20)$$

$$Pos(\alpha \geq g) \geq \theta \Rightarrow g \leq \alpha^o - \theta.(\alpha^o - \alpha^m) \qquad (4.21)$$

$$Nes(\alpha \leq g) \geq \theta \Rightarrow g \geq \alpha^m + \theta.(\alpha^o - \alpha^m) \qquad (4.22)$$

$$Nes(\alpha \geq g) \geq \theta \Rightarrow g \leq \alpha^m - \theta.(\alpha^m - \alpha^p) \qquad (4.23)$$

To formulate the fuzzy possibilistic model for the integrated refinery planning, we decompose our profit function (1) into constraints (4.24-29) and reformulate it for possibility and necessity measures to constraints (30,31) respectively :

Possibility Measure:

$$\Big\{ Revenue\ (fpr) = \sum_{u,c,u'} [Am(bu, fpr, stank) * (Prices^o(fpr) - \theta_{price} * \big(Prices^o(fpr) - Prices^m(fpr)\big))] \qquad (4.24)$$

$$\{ Cost\ (o) = \sum_{u,c,u'} [Am(ctank, o, CDU) * (Prices^p(o) + \theta_{price} * \big(Prices^m(o) - Prices^p(o)\big))] \qquad (4.25)$$

$$\Big\{ Cost\ (EtOH) = \sum_{u,c,u'} [Am(EtOHT, EtOH, GP) * (Prices^p(EtOH) + \theta_{price} * \big(Prices^m(EtOH) - Prices^p(EtOH)\big))]$$

(4.26)

Necessity Measure:

$$\begin{cases} Revenue\ (fpr) = \sum_{u,c,u'} [Am(bu, fpr, stank) * (Prices^m(fpr) - \theta_{price} \\ \quad * \left(Prices^m(fpr) - Prices^p(fpr)\right))] \end{cases} \quad (4.27)$$

$$\begin{cases} Cost\ (o) = \sum_{u,c,u'} [Am(ctank, o, CDU) * (Prices^m(o) + \theta_{price} * \left(Prices^o(o) - Prices^m(o)\right))] \end{cases} \quad (4.28)$$

$$\begin{cases} Cost\ (EtOH) = \sum_{u,c,u'} [Am(EtOHT, EtOH, GP) * (Prices^m(EtOH) + \theta_{price} \\ \quad * \left(Prices^o(EtOH) - Prices^m(EtOH)\right))] \end{cases}$$

(4.29)

Possibility Measure:

$$Profit = \sum_{u,c,u'} [Am(bu, fpr, stank) * \left(Prices^o(fpr) - \theta_{price} * \left(Prices^o(fpr) - Prices^m(fpr)\right)\right) - Am(ctank, o, CDU) * \left(Prices^p(o) + \theta_{price} * \left(Prices^m(o) - Prices^p(o)\right)\right) - Am(EtOHT, EtOH, GP) * \left(Prices^p(EtOH) + \theta_{price} * \left(Prices^m(EtOH) - Prices^p(EtOH)\right) - Fin(c, u) * OC(u)\right] \quad (4.30)$$

Necessity Measure:

$$Profit = \sum\nolimits_{u,c,u'} [Am(bu, fpr, stank)$$

$$* \left(Prices^m(fpr) - \theta_{price} * \left(Prices^m(fpr) - Prices^p(fpr)\right)\right)$$

$$- Am(ctank, o, CDU) * \left(Prices^m(o) + \theta_{price} * \left(Prices^o(o) - Prices^m(o)\right)\right)$$

$$- Am(EtOHT, EtOH, GP)$$

$$* \left(Prices^m(EtOH) + \theta_{price} * \left(Prices^o(EtOH) - Prices^m(EtOH)\right)\right)$$

$$- Fin(c,u) * OC(u)\Big] \quad (4.31)$$

and constraints (4.2,3) for uncertain demand data are reformulated into constraints (4.32-35) for possibility and necessity measures of demand data:

Thus, for the first day of demand data , we have:

Possibility Measure:

$$inv_{t,p}^{total} - Initv_p - \sum_{i \in I} W_{i,t,p} - B_{t,p} \geq Dem_{t,p}^p + \theta_{Demand} * (Dem_{t,p}^m - Dem_{t,p}^p) \quad \forall\, t \in T, t = 1, p \in P \quad (4.32)$$

Necessity Measure:

$$inv_{t,p}^{total} - Initv_p - \sum_{i \in I} W_{i,t,p} - B_{t,p} \geq Dem_{t,p}^m + \theta_{Demand} * (Dem_{t,p}^o - Dem_{t,p}^m) \quad \forall\, t \in T, t = 1, p \in P \quad (4.33)$$

And for other days, we have:

Possibility Measure:

$$inv_{t,p}^{total} - inv_{t-1,p}^{total} - \sum_{i \in I} W_{i,t,p} + B_{t-1,p} - B_{t,p}$$
$$\geq Dem_{t,p}^{p} + \theta_{Demand} * \left(Dem_{t,p}^{m} - Dem_{t,p}^{p} \right) \quad \forall\, t \in T, t > 1, p \in P \quad (4.34)$$

Necessity Measure:

$$inv_{t,p}^{total} - inv_{t-1,p}^{total} - \sum_{i \in I} W_{i,t,p} + B_{t-1,p} - B_{t,p}$$
$$\geq Dem_{t,p}^{m} + \theta_{Demand} * \left(Dem_{t,p}^{o} - Dem_{t,p}^{m} \right) \quad \forall\, t \in T, t > 1, p \in P \quad (4.35)$$

Where $Prices^{p}$, $Prices^{o}$ and $Prices^{m}$ denote the most pessimistic, most optimistic and most possible uncertain price data for the commodities and $Dem_{t,p}^{p}$, $Dem_{t,p}^{o}$ and $Dem_{t,p}^{m}$ represent the most pessimistic, most optimistic and most possible uncertain demand data for the product p in time period t, and θ_{price} and θ_{Demand} denote the confidence level for the uncertain price and demand data.

4.3.4. Two-Stage Stochastic Programming with Financial Risk management

In this type of optimization problems some of the model parameters are considered uncertain random variables with a certain probability distribution. Some decisions are taken at the planning stage, that is, before the uncertainty is revealed, whereas a number of other decisions can be made only after the uncertain data become known. The first class of decisions are called first stage or “here and now” decisions, and their associated period is referred to as the first stage. On the other hand, the decisions made after the uncertainty is unveiled are called second-stage or “wait and see” or recourse decisions and the corresponding period is called the second stage.[128]

The second stage decisions are mitigative decisions in an attempt to adapt the design to the realization of uncertain parameters. The general form of a two-stage mixed-integer linear stochastic problem for a finite number of scenarios can be written as Birge and Louveaux [129] stated:

$$Max\ E[Profit] = \sum_{s \in S} p_s\, q_s^T y_s - c^T x \qquad (4.36)$$

$$s.t.\ Ax \leq b$$

$$T_s x + W y_s \leq h_s \qquad \forall s \in S$$

$$x \geq 0 \qquad x \in X$$

$$y_s \geq 0 \qquad \forall s \in S$$

In the above model, x represents the first-stage mixed-integer decision variables and y_s are the second-stage variables corresponding to scenario s, which has occurrence probability p_s. The objective function is composed of the expectation of the profit generated from operations minus the cost of first-stage model appear in the coefficients q_s, the technology matrix T_s, and in the independent term h_s. If W, the recourse matrix, is deterministic, the problem is referred as fixed recourse and ensures that the second-stage feasible region is convex and closed, and that the recourse function is a piecewise linear convex function in x.[129]

Eppen et al.[130] suggested that a major limitation of the two-stage stochastic models is that it does not take into account the variability of the second-stage profit but only its expected value. They proposed to use the concept of downside risk to measure the recourse cost variability and obtain solutions appealing to a risk-averse investor. To present the concept of downside risk, they assumed $\delta(x, \Omega)$ as the positive deviation from a profit target Ω for design x, that is

$$\delta(x, \Omega) = \begin{cases} \Omega - Profit(x) & if \quad Profit(x) < \Omega \\ 0 & otherwise \end{cases} \qquad (4.37)$$

To incorporate the concept of downside risk in the framework of two-stage stochastic models, $\delta_s(x, \Omega)$ is introduced as the positive deviation from the profit target Ω for design *x* and scenario *s* and defined as follows:

$$\delta_s(x, \Omega) = \begin{cases} \Omega - Profit_s(x) & if \quad Profit_s(x) < \Omega \\ 0 & otherwise \end{cases} \qquad \forall s \in S \qquad (4.38)$$

Because the scenarios are probabilistically independent, the expected value of $\delta(x, \Omega)$ (i.e., downside risk) can be expressed as the following linear function of δ

$$DRisk(x, \Omega) = \sum_{\forall s \in S} p_s \delta_s(x, \Omega) \qquad (4.39)$$

Furthermore, Barbaro and Bagajewicz[128] argued that downside risk is a function not only of the first-stage decisions but also of the aspiration or target profit level and minimizing downside risk at one level does not imply its minimization at another. Moreover, minimizing downside risk does not necessarily lead to minimizing financial risk for the specified target. Thus, they suggested that treating financial risk as a single objective presents some limitations, and proposed that risk to be managed over the entire range of aspiration levels.

To incorporate the downside risk $DRisk(x, \Omega)$ as the measure to control financial risk into two-stage stochastic model with a fixed recourse at different profit targets, Barbaro and Bagajewicz [128] proposed the following model:

$$Max\ \mu \left(\sum_{s \in S} p_s\, q_s^T y_s - c^T x \right) - \sum_{\forall s \in S} p_s \delta_s \qquad (4.40)$$

$$\boldsymbol{s.t.} \qquad \delta_s \geq \Omega + c^T x - q_s^T y_s \quad \forall s \in S$$

$$Ax \leq b$$

$$T_s x + W y_s \leq h_s \quad \forall s \in S$$

$$\delta_s \geq 0$$

$$x \geq 0 \quad x \in X$$

$$y_s \geq 0 \quad \forall s \in S$$

Where μ is referred to as the goal programming weight for downside risk formulations. In this case a full spectrum of solutions is accomplished by varying the profit target Ω from small values around $\Omega = \min_s\{Profit_s(x_{SP}^*)\}$ up to higher values around $\Omega = \max_s\{Profit_s(x_{SP}^*)\}$. In this way, solutions obtained for lower values of Ω will generally respond to a risk-averse investor and solutions obtained with higher Ω will be more appealing to risk-taker investors.

In light of these definitions, our profit objective and constraints containing the uncertain parameters of price and data in equations 4.1-4.3 will be reformulated of into a two-stage stochastic model with downside risk as the risk metrics. The numerical results-obtained by three methodologies discussed here as appraisal methods to assess and model uncertainty- are presented in chapter 5.

Chapter 5

NUMERICAL RESULTS AND DISCUSSIONS

5.1. Empirical Nonlinear Models of Refinery Units

The framework based on the nonlinear unit models, material balances and yield and property requirement constraints are used to develop the entire nonlinear refinery production planning model and is implemented in GAMS [131]/ BARON [132] versions 24.7.4/16.8.24 and solved on a DELL Studio XPS 1645 (Intel®Core™ i7 CPU, 1.73 GHz and 8 GB RAM) running Windows 10.0.16299.

5.1.1.Refinery case studies

A total of 13 different refinery case studies have been created: The first 3 case studies with various product demands and throughputs are used to verify the effectiveness of the nonlinear refinery model utilizing the data-based CDU model (DBNLM) over the linear input-output model (IOM) with fixed yield and property for the products and the impact of introducing process nonlinearity on the total profit improvement.

Table 5.1 shows the results for the oil refinery under consideration in these 3 case studies. In these 3 case studies, the effectiveness of a nonlinear refinery model versus a fixed yield linear input-output model with varying throughput have been investigated. In the first case study the total throughput of the refinery to satisfy the product demands is only 12% of the total distillation capacity of the refinery and nonlinear model shows an apparent 26% improvement in overall profit of the refinery by calculating the yields and product properties through the correlations. The second case study represents a scenario where the total throughput of the refinery to satisfy the product demands is 62% of the total distillation capacity of the refinery and nonlinear model shows an even higher 37% improvement in overall profit of the refinery. The third case study demonstrates a scenario where the total throughput of the refinery to satisfy the product demands is 90% of the total distillation capacity of the refinery and nonlinear model shows a highest 40% improvement in overall profit of the refinery and this trend suggests that if the refinery operates near to or at its full capacity, the overall profit optimization by accounting for the unit processes nonlinearity through the nonlinear unit models will be the highest. Figure 5.1 also consolidates these results and discussions illustratively.

Table 5.1. Improvement in Profit ($)-Data Based Nonlinear vs. Input-Output Model

Case Study	Total Product Demand (BPSD)	Throughput (% of CDU Capacity)	Calculated Profit ($)		CPU Time (Sec)		Improvement in Profit %
			Nonlinear	Input-Output	Nonlinear	Input-Output	
1	28000	11.2	2,037,787	1,487,534	25.12	0.56	26 %
2	140,000	56.0	2,143,006	1,697,926	114.93	1.91	37 %
3	201,000	80.4	2,865,595	2,041,408	171.42	4.75	40 %

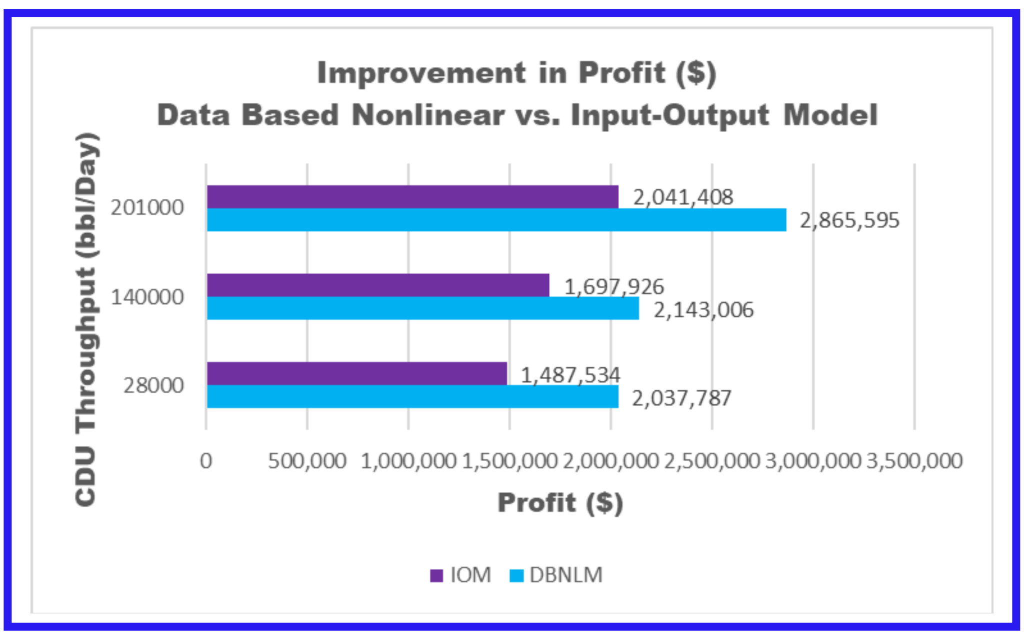

Figure 5.1. Effectiveness of Nonlinear model vs. Input-Output Model

The next 10 case studies have compared two nonlinear planning models utilizing 2 different nonlinear CDU models, that is data-based model versus the model based on fractionation index (FI). The impact of different nonlinear CDU models on the total profit has been investigated by taking into account the effect of calculated cut point temperatures and pseudocomponents yields. Table 5.2 tabulates the data for these 10 case studies. In these case studies the total distillation capacity of the refinery is assumed to be 250,000 BPSD. In case study 4, the total product demand is only 10% of the refining capacity and production planning model with FI-based CDU model demonstrates an obvious 9.4% improvement in profit over the one with data-based CDU model. The higher computational time of the FI-based model is inherently related to the large scale of this model due to the fact that FI-Based model is an MINLP model with more equations and continuous variables in addition to binary variables in comparison with the data-based model which is an NLP model with fewer equations and continuous variables. As the demand increases through the following case studies and reaches the maximum refining capacity in case study 13, both models represent an obvious increase in the calculated profit while improvement in profit by FI-based model over the data-based model reaches a maximum of 14%.In addition, the computational disadvantage of the FI-based model in terms of CPU time dissipates. Figure 5.2 also demonstrates these results graphically.

