DEVELOPMENT OF SUSTAINABILITY EVALUATOR INTERFACE TO EVALUATE ENVIRONMENTAL, ECONOMIC AND SOCIAL INDICES OF CHEMICAL PROCESSES

By

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DEVELOPMENT OF SUSTAINABILITY

EVALUATOR INTERFACE TO EVALUATE

ENVIRONMENTAL, ECONOMIC, AND SOCIAL

INDICES OF CHEMICAL PROCESSES

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Abstract:

Process design engineers have to consider a lot of constraints while designing chemical processes. Engineers have to deal with not only process design and product development details, but also need to consider environmental regulations, social impacts and economic benefits. Sustainable process design should simultaneously maximize the economic and social benefits of the process and minimize adverse impact on the environment. The main challenge engineers must address is, how economic, environmental and social aspects of the chemical process can be incorporated into early stages of process design. So process designers require a well-defined, robust and efficient tool to calculate the sustainability index in order to design sustainable chemical processes. In this work, the SUSTAINABILITY EVALUATOR tool developed by Shadiya and High (2010) is modified and a novel Sustainability Evaluator Interface is developed using Excel VBA to enable engineers to determine sustainability index more effectively. Modified sustainability evaluator allows engineers to customize potency factors of chemicals involved in the process and also weight factors of different index besides built in values to obtain more effective results. The sustainability of the manufacturing process of Lactic Acid has been evaluated using the modified SUSTAINABILITY EVALUATOR and the results was compared with results obtained using previous SUSTAINABILITY EVALUATOR for validation. Details working procedure of the modified SUSTAINABILITY EVALUATOR tool results, reports and graphs generated to determine sustainability of lactic acid process using this SUSTAINABILITY EVALUATOR tool are also described in this work.

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CHAPTER I

INTRODUCTION

1.1 Sustainability

Sustainable processes can be defined as manufacturing processes that minimize negative environmental impacts, conserve natural sources and energy, are safe for employees, consumers, and social communities and are economically feasible. Before going into the details of sustainable process design we need to understand what sustainability is. The Latin word *sustinere* is the origin of the word sustainability meaning *to hold up*. The literal meaning of sustainability is "to maintain" or "to support". The term sustainability was invented as the 21st century was approached because environmental concerns were not the only concern affecting the community all over the world. So, sustainability can be defined as - *economic well being linked to health of the environment and the success of the world citizens* (Schwarz et al., 2002). The World Commission on Environment and Development provided a more relevant definition in 1987 "*development that meets the needs of the present without compromising the ability of future generations to meet their own needs"* (Brundtland, 1987).

Sustainability covers the following fundamentals: environmental protection, economic benefit, resource efficiency and social development as per current level of understanding (Darton, 2003). So the basis of sustainability consists of three main types of factors such as environmental, economic and social where preserving nature is the environmental feature, profitability is the economic feature and social consequences are the social feature of sustainability.

So, we can conclude with a Venn diagram (Figure 1.1) that, a viable process can be defined as the process which takes into account only environmental and economic factors while designing, a bearable process can be defined as the process which takes into account only social and environmental factors while designing and an equitable process can be defined as the process which takes into account only economic and social factors while designing the process. So, a sustainable process is the process which takes all the three factors/concerns into account while designing the process.