Table 5.2 .Improvement in Profit ($)-Nonlinear CDU FI vs. Data-Based Model

Case Study	Total Product Demand (BPSD)	Calculated Profit ($)		CPU Time (Sec)		Improvement in Profit %
		Data-Based	FI	Data-Based	FI	
4	25,000	3,161,030	3,458,167	19.41	68.88	9.4 %
5	50,000	3,205,579	3,516,520	43.30	79.56	9.7 %

6	75,000	3,206,280	3,526,908	57.98	91.44	10 %
7	100,000	3,262,421	3,608,238	81.11	111.92	10.6 %
8	125,000	3,317,281	3,688,816	107.77	139.20	11.2 %
9	150000	3,372,141	3,773,426	124.78	165.53	11.9 %
10	175,000	3,427,001	3,865,657	145.64	193.77	12.8 %
11	200,000	3,481,861	3,937,985	165.52	217.23	13.1 %
12	225,000	3,536,721	4,021,251	188.23	236.13	13.7 %
13	250,000	3,591,581	4,094,402	218.70	257.65	14 %

Table 5.3 represents the calculated optimal cut point temperatures and yields for the major hydrocarbon cuts (HC) and pseudocomponents (PC) for the CDU FI model for case study 13 with highest refinery throughput. The model has notably minimized the first pseudocomponent

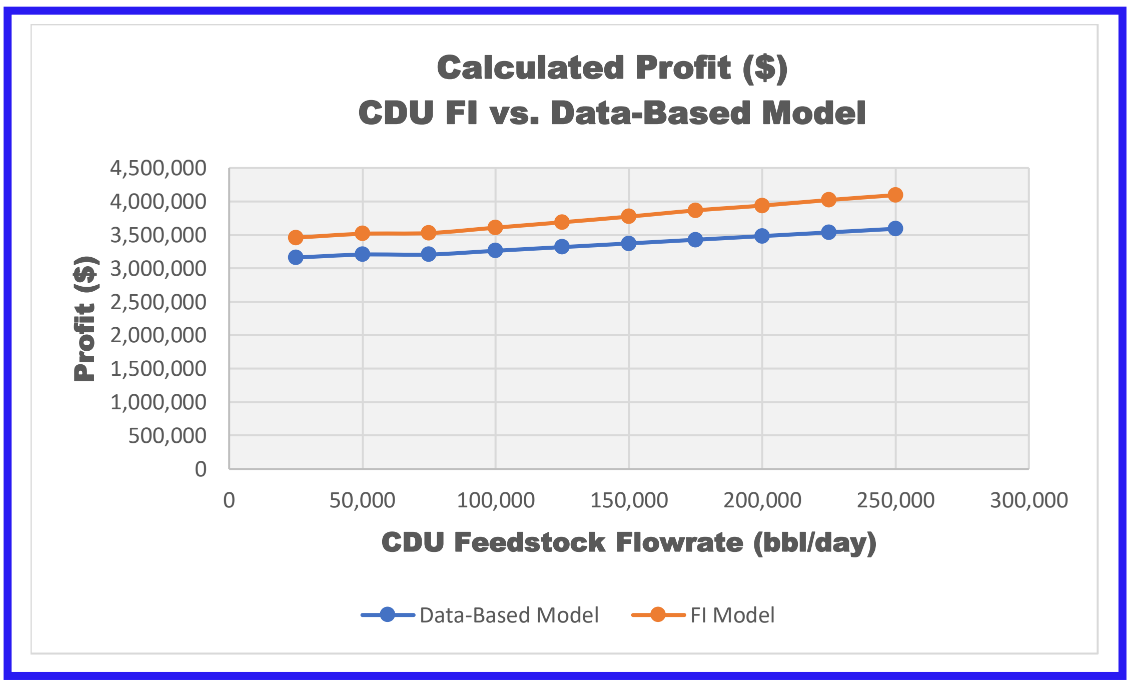

Figure 5.2. Effectiveness of Nonlinear CDU FI vs. Data-Based Model

(PC1) yield to zero as it does not contribute to meet the final product demands. The remaining pseudocomponents will be extracted in their preceding lighter hydrocarbon (HC) stage and their yields are optimized by the model to meet the major hydrocarbon's (HC) demand.

Table 5.3. Optimal Cut Point Temperatures and Yields – CDU FI Model

Hydrocarbon Cuts/ Pseudocomponents	Cut Point Temperature (°K)	Yield (% of CDU Feedstock)
PC1	-	0
Straight Run Gasoline (SRG)	288	10
PC2	-	7.8
Naphtha (N)	364	22.3
PC3	-	7.6
Reference Component	-	0.1
Kerosene (K)	438	16.7
PC4	-	2.3
Gas Oil (GO)	522	25.4
PC5	-	5.8
Residue (R)	603	7.0

Table 5.4 also provides demand data and optimal value of production for the final products calculated by both nonlinear models for the case study 3 while the distillation unit operates at its full capacity. While both models have succeeded to meet the product demands, the FI-based model has judiciously produced more gasoline and less jet fuel regarding the higher sale price of gasoline. In addition, the FI-based model has consumed less ethanol than data-based model which will lead to a higher total profit. The comprehensive product yield and property data are provided through the supporting information.

Table 5.4. Deterministic Product Demand and Production Data Calculated by Nonlinear Models

Final/Intermediate Product	Product Demand (BPSD)	Solver Calculated Production/Consumption (BPSD)	
		CDU Data-Based Model	CDU FI Model
Gasoline	86000	86,791.57	93,142.71
Jet Fuel	29000	34,608.07	29,495.408
Diesel Fuel	72000	72,658.000	72,777.522
Fuel Oil	14000	14,000	14,000
Ethanol	-	9700	8342

Table 5.5 also represents the computational statistics of input-output and nonlinear models for case study 3. As the table has demonstrated and already stated the FI-based model is a larger MINLP model with 870 equations, 884 continuous variables and 55 binary variables and its slightly higher solution time of 226.30 (Sec) could be correlated to its size.

Table 5.5. Computational statistics of input-output and nonlinear models for CS-3

Model	Model Type	# of Equations	# of Continuous Vars.	# of Binary Vars.	Solution Time (Sec)
Input-Output	LP	131	166	-	4.75
Nonlinear/Data-Based CDU	NLP	423	561	-	181.42
Nonlinear/FI-Based CDU	MINLP	870	884	55	226.30

5.2. Deterministic Integrated Refinery Case Study

For the deterministic integrated refinery problem, the mathematical framework based on the crude unloading, blending and inventory management, crude procuring and production planning, final product pooling problem, final product distribution by pipeline, utility system, the overall objective function of the integrated problem and specific constraints for the solution strategy are used to develop the entire integrated refinery planning model and is implemented in GAMS [131] /BARON [132] versions 28.2.0/19.7.13 and solved on Dell R430 and R730 servers with dual E5-2670 v3 12-core CPUs with 64 GB RAM, all running CentOS 7 Linux release 7.3.1611 (Core). An industrial case study has been considered for this study. Table 5.6 compares the results for the economic objectives associated with the sequential and integrated models for the oil refinery under consideration in this case study. It can be clearly identified that the integrated model demonstrates a 7.3% higher production revenue, 27% less unloading cost and overall 10 % improvement in the net profit in comparison with the sequential model. All revenue and cost data are on a million US $ basis.

Table 5.6. Comparison of the Economic Objectives: Integrated vs. Sequential Model

Model	Integrated	Sequential
Production(REV_{PROD})	4,408,290	4,087,100
Utility ($COPR_{UTIL}$)	797,650	797,650
Unloading ($COPR_{UNL}$)	114,880	146,370
Pipeline ($COPR_{PD}$)	0.213	0. 296
Profit	3,495,760	3,143,079

Table 5.7, further clarifies these comparison and variables by demonstrating the operational objectives associated with the sequential and integrated models. The integrated model clearly predicts less consumption of fuel gas (*Ih*) for boiler operations and demonstrates a 31% reduction in fuel consumption. The integrated model avoids costly boiler shut down and start-ups and minimizes fuel consumption during this period (*SI*) to zero while the sequential model can not completely avoid this process and consumes almost 1369 tons of fuel gas. With less fuel

consumption, the turbines produce more electricity (XEL) in the integrated model, an obvious 11% advantage over the sequential model. While neither of the models can meet the electricity demand from the production unit completely and require electricity to be purchased from an outside supplier (ELP), again the integrated model represents 42 times less need for an outsource to meet the electricity demand of the processing units. From an environmental footprint perspective, the integrated model appears to be more environmentally friendly versus the sequential model again: a 21% reduction in the greenhouse gas pollution ($XGHG$) and 11.6% reduction in sulfur oxides emissions ($XSOX$).In regards to charging tank to CDU changeover and storage tank to charging tank setup or switchover the integrated model again surpasses the sequential model with no changeover ($z_{j,l,t} = 0$) and only 2 switchovers ($\alpha_{i,t} = 2$) while the sequential model enforces 1 changeover and 5 switchovers which are all associated with penalties and contribute negatively to the unloading cost. Both models succeed to avoid CDU shut down ($XD_{l,t} = 0$) which has negative effects on the CDU cuts and intermediate product quality and overall refinery processes. Within the pipeline distribution of the final products, the integrated model proves to be even more efficient than the sequential model. *Z1-Z6* are aggregate normalized variables and interim objectives for the pipeline distribution and their results merit more clarifications. *Z1* represents the difference between the total discharged volume of the final products to the pipeline and the total demands of customers normalized over the total demands of customers over the entire scheduling horizon. As the results in Table 5.7 suggest, the value of *Z1* for the integrated model is slightly positive and implies that the integrated model meets the demands and even slightly discharges more products towards the distribution center whereas the sequential model falls short of the demands and results in a negative value (-26) for this variable. The value of *Z2* implies the inventory level of the product with the lowest final inventory level on the last day of the scheduling horizon, which should be maximized. As the numbers suggest from Table 5.7, the integrated model represents a 46% improvement over the sequential model in maximizing the inventory level of the product with the lowest final inventory level on the last day of the scheduling horizon in order to prevent or minimize the lost or back orders in the next time period or scheduling horizon. The value of *Z3* represents the underutilized pipeline capacity during the total hours of the scheduling horizon and while at the first look the sequential model apparently performs better in this regard by minimizing this value to zero, but this better performance comes at the expense of utilizing the pipeline even during the peak electricity hours which will

Table 5.7. Comparison of the Operational Objectives: Integrated vs. Sequential Model

Model	Integrated	Sequential
Ih(ton)	15,693	20,557.73
SI (ton)	0	1369.43
XEL (MWh)	17,744.61	15,792.58
ELP (MWh)	45.89	1997.91
BEL (MWh)	290.50	290.50
XGHG (ton)	3198.78	3869.43
XSOX (ton)	40.66	45.38
$\boldsymbol{z_{j,l,t}}$	0	1
$\boldsymbol{\alpha_{i,t}}$	2	5
$\boldsymbol{XD_{l,t}}$	0	0
Z1	6.79E-04	-0.26
Z2	1.159	0.630
Z3	0.105	0
Z4	0	0.738
Z5	0	0.786
Z6	0	0.213

demonstrate its negative effect on the value of *Z4*. The integrated model leaves the pipeline unutilized during the peak electricity hours and computes a value of 0.105 for *Z3*.This analysis can be further clarified by the value of *Z4* which is zero for the integrated model while 0.738 for the sequential model. The value of *Z5* determines the volume interfaces occurring between the injected batches containing different products and needs to be minimized. As expected, the integrated model minimizes this value to zero by not injecting different products in the subsequent batches into the pipeline while meeting the demand but the sequential model fails to achieve this goal and computes a value of 0.786 for *Z5*. The value of *Z6* encodes the backorders or delays in meeting the demand by the due dates which should be minimized. The integrated model judiciously minimizes this value to zero while the sequential model again fails to accomplish this goal and settles with some lost orders represented by a value of 0.213 for *Z6*.

Table 5.8 demonstrates the results for the economic objectives associated with the integrated model obtained by the proposed methodology versus BARON as a commercial global solver. It can be clearly identified that the proposed methodology demonstrates a 13% higher production revenue, 21% less utility cost, 2.5% less unloading cost and overall 19% improvement in the net profit in comparison with the commercial solver.

Table 5.8. Comparison of the Economic Objectives: Proposed Heuristic vs. BARON

Model	**Proposed Heuristic**	**BARON**
Production(REV_{PROD})	5,093,900	4,408,290
Utility ($COPR_{UTIL}$)	659,322	797,650
Unloading ($COPR_{UNL}$)	112,047	114,880
Pipeline ($COPR_{PD}$)	0.094	0.296
Profit	4,322,531	3,495,760

Table 5.9, presents the results for the operational objectives associated with the integrated model solved by the proposed algorithm and commercial solver. The proposed methodology consumes far more less fuel gas (*Ih*) for boiler operations and demonstrates a 17% reduction in fuel consumption. It produces more electricity (*XEL*) by the turbines, an approximate 5% advantage over the commercial solver. While the integrated model solved by the commercial solver had failed to meet the electricity demand from the processing units and required some electricity to be purchased from an outside supplier (*ELP =45.89 MWh*), the proposed methodology meets this demand and minimizes this value to zero. In regards to the emission of harmful gases, the current algorithm produces more eco-friendly results than the commercial solver: 29% reduction in the greenhouse gas pollution (*XGHG*) and 21% reduction in sulfur oxides emissions (*XSOX*). While both methods succeed to avoid CDU changeover ($z_{j,l,t} = 0$) and CDU shutdowns ($XD_{l,t} = 0$) , proposed methodology also avoids the tank-tank setup or switchover ($\alpha_{i,t} = 0$) while the commercial solver introduces yet 2 switchovers ($\alpha_{i,t} = 2$).

When we arrive at the results related to the pipeline distribution of products, *Z1*-the difference between the total discharged volume of the final products to the pipeline and the total demands of customers normalized over the total demands of customers- is minimized to zero by the proposed algorithm while it was slightly positive obtained by the commercial solver. It implies that the current method meets the demands without incurring extra pumping costs by injecting more products down the pipeline. For the value of *Z2*-the inventory level of the product with the lowest final inventory level on the last day of the scheduling horizon- which should be maximized the proposed method represents a 1.2 % improvement over the results obtained by the commercial solver. The value of *Z3*-the underutilized pipeline capacity within the total hours of the scheduling horizon- is the same for both methods who tend to leave the pipeline unutilized during the peak electricity hours and compute a value of 0.105 for *Z3*. Eventually both methods avoid utilizing the pipeline during the peak electricity hours (*Z4=0*), minimize the contaminated volume of the interfaces between the consecutive injected batches containing different products to zero (*Z5=0*) and avoid the backorders or delays in supplying the demand by the due dates (*Z6=0*).

Table 5.9. Comparison of the Operational Objectives: Proposed Heuristic vs. BARON

Model	Proposed Methodology	BARON
Ih(ton)	13,411	15,693
SI (ton)	0	0
XEL (MWh)	18,657.94	17,744.61
ELP (MWh)	0	45.89
BEL (MWh)	277.15	290.50
XGHG (ton)	2268.54	3198.78
XSOX (ton)	32.07	40.66
$\boldsymbol{z_{j,l,t}}$	0	0
$\boldsymbol{\alpha_{i,t}}$	0	2
$\boldsymbol{XD_{l,t}}$	0	0
Z1	0	6.79E-04
Z2	1.173	1.159
Z3	0.105	0.105
Z4	0	0
Z5	0	0
Z6	0	0

Table 5.10, provides the computational statistics of sequential model and integrated model solved by the commercial solver and proposed methodology (LVL+NMDT). The overall problem size, that is, the number of equations and continuous and binary variables are almost the same for both sequential and integrated model solved by BARON, but as the sequential model

just accounts for a portion of those equations and variables in each run of a sub-model associated with one the refinery activities, it has obviously introduced less CPU time (211.07 Sec) while producing sub- optimal results. The integrated model solved by BARON as discussed through the results of Tables (6.6,7), demonstrates a clear improvement in the economic and operation objectives over the sequential model but at the expense of a high solution time (7115.40 Sec) and yet fails to achieve a global optimal solution. Nevertheless, the integrated model solved by the proposed methodology presents far more improvement in economic and operation objectives but at a very competitive solution time (262.37 Sec) and obtains the global optimal solution.

Table 5.10 . Computational Statistics of Sequential and Integrated Models

Model	Model Type	# of Equations	# of Continuous Vars.	# of Binary Vars.	Solution Time (Sec)	Solution Quality
Sequential	MINLP	3468	2611	466	211.07	Local
Integrated	MINLP	3489	2613	466	7115.40	Local
Integrated + LVL +NMDT	MINLP	12,350	6366	1096	262.37	Global

5.3. Stochastic Integrated Refinery Case Study

In order to demonstrate the performance of the proposed approach in dealing with demand and price uncertainty at the strategic planning of an integrated refinery, the 3 robust, fuzzy and 2-stage stochastic programming strategies to handle uncertainty mentioned earlier have been applied to an industrial case study and solved with the aggregation/disaggregation global optimization scheme for the integrated refinery under study for a 7-year planning horizon. The mathematical framework based on the crude unloading, blending and inventory management, crude procuring and production planning, final product pooling problem, final product distribution by pipeline, utility system, the overall objective function of the integrated problem and specific constraints for the aggregation/disaggregation global optimization solution strategy within 3 different models are integrated with the associated constraints of the robust, fuzzy and 2-stage stochastic model with financial risk consideration to develop the entire stochastic integrated refinery planning model and are implemented in GAMS [131] 28.2.0 and BARON [132] 19.7.13 and solved on Dell R430 and R730 servers with dual E5-2670 v3 12-core CPUs with 64 GB RAM, all running CentOS 7 Linux release 7.3.1611 (Core).

In the robust model (RO), first a (relative) infeasibility tolerance level (δ) of 10% is considered for the normal uncertain parameters and an uncertainty level (ϵ) of 20% and a reliability level (κ) of 10% for the normal uncertain parameters, meaning that there is only a 10% chance of constraint violation.

For the fuzzy model (FUZ), product demand and crude and product prices are considered as fuzzy members. The same notation as $[\alpha^p \;\; \alpha^m \;\; \alpha^o]$ represents the most pessimistic, most possible and most optimistic value of fuzzy number α -which is representing uncertain price and demand data here- to characterize the triangle fuzzy number $\tilde{\alpha}$. α^m is set to be the same value as α in the deterministic problem. α^p and α^o are set to be 20% less and 20% greater than the most possible values, respectively. The confidence level for possibility and necessity are all set to 0.8.

For the 2-stage stochastic model with downside risk metric (2-ST-DR), a Monte Carlo sampling scheme is used to sample 100 independent scenarios for demand and price data from a normal distribution with known mean and standard deviations. The results for this model is averaged over all 100 scenarios.

Table 5.11, provides the computational statistics for the deterministic, Robust, Fuzzy and 2-stage stochastic with downside risk models solved by the proposed methodology (LVL+NMDT). The overall problem size, that is, the number of equations and continuous and binary variables are almost the same for the deterministic, Robust, Fuzzy models while it rises drastically for the stochastic model regarding the higher number of scenario based variables and equations. Intuitively the associated CPU time for these models' solutions and the solution quality follows the same pattern: while the first 3 models are solved within approximately 6 minutes and converge to the global optimum, 2-stage stochastic model with downside risk produces a sub-optimal result while the CPU time also soars to an extreme value of almost 3 hours.

Table 5.11. Computational Statistics-Deterministic, Robust, Fuzzy and Stochastic Models

Model	Model Type	# of Equations	# of Continuous Vars.	# of Binary Vars.	Solution Time (Sec)	Solution Quality
Deterministic	MINLP	12,338	12,443	1566	262.37	Global
Robust	MINLP	12,350	12,443	1566	348.29	Global
Fuzzy	MINLP	12,362	12,534	1566	360.296	Global
2-ST-DR	MINLP	145,307	149,817	7442	10,853.80	Local

Table 5.12 compares the results for the economic objectives associated with the deterministic, Robust, Fuzzy and 2-stage stochastic with downside risk models. As it could be anticipated, accounting for uncertainty causes a sharp decline in the overall refinery's net profit in comparison with the deterministic model. However the difference in the results of the 3 models with uncertainty is also remarkable: While the robust model reports 21% less net profit than the deterministic model as the price to obtain robustness, it demonstrates the best profile among

Table 5.12. Economic Objectives-Deterministic, Robust, Fuzzy and Stochastic Models

Model	Deterministic	Robust	Fuzzy	2-ST-DR
Production(Revenue($M))	30,809.36	24,815.25	23,021.91	24,385.56
Production(cpurchase($M))	24,694.34	19,962.43	20,205.42	20,550.57
Production(ipurchasee($M))	246.25	195.42	344.35	308.07
Utility (COST($M))	291.14	231.05	304.59	275.06
Unloading (COPR ($M))	41.86	33.27	42.32	34.68
Pipeline (ZOF)	0.094	0.096	-0.165	0.189
Net Profit ($M)	5535.77	4393.08	2125.23	3217.18

all three models with uncertainty: notably 41% better than fuzzy model and 20% better than the 2-stage stochastic model which translates to more ($ 2.3 B) and ($ 1.1 B) profit respectively for the refinery over the span of 7 years planning horizon. Table 6.13 tabulates the economic decisions for the overall amount of all crude oils to be purchased in each time interval. While both fuzzy and stochastic models forecast a substantially less profit for the refinery, they require purchasing of more crude oils than deterministic model over the planning horizon. The robust model estimates a slightly less crude purchase while producing higher profit which yet again substantiates a better decision profile than the other 2 models.

Table 5.13 indicates the operational objectives associated with the deterministic, Robust, Fuzzy and 2-stage stochastic with downside risk models. The robust model clearly consumes less fuel gas (*Ih*) for boiler operations and demonstrates a 28% and 33% reduction in fuel consumption in

Table 5.13. Volume of Crude Oils Purchased at Time Periods (Mbbl)

Deterministic, Robust, Fuzzy and Stochastic Models

Time Period/ Model	1	2	3	4	5	6	7	Total
Deterministic	73	71	78	75	72	73	79	521
Robust	68.34	67.21	79.19	73.74	74.12	69.85	81.57	514.02
Fuzzy	71.33	69.96	80.33	77.43	75.68	73.48	78.66	526.87
2-ST-DR	74.58	71.28	75.55	78.37	79.41	77.25	84.37	540.81

comparison with stochastic and fuzzy models respectively. All models judiciously avoid costly boiler shut down and start-ups and minimize fuel consumption during this period (*SI*) to zero. With less fuel consumption, the turbines produce more electricity (XEL) in the robust model, an obvious 40% and 25% advantage over stochastic and fuzzy models respectively. While neither of the models can meet the electricity demand from the production unit completely and require electricity to be purchased from an outside supplier (*ELP*), again the robust model performs 27% and 12% better than fuzzy and stochastic models in terms of need for an outsource to meet the electricity demand of the processing units. From an environmental footprint perspective, the robust model appears to be more environmentally friendly versus the other 2 models: a 24% and 11% reduction in the greenhouse gas pollution ($XGHG$) and 26% and 9% reduction in sulfur oxides emissions (*XSOX*) comparing the fuzzy and stochastic models. In regards to charging tank to CDU changeover and storage tank to charging tank setup or switchover, all models perform well with no changeover ($z_{j,l,t} = 0$) and only 2 switchovers ($\alpha_{i,t} = 2$) which its correspondent penalty contributes negatively to the unloading costs. All models succeed to avoid CDU shut down ($XD_{l,t} = 0$) which has negative effects on the intermediate product quality and overall refinery processes. Within the pipeline distribution of the final products, the results of all models are conspicuous and the previous pattern is not as palpable here. *Z1-Z6* are aggregate normalized variables and interim objectives for the pipeline distribution and their results merit more clarifications. *Z1* represents the difference between the total discharged volume of the final products to the pipeline and the total demands of customers normalized over the total demands of customers over the entire time horizon . As the results in Table 5.14 manifest, the value of *Z1* for the robust model is slightly positive and implies that robust model meets the demands and even slightly discharges more products towards the distribution center whereas the other 2 models result in negative values (-0.012 and -0.021) for this variable. The value of *Z2* implies the inventory level of the product with the lowest final inventory level on the last day of the time horizon, which should be maximized. As the numbers suggest from Table 5.14, all models underperform and represent a negative contribution for this variable highlighting their failure in maximizing the inventory level of the product with the lowest final inventory level on the last day of the time horizon. The purpose of this maximization is to prevent or minimize the lost or back orders in the next scheduling horizon. The value of *Z3* represents the underutilized pipeline capacity within the total hours of the scheduling horizons. All the models fail in minimizing this value to zero, however both robust and fuzzy models perform better than the stochastic model: a 33% and 17% reduction in underutilized pipeline capacity respectively. The models effectiveness in avoiding the utilization of the pipeline during the peak electricity hours are implied through the values of *Z4* and impressively all models have managed to minimize this value to zero. The value of *Z5* determines the volume of contaminated interfaces occurring between the injected batches containing different products and needs to be minimized. While neither of the models have succeeded to avoid this cost, the fuzzy model here outperformed both robust and stochastic models: a reduction of 6% and 27% in the contaminated interface volume better than robust and stochastic models. The value of *Z6* encodes the backorders or delays in supplying the demand by the due dates which should be minimized. All models have accomplished this goal and minimized this value to zero.

Table 5.14. Comparison of the Operational Objectives: Deterministic, Robust, Fuzzy and Stochastic Models

Model	Deterministic	Robust	Fuzzy	2-ST-DR
Ih(ton)	5,727,945	4,430,565	6,002,886	5,178,635
SI (ton)	0	0	0	0
XEL (MWh)	6,976,783	6,349,558	4,795,441	5,850,478
ELP (MWh)	16,750	13,026	17,551	15,095
BEL (MWh)	106,033	81,158	111,472	95,938
XGHG (ton)	1,167,555	916,064	1,223,777	1,055,819
XSOX (ton)	14,841	11,559	15,580	13,406
$\boldsymbol{z_{j,l,t}}$	0	0	0	0
$\boldsymbol{\alpha_{i,t}}$	2	2	2	2
$\boldsymbol{XD_{l,t}}$	0	0	0	0
Z1	6.79E-04	0.002	-0.012	-0.021
Z2	1.159	-0.821	-0.990	-0.931
Z3	0.105	0.128	0.145	0.163
Z4	0	0	0	0
Z5	0	0.810	0.762	0.978
Z6	0	0	0	0
ZOF	0.094	0.096	-0.165	0.189

Eventually, regarding the better performance of robust counterpart model (RC), we conducted 6 case studies to investigate the effect of reliability level (κ) on profit in presence of variations in levels of uncertainty ($\epsilon = 10$ and 20%) and infeasibility ($\delta = 10, 15$ and 20%). Figure 6.3 illustrates the results of these studies. As it's been displayed in Figure 6.3, while the reliability level approaches to 1, that is the probability of violation of the uncertain constraints increases, regardless of the levels of uncertainty and infeasibility, the calculated profit for all studies approaches the value of profit for the deterministic model with no uncertainty, an approximate value of $ 5536 M.

In addition, as it is expected, for a given reliability level, the maximal profit that can be achieved decreases as the uncertainty level increases, which highlights more conservative decisions at the presence of uncertainty. In an opposite manner, at a given reliability level, the maximal achievable profit rises as the infeasibility tolerance level increases, which allows for more audacious planning approach if violations of demand and price constraints can be tolerated to a higher extent.

To draw meaningful conclusions on the dominance of uncertainty (ϵ) and infeasibility (δ) level at a certain reliability level ($\kappa = 30\%$) or higher, it's enough to compare the curves for case study ($\epsilon = 20\%$ & $\delta = 20\%$) and ($\epsilon = 10\%$ & $\delta = 10\%$): while the former has higher uncertainty level and expected to produce less profit, has surpassed the latter and produced higher profit on levels of ($\kappa = 30\%$) or higher. This is an indication that while at lower levels of reliability level (κ), uncertainty (ϵ) might be a dominating factor, at higher levels of reliability level (κ) the infeasibility (δ) level has higher significance.

These results are in agreement with findings of Janak et al.[125] and confirm their results on the correlation of these 3 parameters associated with the robust counterpart model in an even more transparent fashion and with less outlying result data.

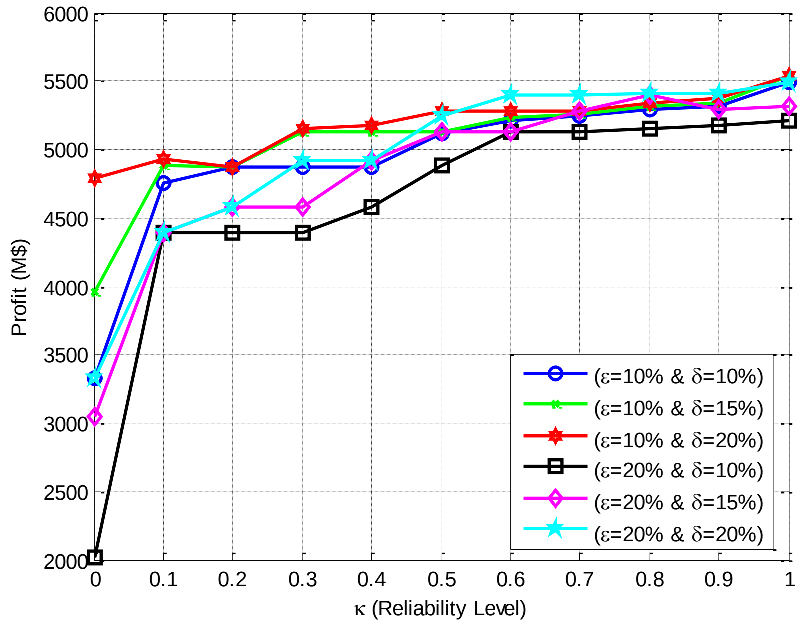

Figure. 5.3. Effect of reliability level on profit at different uncertainty and infeasibility levels.

Chapter 6

CONCLUSION AND FUTURE WORK

Linear process models are not suitable for refinery process modeling, since refinery processes are inherently nonlinear and the refinery planning problem based on the input-output or approximate linear models may sacrifice the refining profitability or product quality. Moreover, different refinery processes are tightly interconnected and coherent entities, and attempting to solve each part in a sequential hierarchical manner may result in infeasible or suboptimal solutions. Furthermore, the oil industry is subject to uncertainties such as unpredictable product demand and unstable market prices and uncertainty, if not taken into account, could lead to infeasible or suboptimal designs.

In this study, to account for the nonlinearity in the refinery processing units, first a complete model for the refinery wide production planning was presented. For the fractionation unit, two nonlinear models were introduced: first a data-based CDU model, then another nonlinear model for CDU based on the Geddes fractionation index (FI). For the remaining refinery units, empirical nonlinear unit models were utilized. On this basis, the nonlinear refinery-wide production planning model created the global maximum solutions for the overall refinery profit in 13 case studies. The results of the case studies substantiate the huge advantage of the nonlinear model over the linear input-output model. In addition, from a fractionation perspective, the effectiveness of the nonlinear CDU model based on fractionation index (FI) over the data-based model was demonstrated. Ultimately, the product yield and quality data calculated by nonlinear model and compared with the final product property requirements prove the effectiveness of this model in computing refinery product yield and properties within reasonable precisions and requirements.

Next to integrate the refinery supply chain sub-systems and solve the refinery planning model within a deterministic enterprise-wide integrated model rather than a hierarchical model, in this study a novel optimization approach with a multi-period mixed-integer nonlinear programming (MINLP) model was presented. The integration of the refinery network was implemented across the different echelons of the refinery supply chain including crude unloading, oil procuring while accounting for the highly nonlinear nature of the processing units, final product pooling and blending, inventory management, product distribution by pipeline and the utility system. The results of the refinery integrated and sequential models both solved by the commercial solver were compared where the integrated model demonstrated clear improvements in both economic and operational objectives. A hybrid aggregation/disaggregation methodology based on lumped variable linearization (LVL) and normalized multiparametric disaggregation technique (NMDT) was presented as a two-level optimization algorithm. In the next step, the integrated model was solved by the proposed methodology, and its results were compared with the ones obtained by the commercial solver. The results from the proposed method introduced even far more improvements in both economic and operational objectives while obtaining ε-global optimal solutions in very competitive solution time. These benefits reinforce the point that planning and process decisions need to be integrated.

Eventually, to account for uncertainties in the final product demand and crude oil and final product market prices, a stochastic integrated refinery planning model was devised. To model the uncertainties, three different methodologies such as robust programming, fuzzy possibilistic programming and two-stage stochastic programming with fixed recourse and downside risk metric were utilized. These methodologies were applied to an industrial case study, comprising the integrated oil refinery operations over a planning horizon of 7 years and solved by the proposed global optimization framework. The results of three different uncertainty appraisal methodologies were compared with the deterministic model at the absence of uncertainty. As it was anticipated, accounting for uncertainty caused a sharp decline in the overall refinery's net profit in comparison with the deterministic model. Among the three different methodologies to treat uncertainty, the robust framework outperformed the other two models in terms of both economic and operational objectives with exception of the pipeline model. In regards to the pipeline model, the results of all models are conspicuous and the same pattern of performance was not obtained. In reference to the robust counterpart parameters, it was demonstrated that while at lower levels of reliability level (κ), uncertainty (ϵ) might be a dominating factor; at higher levels of reliability level (κ) the infeasibility (δ) level becomes more significant.

For future work, the consideration and incorporation of the following research is recommended:

1-The nonlinear CDU model is a complex matter and still subject of ongoing investigations and a computationally less intensive model yet with high fidelity can enhance the effectiveness of the refinery planning model.

2- The use of crude cocktails instead of single crude fed into distillation units should be accommodated in the production planning model.

3-The crude blending problem should also be modeled rigorously through a generalized pooling problem at the refinery's front end.

4- The feeding rate fluctuation of CDU through an Inherent Upset Minimization (IUM) procedure must be accounted for.

5-The environmental impacts of the refining operations should be penalized and accounted for in a more realistic and rigorous manner.

6-For the product distribution through a pipeline, the realistic tree configuration for the pipeline should be considered and deliveries to multiple depots or distribution centers must be incorporated within the design.

7- Transport phenomena specifically fluid dynamical effects, e.g. pressure drops, multiphase flows etc. should be incorporated in pipeline models

8-Maritime or vehicular routing problem should be incorporated within the planning model to accommodate for the crude distribution for multisite refineries or distribution of final products by trucks from depots to final consumer markets such as gas stations.

9-Crude selection, purchase policy and cross-hedging with future contracts should be considered.

10-Price elasticity, symmetry/asymmetry between price of crude oil and petroleum products should be accounted for

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NOMENCLATURE

Unloading Model

Indices

c	*crude type*
i	*storage tank*
j	*charging tank*
k	*key component*
l	*crude distillation unit*
m	*alias for time interval*
t	*time interval*
v	*crude oil vessel*

Parameters

CC	*charging tanks changeover cost*
$CINBT_j$	*charging tanks j inventory cost per unit time per unit volume*
$CINST_i$	*storage tanks i inventory cost per unit time per unit volume*
CS	*cost penalty for shutdown*
$CSEA_v$	*sea waiting cost for vessel v*
CSSU	*cost penalty for switching to another tank during tank-tank transfers*
$CUNL_v$	*unloading cost for vessel v*
DM_q	*demand of crude mix q*
H	*Length of scheduling horizon*

NBT *number of charging (blending) tanks*

NCDU *number of CDUs*

NCOMP *number of key components*

NST *number of storage tanks*

NSCH *number of time intervals in scheduling horizon*

NV *number of vessels*

NC *number of crude types*

$TARR_v$ *arrival time of vessel v*

TF_v *time vessel v begins to unload*

TL_v *time vessel v finishes unloading*

ε_{1q} *violation parameter due to decrease in demand*

ε_{2q} *violation parameter due to increase in demand*

μ_1 *user defined parameter that determines interval–interval variations for CDU l throughput*

Variables

$COPR_{UNL}$ *operating cost*

$CB_{b,i}$ *end time for discharge of batch $b \in B_i$ from storage tank i into a charging tank*

$LB_{b,i}$ *length of unloading operation of batch $b \in B_i$ from storage tank i*

$SB_{b,i}$ *starting time for discharge of batch $b \in B_{tk}$ from storage tank i*

dd_i *emptying due date for storage tank i*

rt_i *release time of storage tank i denoting the time the content of tank i is available*

$fbc_{j,l,k,t}$ *volumetric flow rate of component k from charging tank j to CDU l at time t*

$fsb_{i,j,k,t}$ *volumetric flow rate of component k from storage tank i to charging tank j at time t*

$fvs_{v,i,k,t}$ *volumetric flow rate of component k from vessel v to storage tank i at time t*

$FBC_{j,l,t}$ *volumetric flow rate from charging tank j to CDU l at time t*

$FBCmax_{j,l}$ *maximum volumetric flow rate from charging tank j to CDU l*

$FBCmin_{j,l}$ *minimum volumetric flow rate from charging tank j to CDU l*

$FSB_{i,j,t}$ *volumetric flow rate from storage tank i to charging tank j at time t*

$FSBmax_{i,j}$ *maximum volumetric flow rate from storage tank i to charging tank j*

$FSBmin_{i,j}$ *minimum volumetric flow rate from storage tank i to charging tank j*

$FVS_{v,i,t}$ *volumetric flow rate from vessel v to storage tank i at time t*

$FVSmax_{v,i}$ *maximum volumetric flow rate from vessel v to storage tank i*

$FVSmin_{v,i}$ *minimum volumetric flow rate from vessel v to storage tank i*

M *big M takes a value equal to the storage capacity of the tanks*

$vb_{j,k,t}$ *volume of component k in charging tank j at time t*

$vs_{i,k,t}$ *volume of component k in storage tank i at time t*

$VB_{j,t}$ *volume of charging tank j at time t*

$VBmax_{j}$ *maximum volume of charging tank j*

$VBmin_{j}$ *minimum volume of charging tank j*

$VS_{i,t}$ *volume of storage tank i at time t*

$VSmax_{i}$ *maximum volume of storage tank i*

$VSmin_{i}$ *minimum volume of storage tank i*

$VV_{v,t}$ *volume of crude oil vessel v at time t*

$ws_{i,k}$ *concentration of component k in storage tank i*

$wsmax_{i,k}$ *maximum concentration of component k in storage tank i*

$wsmin_{i,k}$ *minimum concentration of component k in storage tank i*

$wb_{j,k}$ *concentration of component k in charging tank j*

$wbmax_{j,k}$ *maximum concentration of component k in charging tank j*

$wbmin_{j,k}$ *minimum concentration of component k in charging tank j*

$wv_{v,k}$ *concentration of component k in crude oil vessel v*

$D_{j,l,t}$ *binary variable that denotes charging tank j is charging CDU l at time interval t*

$XD_{l,t}$ *binary variable that indicates shutdown of CDU l at time t*

$XF_{v,t}$ *binary variable that denotes that vessel v starts unloading at time t*

$XL_{v,t}$ *binary variable that denotes that vessel v stops unloading at time t*

$XW_{v,t}$ *binary variable that denotes that vessel v is unloading to a storage tank at time t*

$XWS_{i,j,t}$ *binary variable that denotes that storage tank i transferring to charging tank j at time t*

$XV_{v,i,t}$ *binary variable that denotes that vessel v is connected to storage tank i at time t*

$YC_{c,i}$ *binary variable that denotes that crude type c is stored in storage tank i*

$Z_{j,l,t}$ *binary variable that denotes that charging tank j charges the CDU l at time t*

$\alpha_{i,t}$ *binary variable that denotes that storage i tank is set up for tank-tank transfer*

Refinery Production Model

Sets

C= set of all commodities c

U = set of all units u

BU=set of blending units (GP,JFP,DFP,FOP)

Ptank = set of final product tanks (GT,JFT,DFT,FOT)

Ctank = set of crude tanks

CT = crude tank

P_s *= set of all the properties calculated for the specified CDU fraction s*

S_{CDU} *= set of CDU fractions*

$QO_{u,c}$ *=set of properties q of product c leaving unit u*

upr *= set of products from unit* u

fpr *= set of final products*

fccpr = product streams set from the FCC unit

crupr = product streams set from the CRU unit

hcpr = product streams set from the HC unit

Vbpr = product streams set from the VB unit

dcpr = product streams set from the DC unit

$pathu(u, c, u')$ *= a set that verifies the product* c *is on that flow path from unit* u *to unit* u'

i crude component i in FI model

j crude cut or separation unit j in FI model

HC set of hydrocarbon components in crude oil feed to the CDU in FI model

PsC set of pseudocomponents in crude oil feed to the CDU in FI model

<u>Continuous Variables</u>

$F_{in}(f, u)$ *= inlet flowrate of feedstock into unit u*

$F_{out}(u, c)$ *= outlet flowrate of commodity c from unit u*

$A_m(u', c, u)$ = *the amount of commodity* c *coming from unit* u' *to unit* u

Vol_frac(c,u)=volume fraction of commodity c in unit u

$Y(c, u)$ = *volumetric yield of commodity c from unit u*

$Y_w(c, u)$ = *weight yield of commodity c from unit u*

$yield_{u,c}$ = *constant percent yield of unit u for product c for a specific crude*

PO_{ucq} = *property q of product* c *leaving unit u*

$pro(u', c', q)$ = *property* q *of commodity* c' *coming from unit* u' *to unit* u

$F_{j,i}$ *feed stream of component i to crude cut j*

$PB_{j,i}$ *bottom product stream of crude cut j of component i*

$PD_{j,i}$ *top product stream of crude cut j of component i*

F_total_j *total feed stream to fractionation unit crude cut j*

PD_total_j *total top product stream to fractionation unit crude cut j*

PB_total_j *total bottom product stream to fractionation unit crude cut j*

$K_{j,i}$ *equilibrium constant in crude cut j for component i*

$\alpha_{j,i}$ *relative volatility in crude cut j for component i with component ref*

$Pv_{j,i}$ *vapor pressure in crude cut j for component i*

Tb_i *boiling point temperature of component i (K)*

TI_j *initial boiling point temperature for crude cut j*

TE_j *end boiling point temperature for crude cut j*

T_j *separation temperature of crude cut j(cut point temperature)*

$Tr_{j,i}$ *reduced temperature of component i in crude cut j*

$x\_PB_{j,i}$ *component i composition fraction in bottom product stream PB of crude cut j*

$x\_PD_{j,i}$ component i composition fraction in top product stream PD of crude cut j

$\gamma_{i,j}$ place holder for the selected FI value for component i at the crude cut j

<u>Binary Variables</u>

Y(i,j) 0-1 variable for stripping (FIs) or rectifying (FIr) value of the fractionation index associated with component i for crude cut j

<u>Parameters</u>

C = Conversion Level, LV.PCT.

FQP = Feed Quality Parameter

P = Operating pressure, psig

ASF = Aromatic Saturation Factor

CCR = Conradson Carbon Residue, Wt%

EP= End-Point Temperature

FCC = Volume Fraction FCC Stocks in Feedstock

VGC = Viscosity-Gravity Constant

NC5 = Normal Pentane Insolubles Content, Wt. Pct.

VBN = Viscosity Blending Number

$pn_{c,q}$ *= lower bound on the property q of product c*

$px_{c,q}$ *= upper bound on the property q of product c*

$Demand\ (fpr)$*= demand of product fpr*

x =Operating variable

N2A = Naphthene content plus 2 times the aromatic content of feedstock, volume fraction

GASO/ C_3 PROD = Ratio of C_5/400 (Gasoline) to C_3/400 Product (400 °F end point gasoline)

M_L   big M value for separation temperatures greater than the component boiling point

M_U   big M value for separation temperatures smaller than the component boiling point

Tc(i)   critical temperature of pseudocomponent i (K)

Pc(i)   critical pressure of pseudocomponent i (Bar)

PVA(i) parameter A for the vapor pressure of component i in Antoine's equation

PVB(i) parameter B for the vapor pressure of component i in Antoine's equation

PVC(i) parameter C for the vapor pressure of component i in Antoine's equation

w(i)   Acentric factor of pseudocomponent i

Commodities

O = Crude Oil Feedstock

G = Gasoline

DF = Diesel Fuel

JF = Jet Fuel

FO = Fuel Oil

ETOH =Ethanol

GASO= total gasoline

LCO= light cycle oil

HCO= heavy cycle oil

COKE= coke

REF= Reformate

RG= Refinery Gas

NAP= Naphtha

MD= Middle Distillate

FG = Fuel Gas

LPG= Liquefied Petroleum Gas

LGO= Light Gas Oil

HGO= Heavy Gas Oil

R= Residue

SRLN= straight-run light naphtha

SRHN= straight-run heavy naphtha

Kero= kerosene

Diesel= diesel

VGO= vacuum gas oil

VR= vacuum residue

Rsd= residue (CDU Model)

C3/400= C3(at operational mode to produce maximum yield of gasoline at 400 ℉ end point)

Product Yield

RG = Refinery GAS (C_1 through C_3) Yield, Wt. Pct.

FG = Fuel Gas Yield, Wt. Pct.

FO = Low Sulfur Fuel Oil Yield (Wt. Pct.)

C_3 LPG = C_3 LPG Yield, LV Pct.

C_4 LPG = C_4 LPG Yield, LV Pct.

LPG = Total Liquefied Petroleum Gas Yield, LV Pct.

H = Hydrogen Consumption (Wt. Pct.)

H_O = Hydrogen Consumption (SCF/Bbl)

H_2S = Hydrogen Sulfide Yield, Wt. Pct.

NH_3 = Ammonia Yield, Wt. Pct.

NAP = Naphtha Yield, Wt. Pct.

LGO = Light Gas Oil Yield, Wt. Pct.

HGO = Heavy Gas Oil Yield, Wt. Pct.

TGO = Total Gas Oil Yield, Wt. Pct.

COKE = Coke Yield, Wt. Pct.

C_3/400= Yield of C_3/400 Product (LV PCT.)

REFBASE = Base reformate yield at 200 psig, vol. pct.

REFORMATE = Reformate yield corrected for operating pressure, scf/bbl

HC = Hydrocarbon Product Yield (WT. PCT.)

LG = Light Gasoline Yield, Wt. Pct.

KERO = Kerosene/Jet Fuel Yield, Wt. Pct.

HN = Hydrotreated Naphtha Yield (Wt. Pct.)

MD = Hydrotreated Middle Distillate Yield (Wt. Pct.)

VN = Visbreaker Naphtha Yield, LV Pct.

ATB = Atmospheric Residue Yield, LV Pct.

VTB = Vacuum Residue Yield, LV Pct.

VFO = Visbreaker Fuel Oil Yield, LV Pct.

VTB = Vacuum Residue Yield, LV Pct.(Visbreaker)

Product Quality

RVP = Reid vapor pressure, psia

RONCL = Research Octane Number (Clear)

MONCL = Motor octane number (clear)

RON = Research octane number (clear) of C_{5^+} reformate divided by 100

PON= Posted octane number (clear)

CI = Cetane Index

K = Watson Characterization Factor

VABP = Volumetric Average Boiling Point, ℉

S = Sulfur Content, Wt. Pct.

N = Nitrogen Content, Wt. Pct.

SG = Specific gravity (60 ℉/60 ℉)

PP = Pour Point, ℉

FP = Freeze Point, ℉

API = API Gravity, °API

B = Bromine Number

AP = Aniline Point, ℉

A = Aromatic Content, LV Pct.

SP = Smoke Point, mm

LN = Luminometer Number

P = Paraffin Content (Wt. Pct.)

O = Olefin Content (Wt. Pct.)

CP = Naphthene Content (Wt. Pct.)

M = Metals (Nickel and Vanadium) Content (ppm wt)

BP = Boiling Point, °F

FPBI= freezing point blending index

PPBI= pour point blending index

VBI122 = viscosity blending index at 122 °F

VBI210 = viscosity blending index at 210 °F

Vis122 = viscosity at 122 °F, centistokes (cSt)

Vis210 = viscosity at 210 °F, centistokes (cSt)

SUS210 =Saybolt Universal Viscosity at 210 °F, SSU

CS122 = Viscosity at 122 °F, CS

CS210 = Viscosity at 210 °F, CS

Subscripts

f = feedstock

g = gas (C_1 through C_4) (HT&HDS)

g = light gasoline (HC)

n = naphtha

k = kerosene/jet fuel

d = distillate

lgo = light gas oil

hgo = heavy gas oil

atb = atmospheric residue

vtb = vacuum residue

vfo = visbreaker fuel oil

r = residual fuel oil

s=CDU fraction

Units

BPSD = barrel per stream day

Pipeline Distribution Model

Sets

i,j discharging batches during a day

p, q refined petroleum products

t, tt daily periods of the time horizon

Parameters

dd_t *last hour of the time period t*

$Dem_{t,p}$ *demand for product p on day t*

Initvp initial inventory level of product p at DC

Init- volume$_{i,t,p}$ *volume of initial batches*

Init-$T_{i,t}$ *discharging time of initial batches*

$Inv_p^{clients-min}$ *minimum allowed storage capacity of clients for product p at DC*

$Inv_p^{clients-max}$ *maximum allowed storage capacity of clients for product p at DC*

$Inv_p^{total-min}$ *minimum allowed total storage capacity for product p at DC*

$Inv_p^{total-max}$ *maximum allowed total storage capacity for product p at DC*

$Lotmin_p$ *minimum allowed volume for every discharged batch of product p*

$lotmax_p$ maximum allowed volume for every discharged batch of product p

M a very large number

$peak_t$ peak hours in time period t

$prate_{t,p}$ produced output volume of product p on day t

pw maximum allowable interference

$Rinitv_p$ initial inventory level of product p at the refinery

$Rinv_p^{min}$ *minimum allowed storage capacity for product p at the refinery*

$Rinv_p^{max}$ *maximum allowed storage capacity for product p at the refinery*

$setl_p$ duration of the settling period for a batch of product p

vb_{min}; vb_{max} minimum and maximum allowed continuous flow rates

vp pipeline volume

$waste_{p,q}$ contamination volume between consecutive batches of products p and q

<u>Continuous variables</u>

$Cub_{i,t,p}$ cumulative volume of a sequence of successive batches of product p up to the ith batch on day t

$B_{t,p}$ shortage volume of product p at the DC to meet the demand on day t

$D_{i,t,tt}$ volumetric distance between the ith batch on day t and the first batch on day tt

diff difference between the total discharged volume and total demand for all products

$inf_{i,t}$ contaminated volume of the ith batch on day t

$inj_{i,t,p,tt}$ size of the ith discharged batch on day t, including product p injected on day tt

$inv_{t,p}^{clients}$ *inventory level of product p at the DC on day t ready to supply the customer demand*

$inv_{t,p}^{total}$ *total inventory level of product p at DC on day t* *minid lowest total inventory among all products on the last day*

ph_t *used peak hours on day t*

$Rinv_{t,p}$ *inventory level of product p at the refinery on day t*

$T_{i,t}^{dis}$ *discharging time of the ith batch on day t*

$W_{I,t,p}$ *size of the ith batch on day t, including product p*

Binary variables

$x_{i,t,tt}$ *= 1 if injection of the ith batch on day t starts on day tt; otherwise, 0*

$y_{i,t,p}$ *= 1 if the ith batch on day t contains product p; otherwise, 0*

Utility System Model

Indices

I fuels

j units (processing equipment /boilers/turbines)

q piecewise segment of efficiency curve

t time period

v utility

Sets

BOIL set of boilers in CHP plant

FUEL set of fuels in CHP plant

J set of processing equipment in manufacturing unit

TURB set of turbines in CHP plant

UTILITY set of utilities provided by CHP plants; {LP, MP, HP, electricity}

Parameters

a_j consumption coefficient for MP steam redirected towards boiler

b_j consumption coefficient for electricity required to carry out boiler operation

cc_i calorific value of fuel (MJ/kg)

cf_i cost of fuel (V/ton)

CEL electricity purchase cost (V/MWh)

CGHG cost incurred for emissions of GHG (V/ton)

CSOX cost incurred for emissions of SOx (V/ton)

cpt_i capacity of storage repository for fuel i (tons)

ghg_i coefficient of GHG released from boiler due to fuel i

$ehst_i$ exhaust steam parameter for turbine j (defined as a fraction of $TXHP_{t,j}$)

h enthalpy values based on steam temperature and pressure (MJ/kg)

$Imax_{j,i}$ quantity of fuel i that is required to attain maximum steam level in boiler j

$Imin_{j,i}$ quantity of fuel i that is required to attain minimum steam level in boiler j

$\bar{I}_{q,j,i}$ *fuel threshold of the piecewise efficiency curve segment q*

Q total number of piecewise segments

$SIdem_{j,i}$ quantity of fuel i that is used during starting-up phase of boiler j

sox_i coefficient of SOx released from boiler due to fuel i

ssfi safety stock parameter for fuel i (defined as a fraction of cpt_i)

T time horizon

$TXHPmax_{t,j}$ maximum amount of steam that can enter turbine j in time period t

$TXHPmin_{t,j}$ minimum amount of steam that can enter turbine j in time period t

$XHPmax_j$ maximum amount of steam that can be produced by boiler j

$XHPmin_j$ *minimum amount of steam that can be produced by boiler j*

$\overline{XHP}_{q,j,i}$ *steam threshold of the piecewise efficiency curve segment q*

$\eta_{j,i}$ *efficiency of boiler j with fuel i*

η_j *efficiency of the turbine j*

<u>Binary variables</u>

$A_{q,t,j,I}$ *to determine the boiler efficiency as a function of boiler load factor*

$SB_{t,j,i}$ *to determine whether boiler j is operational during time period t using fuel i*

$FSB_{t,j,i}$ *to determine whether boiler j is being restarted during time period t using fuel i*

Appendices

Appendix A.

The following is a brief representation of the crude oil unloading model adopted from Hamisu et al. (2013).

A.1. Operating rules

1. Vessel unloading sequence:

a. Vessel arrives and leaves the docking station only once throughout the scheduling horizon.

$$\sum_{t=1}^{NSCH} XF_{v,t} = 1 \qquad v = 1, \dots, NV \quad (\boldsymbol{A-1})$$

$$\sum_{t=1}^{NSCH} XL_{v,t} = 1 \qquad v = 1, \dots, NV \quad (\boldsymbol{A-2})$$

b. A vessel can only unload after it arrives at the docking station as determined at the planning level.

$$TF_v \geq T_{ARR,v} \qquad v = 1, \dots, NV \quad (\boldsymbol{A-3})$$

c. The initiation and completion times are defined as:

$$TF_v = \sum_{t=1}^{NSCH} tXF_{v,t} \qquad v = 1, \dots, NV \quad (\boldsymbol{A-4})$$

$$TL_v = \sum_{t=1}^{NSCH} tXL_{v,t} \qquad v = 1, \dots, NV \quad (\boldsymbol{A-5})$$

d. Two vessels cannot unload their contents at the same time. Therefore the preceding vessel must finish unloading one time interval before the later vessel begins to unload.

$$TF_{v+1} \geq TL_v + 1 \qquad v = 1, \dots, NV \quad (\boldsymbol{A-6})$$

e. A vessel unloading is accomplished between two time intervals: initiation time, TF_v and completion time, TL_v

$$XW_{v,t} \leq \sum_{m=1}^{t} XF_{v,m}$$

$$XW_{v,t} \leq \sum_{m=t}^{NSCH} XL_{v,m}$$

$$v = 1, \dots, NV, \qquad t = 1, \dots, NSCH \quad (\boldsymbol{A-7})$$

f. The unloading duration is bounded by TF_v and TL_v.

$$TL_v - TF_v \geq 1 \qquad v = 1, \dots, NV \quad (\boldsymbol{A-8})$$

3. Standing gauge operation:

Flow in and out of tanks simultaneously is not allowed.

a. For storage tanks:

$$XWS_{i,j,t} \leq 1 - XWS_{v,i,t} \qquad (\boldsymbol{A-9})$$

$$v = 1, \dots, NV, i = 1, \dots, NST, j = 1, \dots, NBT, t = 1, \dots, NSCH$$

b. For charging tanks:

$$D_{j,l,t} \leq 1 - XWS_{i,j,t} \qquad (\boldsymbol{A-10})$$

$$i = 1, \dots, NST, j = 1, \dots, NBT, l = 1, \dots, NCDU, t = 1, \dots, NSCH$$

4.Only one connection is allowed at any time period t:

a. Flow from vessel to storage tank

$$\sum_{i}^{NST} XV_{v,i,t} = 1 \quad (\boldsymbol{A-11})$$

$$v = 1, \dots, NV, t = 1, \dots, NSCH$$

$$\sum_{v}^{NV} XV_{v,i,t} = 1 \quad (\boldsymbol{A-12})$$

$$i = 1, \dots, NST, t = 1, \dots, NSCH$$

b. Flow from storage tank to charging tank

$$\sum_{j}^{NBT} XWS_{i,j,t} = 1 \quad (\boldsymbol{A-13})$$

$$i = 1, \dots, NST, t = 1, \dots, NSCH$$

$$\sum_{i}^{NST} XWS_{i,j,t} = 1 \quad (\boldsymbol{A-14})$$

$$j = 1, \dots, NBT, t = 1, \dots, NSCH$$

c. Flow from charging tank to CDU

$$\sum_{l}^{NCDU} D_{j,l,t} = 1 \quad (\boldsymbol{A-15})$$

$$j = 1, \dots, NBT, t = 1, \dots, NSCH$$

$$\sum_{j}^{NBT} D_{j,l,t} = 1 \quad (\boldsymbol{A-16})$$

$$l = 1, \dots, NCDU, t = 1, \dots, NSCH$$

5. Semi-continuous constraints are applied for feedstock to CDU

These ensure operation of the unit within the design flow rate and assumes no flow when CDU shut down. For normal operation the constraint is represented as:

$$FBCmin_{j,l} \le FBC_{j,l,t} \le FBCmax_{j,l} \qquad (\boldsymbol{A-17})$$

$$j = 1, \dots, NBT, l = 1, \dots, NCDU, t = 1, \dots, NSCH$$

When CDU shuts down,

$$FBC_{j,l,t} = 0 \qquad (\boldsymbol{A-18})$$

$$j = 1, \dots, NBT, l = 1, \dots, NCDU, t = 1, \dots, NSCH$$

6. Flow constraint from storage tank to charging tank:

The total quantity received by charging tank (s) must not exceed the maximum flow rate from storage tanks.

$$\sum_{i}^{NST} FSB_{i,j,t} \le FSBmax_{i,j} \qquad (\boldsymbol{A-19})$$

$$j = 1, \dots, NBT, t = 1, \dots, NSCH$$

7. Demand violation constraints:

For demand of crude blend q from charging tank j, Equation (A-20) represents supply to meet exact or below actual demand and Equation(A-21) to account for supply to meet the exact or above actual demand.

$$\sum_{l=1}^{NCDU} \sum_{t=1}^{NSCH} FBC_{j,l,t} \geq DM_q(1 - \varepsilon_{1q}) \quad (\boldsymbol{A-20})$$

$$j = 1, \dots, NBT, q = 1, \dots, NBT$$

$$\sum_{l=1}^{NCDU} \sum_{t=1}^{NSCH} FBC_{j,l,t} \leq DM_q(1 - \varepsilon_{2q}) \quad (\boldsymbol{A-21})$$

$$j = 1, \dots, NBT, q = 1, \dots, NBT$$

ε_{1q} is a parameter that specifies the demand violation of crude blend q in the negative direction (below the actual demand) and ε_{2q} in the positive direction (above the actual demand). When each of these parameters is 0, a demand violation is not allowed.

8. Continuous flow constraint:

At any time, a charging tank should be charging the CDU:

$$\sum_{j}^{NBT} D_{j,l,,t} = 1 \quad (\boldsymbol{A-22})$$

$$l = 1, \dots, NCDU, t = 1, \dots, NSCH$$

9. Flow fluctuation constraints:

Flow fluctuations in CDU charging rate should be avoided because it disrupts CDU operation and may generate off specification cuts.

$$FBC_{j,l,t-1} \geq FBC_{j,l,t}(1-\mu_1) \qquad (\boldsymbol{A-23})$$

$$j = 1, \dots, NBT, l = 1, \dots, NCDU, t = 1, \dots, NSCH - 1$$

$$FBC_{j,l,t-1} \leq FBC_{j,l,t}(1+\mu_1) \qquad (\boldsymbol{A-24})$$

$$j = 1, \dots, NBT, l = 1, \dots, NCDU, t = 1, \dots, NSCH - 1$$

μ_1 is a user defined parameter with values ranging between zero and one. If μ_1 is set at zero, no variation is allowed in interval–interval quantity. For the purpose of our study a value of 0.1 has been used.

10. Changeover penalty:

This is to consider a penalty cost associated with the changeover of CDU with the charging tanks.

$$Z_{j,l,t} \geq D_{j,l,t} - D_{j,l,t-1} \qquad (\boldsymbol{A-25})$$

$$j = 1, \dots, NBT, l = 1, \dots, NCDU, t = 1, \dots, NSCH - 1$$

$$Z_{j,l,t} \geq D_{j,l,t-1} - D_{j,l,t} \qquad (\boldsymbol{A-26})$$

$$j = 1, \dots, NBT, l = 1, \dots, NCDU, t = 1, \dots, NSCH - 1$$

The term $CC \times Z_{j,l,t}$ is added to the objective function. *CC* is the cost penalty for changeover.

11. Shutdown constraints:

These are included to permit both shutdown and continual operations for CDU.

$$FBC_{j,l,t} \geq (1 - XD_{l,t})FBClo_{j,l,t} \quad (\boldsymbol{A-27})$$

$$j = 1, \dots, NBT, l = 1, \dots, NCDU, t = 1, \dots, NSCH - 1$$

$$FBC_{j,l,t} \leq (1 - XD_{l,t})FBCup_{j,l,t} \quad (\boldsymbol{A-28})$$

$$j = 1, \dots, NBT, l = 1, \dots, NCDU, t = 1, \dots, NSCH - 1$$

The binary variable $XD_{l,t}$ is zero during normal operation and takes on the value of 1 when CDU shuts down. The term $CS \times XD_{l,t}$ is added to the objective function. *CS* is the cost penalty for shutdown.

12. Set-up or tank switchover constraint:

A set-up cost is incurred anytime switching occurs between storage tanks and charging tanks transfer. The term $CSSU \times \alpha_{i,t}$ is added to the objective function. *CSSU* is the cost penalty for switching from tank to tank during tank-tank transfers.

$$\alpha_{i,t} \geq XWS_{i,j,t} - XWS_{i,j,t-1} \qquad (\boldsymbol{A-29})$$

$$i = 1, \dots, NST, j = 1, \dots, NBT, t = 1, \dots, NSCH - 1$$

A.2. Hydraulic capacities

1. Flow constraints:

Flow of the crude oil is bounded by the capacity of the pumping system available.

a. Flow from vessel to storage tank

$$FVSmin_{v,i}XW_{v,i,t} \leq FVS_{v,i,t} \leq FVSmax_{v,i}XW_{v,i,t} \quad (\boldsymbol{A-30})$$

$$v = 1, \dots, NV, i = 1, \dots, NST, t = 1, \dots, NSCH$$

b. Flow from storage tank to charging tank

$$FSBmin_{i,j}XWS_{i,j,t} \leq FSB_{i,j,t} \leq FSBmax_{i,j}XWS_{i,j,t} \quad (\boldsymbol{A-31})$$

$$i = 1, \dots, NST, j = 1, \dots, NBT, t = 1, \dots, NSCH$$

c. Flow from charging tank to CDU.

$$FBCmin_{j,l}D_{j,l,t} \leq FBC_{j,l,t} \leq FBCmax_{j,l}D_{j,l,t}$$

$$j = 1, \dots, NBT, l = 1, \dots, NCDU, t = 1, \dots, NSCH \qquad (\boldsymbol{A-32})$$

2. Capacity constraints:

The volume of crude oil in storage and charging tanks at any time must be within the upper and lower bounds of the containing medium.

a. Storage tank capacity limitation

$$VSmin_i \leq VS_{i,t} \leq VSmax_i \qquad (\boldsymbol{A-33})$$

$$i = 1, \dots, NST, t = 1, \dots, NSCH$$

b. Charging tank capacity limitation.

$$VBmin_j \leq VB_{j,t} \leq VBmax_j \qquad (\boldsymbol{A-34})$$

$$j = 1, \dots, NBT, t = 1, \dots, NSCH$$

3. Crude oil material balance.

a. Crude oil vessel: volume of crude oil in vessel *v* at time t equals the difference between the initial crude volume and the overall volume transferred from the vessel up to time t.

$$VV_{v,t} = VV_{v,0} - \sum_{i=1}^{NST} \sum_{m=1}^{t} FVS_{v,i,m} \qquad (\boldsymbol{A-35})$$

$$v = 1, \dots, NV, t = 1, \dots, NSCH$$

b. Storage tank: volume of crude oil in storage tank *i* at time t equals the sum of the initial volume stored in the storage tank with the volume transferred into the storage tank up to time t, less volume transferred from the storage tank up to time t.

$$VS_{i,t} = VS_{i,0} + \sum_{v=1}^{NV} \sum_{m=1}^{t} FVS_{v,i,m} - \sum_{j=1}^{NBT} \sum_{m=1}^{t} FSB_{i,j,m} \quad (\boldsymbol{A-36})$$

$$i = 1, \dots, NST, t = 1, \dots, NSCH$$

c. Charging tank: volume of crude mix in charging tank j at time t equals the sum of the initial volume of crude mix in the charging tank with the volume transferred into the charging tank up to time t, less volume transferred from the charging tank up to time t.

$$VB_{j,t} = VB_{j,0} + \sum_{i=1}^{NST} \sum_{m=1}^{t} FSB_{i,j,m} - \sum_{l=1}^{NCDU} \sum_{m=1}^{t} FBC_{j,l,m} \qquad (\boldsymbol{A-37})$$

$$j = 1, \dots, NBT, t = 1, \dots, NSCH$$

Appendix B.

The following is a brief representation of the product distribution by pipeline model adopted from Moradi & MirHassani (2015).

1.Allocating products to the batches

Each day, a newly discharged batch is one of the products or it is empty.

$$\sum_{p \in P} y_{i,t,p} \leq 1 \qquad \forall\, i \in I, t \in T \quad (\boldsymbol{B-1})$$

The empty batches should be left at the end of the sequence of batches each day, i.e., if one of the considered batches contains no product, then all of the subsequence batches on the day will be considered empty.

$$\sum_{p \in P} y_{i+1,t,p} \leq \sum_{p \in P} y_{i,t,p} \qquad \forall\, i \in I, i < |I|, t \in T \quad (\boldsymbol{B-2})$$

In addition, if on day *t*, no batch is to be discharged ($\sum_p y_{1,t,p} = 0$) , then on the subsequent days, no batches will be discharged.

$$\sum_{p \in P} y_{i,t+1,p} \leq \sum_{p \in P} y_{i,t,p} \qquad \forall\, i \in I, i = 1, t \in T, t < |T| \quad (\boldsymbol{B-3})$$

2.Lot-sizing

The size of a batch of product p should be in a specific range ([$minlot_p$; $maxlot_p$]). In addition, the volume of fictitious batches is zero; therefore:

$$y_{i,t,p} \times lotmin_p \leq W_{i,t,p} \leq y_{i,t,p} \times lotmax_p \qquad \forall\, i \in I, t \in T, p \in P \quad (\boldsymbol{B-4})$$

If only the constraint above is considered, it is possible for some consecutive nonempty batches to include product *p* and to comprise a single lot of *p*, and thus the maximum batch size may be violated. Supposing that $Cub_{i,t,p}$ is the cumulative volume of a sequence of successive batches of product *p* up to the *i*th batch on day *t*, this variable is determined by Equations (B-5) and (B-6), and it should be lower than the maximum batch size.

$$Cub_{i,t,p} \geq Cub_{i-1,t,p} + W_{i,t,p} - lotmax_p \left(\sum_{q \in P-\{p\}} y_{i,t,q} \right) \quad \forall\, i \in I, i > 1, t \in T, p \in P \quad (\boldsymbol{B-5})$$

$$Cub_{i,t,p} \geq Cub_{j,t-1,p} + W_{i,t,p} - lotmax_p \left(\sum_{q \in P-\{p\}} y_{i,t,q} \right) \forall\, i,j \in I, i = 1, t \in T, t > 1, p \in P \quad (\boldsymbol{B-6})$$

The nonnegative variable *diff* is defined as being equal to the difference between the total discharged volume and total customer demand in the time horizon, which is minimized by the objective function.

$$diff = \sum_{i \in I} \sum_{t \in T} \sum_{p \in P} W_{i,t,p} - \sum_{t \in T} \sum_{p \in P} Dem_{t,p} \quad (\boldsymbol{B-7})$$

3.Product inventories at the DC

The total inventory level of product *p* at the end of day *t* ($inv_{t,p}^{total}$) is equal to the sum of inventory from the previous day and any inventory discharged during day *t* ($\sum_i W_{i,t,p}$), which backorders from the previous day ($B_{t-1,p}$), and the demand on day *t* ($Dem_{t,p}$) will be excluded. In addition, it is possible for the DC to encounter an inventory shortage as high as $B_{t,p}$. Thus, for the first day, we have:

$$inv_{t,p}^{total} = Initv_p + \sum_{i \in I} W_{i,t,p} - Dem_{t,p} + B_{t,p} \quad \forall\, t \in T, t = 1, p \in P \quad (\boldsymbol{B-8})$$

For other days, we have:

$$inv_{t,p}^{total} = inv_{t-1,p}^{total} + \sum_{i \in I} W_{i,t,p} - Dem_{t,p} - B_{t-1,p} + B_{t,p} \quad \forall\, t \in T, t > 1, p \in P \quad (\boldsymbol{B-9})$$

The total and available inventory levels of each product on each day should lie within a specified range, as follows.

$$inv_p^{total-min} \le inv_p^{total} \le inv_p^{total-max} \qquad \forall t \in T, p \in P \quad (\boldsymbol{B-10})$$

4.Interface volume between consecutive batches

If the *i*th batch of day *t* contains product *p* and the next batch contains product *q*, the contaminated volume of the *i*th batch on day *t* is assumed to equal $waste_{p,q}$. The continuous variable $inf_{i,t}$ represents the amount of the contaminated volume of the *i*th batch on day *t*.

On each day, a batch is mixed with the next batch. If batch *i* is not the last batch of day *t*, its interface can occur with the (*i + 1*)th batch of day *t*.

$$inf_{i,t} \ge waste_{p,q}\left(y_{i,t,p} + y_{i+1,t,q} - 1\right) \qquad \forall\, i \in I, i < |I|, t \in T, p, q \in P \quad (\boldsymbol{B-11})$$

If batch *i* is the last batch of day *t*, its interface can occur with the first batch of day *t + 1*.

$$inf_{i,t} \ge waste_{p,q}\left(y_{i,t,p} + y_{j,t+1,q} - 1\right) \quad \forall\, i, j \in I, i = |I|, j = 1, t \in T, t < |T|, p, q \in P \quad (\boldsymbol{B-12})$$

5.Discharging time

During each day, one or more batches are discharged at the DC. The discharge duration of each batch depends on the flow rate. Discharging the first batch of day *t* starts from the earliest hour of day (dd_{t-1}) and finishes at time ($dd_{t-1} + (\frac{1}{vb}) \times \sum_p W_{i,t,p}$).Thus,

$$dd_{t-1} + \left(\frac{1}{vb_{max}}\right)\sum_{p\in P} W_{i,t,p} \le T_{i,t}^{dis} \le dd_{t-1} + \left(\frac{1}{vb_{min}}\right)\sum_{p\in P} W_{i,t,p} \quad \forall\, i \in I, i = 1, t \in T \quad (\boldsymbol{B-13})$$

The discharging of the other batch starts after the previous batch $T_{i-1,t}^{dis}$ and finishes at time $T_{i-1,t}^{dis} + (\frac{1}{vb}) \times \sum_p W_{i,t,p}$ .Thus,

$$T_{i-1,t}^{dis} + \left(\frac{1}{vb_{max}}\right)\sum_{p\in P} W_{i,t,p} \le T_{i,t}^{dis} \le T_{i-1,t}^{dis} + \left(\frac{1}{vb_{min}}\right)\sum_{p\in P} W_{i,t,p} \quad \forall\, i \in I, i > 1, t \in T \quad (\boldsymbol{B-14})$$

6.Peak electricity hours

Discharging the last batch on day *t* should be finished before the peak hours unless the required pumping is performed during ph_t hours in the peak hours.

$$T_{i,t}^{dis} \le dd_t - peak_t + ph_t \quad \forall\, i \in I, i = |I|, t \in T \quad (\boldsymbol{B-15})$$

The used peak hours are less than or equal to the total peak hours on day t and these variables are minimized in the objective function.

$$ph_t \le peak_t \quad \forall\, t \in T \quad (\boldsymbol{B-16})$$

7.Inventory management at the refinery

The variable $D_{i,t,tt}$ is defined as equal to the volumetric distance between the *i*th discharged batch on day *t* and the first batch on day *tt* ($tt \le t$), which is obtained from Equations (B-(17-19)). The volumetric distance between the $(i-1)$th discharged batch on day *t* and first batch on day *tt* ($D_{i-1,t,tt}$) plus the volume of this batch is equal to the volumetric distance between the next and first batches on day *tt*.

$$D_{i,t,t} = 0 \quad \forall\, i \in I, i = 1, t \in T \quad (\boldsymbol{B-17})$$

$$D_{i,t,tt} = D_{j,t-1,tt} + \sum_{p \in P} W_{j,t-1,p} \quad \forall\, i,j \in I, i = 1, j = |I|, t, tt \in T, tt < t \quad (\boldsymbol{B-18})$$

$$D_{i,t,tt} = D_{i-1,t,tt} + \sum_{p \in P} W_{i-1,t,p} \quad \forall\, i \in I, i > 1, t, tt \in T, tt < t \quad (\boldsymbol{B-19})$$

If the volumetric distance between the *i*th batch on day *t* and the first batch on day *tt* belongs to the interval $[vp, vp + \sum_{i \in I} \sum_{p \in P} W_{i,tt,p}]$, then injecting this batch causes the discharge of some batches of day *tt*, and thus its discharge starts on day *t* and the binary variable $x_{i,t,tt}$will be equal to 1. Equations (B-(20-22)) provide these conditions.

$$D_{i,t,tt} \geq vp \times x_{i,t,tt} \quad \forall\, i \in I, t, tt \in T, tt \leq t \quad (\boldsymbol{B-20})$$

$$D_{i,t,tt} \leq vp + \sum_{i \in I} \sum_{p \in P} W_{i,tt,p} + M(1 - x_{i,t,tt}) \quad \forall\, i \in I, tt \in T, tt \leq t \quad (\boldsymbol{B-21})$$

$$\sum_{tt \in T, tt \leq t} x_{i,t,tt} = 1 \qquad \forall\, i \in I, t \in T, ((i,t) \notin O) \quad (\boldsymbol{B-22})$$

If the injection of the *i*th batch on day *t* starts during day *tt*, then the injected volume must be equal to $W_{i,tt,p}$; otherwise, it must be equal to zero and thus:

$$inj_{i,t,p,tt} \leq M x_{i,t,tt} \quad \forall\, i \in I, \forall\, t, tt \in T, tt \leq t, \forall\, p \in P \quad (\boldsymbol{B-23})$$

$$W_{i,t,p} - M(1 - x_{i,t,tt}) \leq inj_{i,t,p,tt} \leq W_{i,t,p} \quad \forall\, i \in I, \forall\, t, tt \in T, tt \leq t, \forall\, p \in P \quad (\boldsymbol{B-24})$$

The inventory level of product *p* at the refinery on day *tt* is equal to the sum of the inventory level on the previous day plus the production volume of product *p* on day *tt* minus the injected volume. To calculate the inventory level at the refinery, it is assumed that the daily output of each product is known ($prate_{tt,p}$). In addition, when the injection of a batch starts on day *tt*, the total volume of this batch is subtracted from the refinery inventory on day *tt*.

$$Rinv_{tt,p} = Rinitv_p + prate_{tt,p} - \sum_{i \in I} \sum_{t \in T} inj_{i,t,p,tt}, \quad \forall\, p \in P, tt = 1 \quad (\boldsymbol{B-25})$$

$$Rinv_{tt,p} = Rinv_{tt-1,p} + prate_{tt,p} - \sum_{i \in I} \sum_{t \in T} inj_{i,t,p,tt}, \quad \forall\, p \in P, tt > 1 \quad (\boldsymbol{B-26})$$

Appendix C.

The following is a brief representation of the utility system model adopted from Agha et al. (2010).

1.Fuel storage model

The amount of fuel i entering the boiler j and producing HP steam (high pressure) in the period t is represented by $I_{t,j,i}$. The fuel repository has a certain capacity and initial amount of fuel $ORF_{0,i}$ stored in it is assumed as known. The Equation (C-1) models the fuel tank mass balance. Fuel leaving the repository depends on the demands of the boiler.

$$ORF_{t,i} = ORF_{t-1,i} + PRF_{t,i} - \sum_{j \in BOIL} (I_{t,j,i} + SI_{t,j,i}) \quad (\boldsymbol{C-1})$$

$$\forall\, i \in FUEL, \forall\, t = 1, \dots, T$$

2.Boiler model

Equation (C-2) models the fuel *i* consumption in boiler j as a function of the amount of high pressure (HP) steam produced, calorific value of fuel, boiler efficiency and the enthalpy difference between superheated steam and feed-water heaters. This is a nonlinear equation but simplifying assumptions are used to develop a representative linear equation. There are still two variables in the equation, boiler efficiency $\eta_{j,i}$ and fuel consumption $\bar{I}_{q,j,i}$.

$$\bar{I}_{q,j,i} = \frac{(h_b - h_{fw}) * \overline{XHP}_{q,j,i}}{cc_i . \eta_{q,j,i}} \quad (\boldsymbol{C-2})$$

$$\forall\, q \in Q, \forall\, j \in BOIL, \forall\, i \in FUEL$$

In order to include the effect of the efficiency variation with the varying load factor and at the same time guarding the condition of linearity, piecewise linear approximation is used and three linear discretized pieces are considered (Q= 3), where:

$$\overline{XHP}_{0,j,i} = XHPmin_j; \qquad \overline{XHP}_{1,j,i} = 0.5 * XHPmax_j; \;\; (\boldsymbol{C-3})$$

$$\overline{XHP}_{2,j,i} = 0.75 * XHPmax_j; \qquad \overline{XHP}_{3,j,i} = XHPmax_j;$$

Equations (E-(4-6)) develop this piecewise linear approximation curve, quantifying fuel consumption with the varying load factor. Equation (E-4) determines $XHP_{t,j,i}$ the amount of HP steam being generated in the boiler. It joins q linear equations by use of binary variables $A_{q,t,j,i}$ and continuous variables $x_{q,t,j,i}$.

$$XHP_{t,j,i} = \sum_{q=1}^{Q} A_{q,t,j,i} * \overline{XHP}_{q-1,j,i} + x_{q,t,j,i} * (\overline{XHP}_{q,j,i} - \overline{XHP}_{q-1,j,i}) \quad (\boldsymbol{C-4})$$

$$\forall\, t = 1, \dots, T, \forall\, j \in BOIL, \forall\, i \in FUEL$$

$$I_{t,j,i} = \sum_{q=1}^{Q} A_{q,t,j,i} * \bar{I}_{q-1,j,i} + x_{q,t,j,i} * \left(\bar{I}_{q,j,i} - \bar{I}_{q-1,j,i}\right) \quad (\boldsymbol{C-5})$$

$$\forall\, t = 1, \dots, T, \forall\, j \in BOIL, \forall\, i \in FUEL$$

Equation (E-6) enforces that, at maximum, only one binary variable $A_{q,t,j,i}$ will have the value ‘‘1’’, while Equation (E-7) limits the value of continuous variable $x_{q,t,j,i}$ between 0 and 1.

$$\sum_{q=1}^{Q} A_{q,t,j,i} \le 1 \qquad \forall\, t = 1, \dots, T, \forall\, j \in BOIL, \forall\, i \in FUEL \quad (\boldsymbol{C-6})$$

$$0 \le x_{q,t,j,i} \le A_{q,t,j,i} \qquad \forall\, q \in Q, \forall\, t = 1, \dots, T, \forall\, j \in BOIL, \forall\, i \in FUEL \quad (\boldsymbol{C-7})$$

2.2. Boiler shutdown and restart constraints

Once the boiler is shutdown, it will require a minimum of two time periods before it can start generating steam again. During the restart phase, the boiler uses $SIdem_{t,j,i}$ amount of fuel without producing any steam. The boiler is in its operational phase when ($SB_{t,j,i} = 1$) and when ($SB_{t,j,i} = 0$) the boiler is in the shutdown state

Equation (C-8) determines that boiler being operational in the future time period depends on the current state of the boiler as well as the state of boiler in the previous time interval .

$$SB_{t+1,j,i} \le SB_{t,j,i} + \left(1 - SB_{t-1,j,i}\right) \qquad (\boldsymbol{C-8})$$

$$\forall\, t = 2, \ldots, T-1, \forall\, j \in BOIL, \forall\, i \in FUEL$$

Equations (C-9) and (C-10) establish that 'boiler restart' in a given time interval will occur only if it is operational in the future period and it is not operational in the current time interval.

$$FSB_{t+1,j,i} \leq SB_{t+1,j,i} \quad \forall\, t = 1, \ldots, T-1, \forall\, j \in BOIL, \forall\, i \in FUEL \quad (\mathbf{C-9})$$

$$FSB_{t+1,j,i} \geq SB_{t+1,j,i} - SB_{t,j,i} \quad \forall\, t = 1, \ldots, T-1, \forall\, j \in BOIL, \forall\, i \in FUEL \quad (\mathbf{C-10})$$

Fuel consumed during the restart phase without producing steam is represented by Equation (C-11).

$$SI_{t,j,i} = FSB_{t,j,i} * SIdem_{j,i} \quad \forall\, t = 1, \ldots, T, \forall\, j \in BOIL, \forall\, i \in FUEL \quad (\mathbf{C-11})$$

2.3. Emission constraints

Eqs (C-12) and (C-13) model the amount of SO_x and greenhouse gas (GHG) emissions from the boiler.

$$XSOX_{t,j} = \sum_{i \in FUEL} sox_i * (I_{t,j,i} + SI_{t,j,i}) \quad \forall\, t = 1, \ldots, T, \forall\, j \in BOIL \quad (\mathbf{C-12})$$

$$XGHG_{t,j} = \sum_{i \in FUEL} ghg_i * (I_{t,j,i} + SI_{t,j,i}) \quad \forall\, t = 1, \ldots, T, \forall\, j \in BOIL \quad (\mathbf{C-13})$$

2.4. Boiler electricity and steam return constraints

The amount of medium pressure steam redirected back to preheat water and electricity used by the feed water pump to inject water into the boiler are modeled by Equations (C-14) and (C-15).

$$RET_{t,j} = a_j * \sum_{i \in FUEL} XHP_{t,j,i} \quad \forall\, t = 1, \ldots, T, \forall\, j \in BOIL \quad (\mathbf{C-14})$$

$$BEL_{t,j} = b_j * \sum_{i \in FUEL} XHP_{t,j,i} \quad \forall\, t = 1, \ldots, T, \forall\, j \in BOIL \quad (\mathbf{C-15})$$

3.Turbine model

The high pressure steam comes into the first stage of the multi-stage back pressure steam turbine where it expands and ultimately leaves as medium pressure steam. This medium pressure steam then enters the second turbine stage and leaves as low pressure steam. Finally the low pressure steam enters the third stage of the turbine and exits at a very low pressure. This ‘exhaust steam’ is above the saturated steam level but it is not fit for the process requirements.

After each stage, some quantities of medium pressure (MP) and low pressure (LP) steam are extracted from the turbine to meet the steam demands of the manufacturing unit. Another source for meeting MP and LP steam demands is by expanding the steam through pressure release valves (PRVs). Equation (C-16) models the turbine mass balance.

$$TXHP_{t,j} = XMP_{t,j} + XLP_{t,j} + XEHST_{t,j} \quad \forall\, t = 1, \dots, T, \forall\, j \in TURB \quad (\mathbf{C-16})$$

Equation (C-17) places limiting constraint on quantity of steam that can be extracted from the turbine.

$$XEHST_{t,j} \geq ehst_j * TXHP_{t,j} \qquad \forall\, t = 1, \dots, T, \forall\, j \in TURB \quad (\mathbf{C-17})$$

Equation (C-18) furnishes the turbine energy balance which quantifies the electricity generated by the turbine. It is further assumed that the turbine efficiency η_j remains constant.

$$XEL_{t,j} = \eta_j * [TXHP_{t,j} * (h_b - h_m) + \left(TXHP_{t,j} - XMP_{t,j}\right) * (h_m - h_l)$$

$$+(TXHP_{t,j} - XMP_{t,j} - XLP_{t,j}) * (h_l - h_e)] \quad (\mathbf{C-18})$$

$$\forall\, t = 1, \dots, T, \forall\, j \in TURB$$

4. Mixer model

Mixers are hypothetical devices and are only used to achieve the material balance of HP, MP and LP steam. Equations (C-(19-21) provide the mass balance of the HP, MP and LP steam respectively.

$$\sum_{i \in FUEL} \sum_{j \in BOIL} XHP_{t,j,i} - LXHP_t - \sum_{j \in TURB} TXHP_{t,j} \geq DemHP_t \qquad (\mathbf{C-19})$$

$$\forall\, t = 1, \dots, T$$

$$LXHP_t + \sum_{j \in TURB} XMP_{t,j} - LXMP_t - \sum_{j \in BOIL} RET_{t,j} \geq DemMP_t \qquad (\mathbf{C-20})$$

$$\forall\, t = 1, \dots, T$$

$$LXMP_t + \sum_{j \in TURB} XLP_{t,j} \geq DemLP_t \quad \forall\, t = 1, \dots, T \qquad (\mathbf{C-21})$$

Equation (C-22) models the amount of electricity generated onsite and the electricity purchased from an external source:

$$\sum_{j \in TURB} XEL_{t,j} + ELP_t \geq DemEL_t + \sum_{j \in BOIL} BEL_{t,j} \quad \forall\, t = 1, \dots, T \quad (\mathbf{C-22})$$

Appendix D.

The following is a brief representation of the aggregation/disaggregation global optimization scheme based on normalized multiparametric disaggregation technique (NMDT) proposed by Castro (2016) and lumped variable linearization (LVL) technique used in this study. Figure 3.8 illustrates an algorithmic flowchart for this proposed methodology.

The integrated refinery problem $(\boldsymbol{P})$ considered in this study, can be classified as a nonconvex, mixed-integer nonlinear constrained problem (MINLP) with the following general form as outlined by Castro (2016):

$$\max f_0(x,y) \qquad (\boldsymbol{D-1})$$

$$\text{subject to} \quad f_q(x,y) \leq 0 \quad \forall q \in Q \setminus \{0\}$$

$$f_q(x,y) = \sum_{(i,j)\in BL} a_{ijq}\, x_i\, x_j + B_q(x) + C_q(y) + d_q \qquad \forall q \in Q$$

$$0 \leq x^L \leq x \leq x^U$$

$$x \in R^m, y \in \{0,1\}^r \quad (\boldsymbol{i},\boldsymbol{j}) \qquad (\boldsymbol{P})$$

where $\boldsymbol{x}$ is a vector of continuous non-negative variables and $\boldsymbol{y}$ are binary variables. *BL* is an (i,j)-index set that defines the bilinear $x_i x_j$ terms present in the problem and it is assumed that it is possible to infer finite upper bounds x^U on variables x_i and x_j. $B_q(x)$ is nonlinear in x and $C_q(y)$ includes binary variables. Set Q includes all functions f_q, the objective function f_0 and all the constraints, a_{ijq} and d_q are scalars.

Given a nonconvex bilinear term $w_{i,j} = x_i x_j$, multiparametric disaggregation works by discretizing x_j over a set of powers , $l \in \{p, \ldots, P\}$,where $P = \lfloor \log_{10} x_j^U \rfloor$ and p is chosen by the user so as to reach a certain accuracy level. [S.13-15] The formula for P assumes discretization with base 10 in this study. Normalized version of multiparametric disaggregation technique discretizes $\lambda_j \in [0, 1]$, an auxiliary variable that is used to compute x_j as a linear combination of its lower x_j^L and upper x_j^U bounds:

$$x_j = x_j^L + \lambda_j\left(x_j^U - x_j^L\right) \quad \forall\, j \qquad (\boldsymbol{D-2})$$

The exact representation of λ_j can be achieved by considering an infinite number of positions $l \in Z^-$ in the decimal system,

$$\lambda_j = \sum_{l \in Z^-} \lambda_{jl} \qquad \forall\, j \qquad (\boldsymbol{D-3})$$

and by picking the appropriate digit $k \in \{0, 1, . . . , 9\}$ for each power l. This can be stated as a disjunction (Balas, 1979 ; Raman and Grossmann, 1994), where binary variables z_{jkl} take the value of one if digit k is selected

for position l for discretized variable λ_j:

$$\bigvee_{k=0}^{9} \begin{bmatrix} z_{jkl} \\ \lambda_{jl} = 10^l . k \end{bmatrix} \qquad \forall\, j\,, l \;\in\; Z^- \qquad (\boldsymbol{D-4})$$

The convex hull reformulation (Balas,1985) of the disjunction in (F-4) can be simplified so as to generate a sharp formulation without disaggregated variables. (Oral and Kettani,1992)

$$\lambda_j = \sum_{l \in Z^-} \sum_{k=0}^{9} 10^l . k.\; z_{jkl} \qquad \forall\, j \qquad (\boldsymbol{D-5})$$

$$\sum_{k=0}^{9} z_{jkl} = 1 \qquad \forall\, j, l \;\; \in Z^- \qquad (\boldsymbol{D-6})$$

Multiplying variable x_i by (D-6) and substituting $x_i x_j$ and $x_i \lambda_j$ with bilinear variables w_{ij} and v_{ij} leads to,

$$w_{ij} = x_i x_j^L + v_{ij}\left(x_j^U - x_j^L\right) \quad \forall\, (i, j) \qquad (\boldsymbol{D-7})$$

Substituting (D-5) into the definition of v_{ij} leads to the appearance of bilinear terms involving the product of a continuous and a binary variable.

$$v_{ij} = \sum_{l \in Z^-} \sum_{k=0}^{9} 10^l . k . x_i \ z_{jkl} \qquad \forall\,(i,j) \qquad (\boldsymbol{D-8})$$

An exact linearization can be performed by introducing new continuous variables $\hat{x}_{ijkl} = x_i\, z_{jkl}$ so that:

$$v_{ij} = \sum_{l \in Z^-} \sum_{k=0}^{9} 10^l . k . \hat{x}_{ijkl} \qquad \forall\,(i,j) \qquad (\boldsymbol{D-9})$$

$$z_{jkl} x_i^L \leq \hat{x}_{ijkl} \leq z_{jkl} x_i^U \qquad \forall\,(i,j),\ \ k \in \{0, \dots, 9\}, l \in Z^- \qquad (\boldsymbol{D-10})$$

Finally, multiplying (D-6) by x_i and replacing the bilinear terms by the new continuous variables results in,

$$x_i = \sum_{k=0}^{9} \hat{x}_{ijkl} \qquad \forall\,(i,j), l \ \in Z^- \quad (\boldsymbol{D-11})$$

Since it is impossible to compute the infinite sums over all negative integers, λ_j will be represented to a finite accuracy level by replacing $l \in Z^-$ with $l \in \{p, p+1, \dots, -1\}$, where p is a negative integer chosen by the user. In order to close the gap between discretization points so as to allow for all possible values for λ_j , slack variables $\Delta\lambda_j$ are introduced that are bounded between 0 and 10^p. The continuous representation of λ_j is then given by:

$$\lambda_j = \sum_{l=p}^{-1} \sum_{k=0}^{9} 10^l . k . z_{jkl} + \Delta\lambda_j \qquad \forall j \quad (\boldsymbol{D-12})$$

$$0 \leq \Delta\lambda_j \leq 10^p \qquad \forall j \quad (\boldsymbol{D-13})$$

Following the same reasoning as before, the continuous representation of the bilinear term v_{ij}= $x_i\,.\,\lambda_j$ is,

$$v_{ij} = \sum_{l \in Z^-} \sum_{k=0}^{9} 10^l . k . \hat{x}_{ijkl} + x_i\,.\,\Delta\lambda_j \qquad \forall (i,j) \quad (\boldsymbol{D-14})$$

The newly appeared bilinear terms $x_i\,.\,\Delta\lambda_j$ are going to be relaxed using the McCormick envelopes (McCormick,1976), which in this case coincide with the reformulation linearization technique bound factor products $x_i - x^L \geq 0,\ x^U - x_i \geq 0$, $\Delta\lambda_j \geq 0$ and $10^p - \Delta\lambda_j \geq 0$ [65,66]. Variables Δv_{ij} replace $x_i\,.\,\Delta\lambda_j$ in Equation (D-14).

$$x_i^L . \Delta\lambda_j \leq \Delta v_{ij} \leq x_i^U . \Delta\lambda_j \quad \forall\,(i,j) \quad (\boldsymbol{D-15})$$

$$(x_i - x^U). 10^p + x_i^U . \Delta\lambda_j \leq \Delta v_{ij} \leq (x_i - x^L). 10^p + x_i^L . \Delta\lambda_j \quad \forall\,(i,j) \quad (\boldsymbol{D-16})$$

The full set of mixed integer linear constraints for the exact representation of bilinear terms

$w_{ij} = x_i x_j$ is thus given by Equations (D-2, D-7, D-(11-16)), leading to the new optimization problem

(PR) that is a relaxation of (P). In other words, (PR) is feasible for values of w_{ij} , x_i and x_j

that do not satisfy w_{ij}= $x_i x_j$

$$\max \quad f_0'(x,y) \qquad\qquad (\boldsymbol{D-17})$$

$$subject\ to \qquad f_q'(x,y) \leq 0 \qquad \forall q \in Q\ \setminus \{0\}$$

$$f_q'(x,y) = \sum_{(i.j) \in BL} a_{ijq}\, w_{ij} + B_q(lv) + C_q(y) + d_q \qquad \forall q \in Q$$

$$\left.\begin{array}{c} x_j = x_j^L + \lambda_j\left(x_j^U - x_j^L\right) \\ \lambda_j = \sum_{l=p}^{-1}\sum_{k=0}^{9} 10^l.k.z_{jkl} + \Delta\lambda_j \\ 0 \le \Delta\lambda_j \le 10^p \end{array}\right\} \quad \forall j \in \{j|(i,j) \in BL\}$$

$$\left.\begin{array}{c} w_{ij} = x_i x_j^L + v_{ij}\left(x_j^U - x_j^L\right) \\ v_{ij} = \sum_{l=p}^{-1}\sum_{k=0}^{9} 10^l.k.\hat{x}_{ijkl} + \Delta v_{ij} \\ x_i^L.\Delta\lambda_j \le \Delta v_{ij} \le x_i^U.\Delta\lambda_j \\ \Delta v_{ij} \le (x_i - x^L).10^p + x_i^L.\Delta\lambda_j \\ \Delta v_{ij} \ge (x_i - x^U).10^p + x_i^U.\Delta\lambda_j \end{array}\right\} \quad \forall (i,j) \in BL$$

$$x_i = \sum_{k=0}^{9} \hat{x}_{ijkl} \qquad \forall (i,j) \in BL, l \in \{p, \dots, -1\}$$

$$\sum_{k=0}^{9} z_{jkl} = 1 \qquad \forall j \in \{j|(i,j) \in BL\}, l \in \{p, \dots, -1\}$$

$$z_{jkl}x_i^L \le \hat{x}_{ijkl} \le z_{jkl}x_i^U \qquad \forall\ (i,j),\ \ k \in \{0, \dots, 9\}, l \in \{p, \dots, -1\}$$

$$0 \le x^L \le x \le x^U$$

$$x \in R^m, w_{ij}, \lambda_j, v_{ij}, \hat{x}_{ijkl}, \Delta\lambda_j, \Delta v_{ij} \in R$$

$$y \in \{0,1\}^r, z_{jkl} \in \{0,1\} \qquad (\boldsymbol{PR})$$

Appendix E.

Tables E1-E5 with deterministic system information for integrated refinery model

Table E1. Maximum Capacity of Refinery Unit u (bb/d)	
Refinery Unit	**Capacity**
CDU	250000
FCC	140000
CRU	80000
HC	70000
HT1	50000
HT2	50000
HDS	80000
VB	80000
DC	84000
GT	100000
DFT	95000
EtOHT	15000

Table E2. Deterministic Demand Data for Commodity c (Mbbl/yr)							
Commodity	**Time Period**						
	1	**2**	**3**	**4**	**5**	**6**	**7**
G	31.40	28.11	29.56	32.74	29.57	28.74	27.63
DF	26.28	29.82	30.10	25.33	27.43	29.17	28.96

Table E3. System information for pipeline distribution model

Product	IDmin(p) (m^3)	IDmax(p) (m^3)	Minlotp (m^3)	Maxlotp (m^3)	Setlp (day)	Interface Volume (m^3)	
						P1	P2
P1	4000	88,742	8000	30000	1	0	15
P2	8000	38,833	8000	30000	1	15	0

Peak(t) Peak hours in time period t	1	2	3	4	5	6	7
	8	6	5	6	7	6	7

	P1	P2
Initv(p) Initial Inventory for Each Product at DCs (m3)	28,420	10,505
IR0(P) Initial inventory level of product p at the refinery (m3)	23,567	9271
IRmin(p) Minimum allowed storage capacity for product p at the refinery (m3)	10,000	10,000
IRmax(p) Maximum allowed storage capacity for product p at the refinery (m3)	100,000	100,000

Bmax Maximum Backorder or Lost Demand	8600
vp Pipeline volume(m)	141,810
frmax Maximum allowed pumping flow rate (m3\h)	100,000

Table E4. Deterministic Price Data for Commodity c ($/bbl)

Commodity	Time Period						
	1	**2**	**3**	**4**	**5**	**6**	**7**
G	117.13	118.49	120.74	122.52	119.98	116.37	121.30
DF	137.25	139.62	136.81	135.24	141.55	140.29	138.66

Table E5. System information and operating characteristics for the CHP based utility plant		
a_j consumption coefficient for MP steam redirected towards boiler	**BOIL1**	**BOIL2**
	0.1	0.1
b_j consumption coefficient for electricity required to carry out boiler operation	0.002	0.003
XHPmax maximum amount of steam that can be produced by boiler j (kg)	16000	17000
XHPmin minimum amount of steam that can be produced by boiler j (kg)	8000	8500
h_{fw} enthalpy of boiler feed-water (MJ\kg)	0.56677	0.56677
h_b enthalpy of superheated steam from boilers to turbines (MJ\kg)	3.06677	3.06677
SIdem quantity of fuel gas used during starting-up phase of boiler (ton)	2.024	4.093
ehst exhaust steam parameter for turbine j	**TURB1**	**TURB2**
	0.05	0.05
TXHPmax maximum amount of steam that can enter turbine j in time period t (kg)	500	500
η efficiency of the turbine j	0.8	0.8
h_m enthalpy of MP steams from turbines (MJ\kg)	2.95509	2.95509
h_l enthalpy of LP steams from turbines (MJ\kg)	2.83875	2.83875
h_e enthalpy of Exhaust steams from turbines (MJ\kg)	2.75268	2.75268
cc_i calorific value of fuel (MJ\kg)	23	
C_f cost of fuel (US$\ton)	55.49	
C_{EL} electricity purchase cost (US$\MWh)	88.79	
CGHG cost incurred for emissions of GHG (US$\ton)	19.98	
CSOX cost incurred for emissions of SOx (US$\ton)	25.53	
Cpt_i capacity of storage repository for fuel i (tons)	10,000	
ghg_i coefficient of GHG released from boiler due to fuel i	2.466	