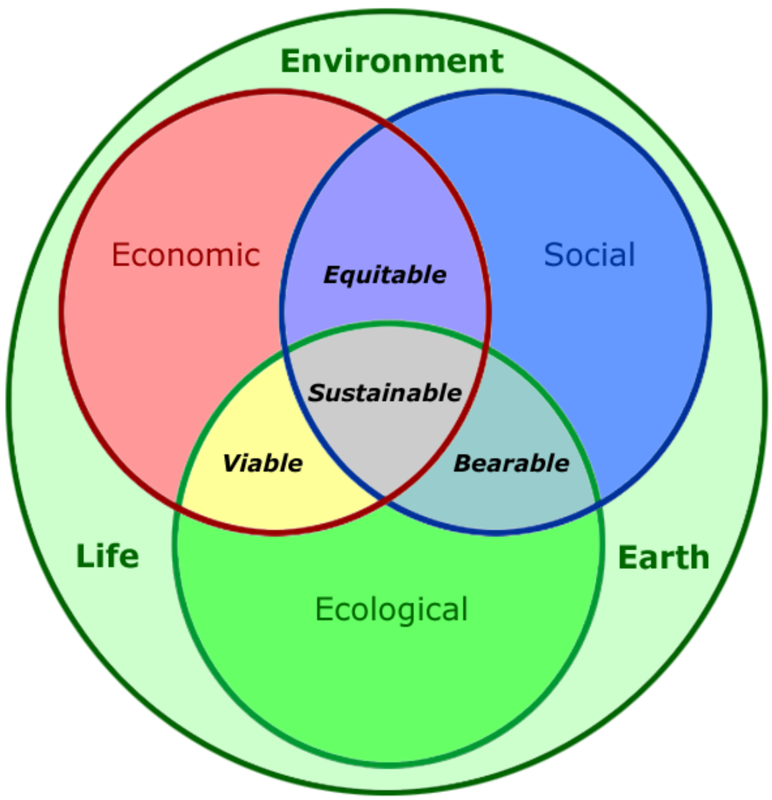


Figure 1.1: Factors/concerns explaining sustainable process (Andrew, 2009)

With industrial development and increasing need of commodities there is an increasing impact of these three aspects of sustainability. We cannot declare a process to be good only if it is viable or bearable or equitable. It needs to be viable, bearable and equitable at the same time and we refer to this process as the sustainable process. Concerns regarding sustainable process design has been growing and researches have been going on in the past few years to devise a procedure to evaluate sustainability of a process.

1.2 Sustainability Concerns

Important groups which include academia, industry, the United Nations, the United States Government are all alarmed with the sustainability challenges. Here are some concerns regarding the necessity of sustainability development given by United Nations Environmental Program's GEO-2002 (Azapagic et al., 2004):

- 15% of earth land (2 billion ha) is considered to be degraded.
- All river water (about half of the water supply system around the world) is considered to be unusable and contaminated.
- 12% of bird species and 24% of mammal species are endangered worldwide.
- Safe drinking water is accessible to 40% of humankind (around 80 countries) in inadequate amounts.
- The daily income of about 2.8 million people is only $2 or less.
- Increased death rate of around 11 million people due to poor nutrition, health education and sanitation are the reasons for increase in death rate to around 11 million.
- Increase in chlorofluorocarbon emissions is making the ozone layer depletion steady.
- Concentration of CO2 has been increased 25% higher than that is 150 years ago.

These concerns are related to all the processes, so sustainability quantification in both chemical and petroleum processes have become very important issue for researchers. They invented some methods also but there were limitations in those methods. The method of quantifying overall sustainability of a process should take into account all three factors involved because they are interdependent which made the decision making process very complex. elaborated list of sustainability concerns is given below as Table 1.1:

Table 1.1: Sustainability Concerns (de Haes et al., 1999; Fiksel et al., 1999; IChemE Metrics, 2002; Azapagic et al., 2004)

Economic concerns	**Environmental concerns**	**Social concerns**
Micro-Economic	Energy Use	Health and Safety
Capital Costs	Water Use	Illness & Disease Reduction*
Operating Costs	Water Discharge	Accident & Injury Reduction*
Profitability	Solid Waste	Peace of Mind*
Decommissioning Costs	Abiotic Reserve Depletion	Quality of Life*
Macro-Economic Costs	Global Warming	Complaints*
Value- added	Ozone Depletion	Employment opportunities*
Taxes paid on investment (e.g.	Acidification	External stakeholders*
pollution prevention, health and	Eutrophication	Community benefits*
safety, decommissioning and	Eco-toxicity	Work force capability*
ethical investments		Public reporting*
Environmental Liability		Organizational learning
		Remuneration*
		Management attention to HR*

"*" mark represents not considered in this study

1.3 Tool to evaluate sustainability of a process

There are several tools available which assist in measuring the parameters listed below as Table 1.2

Table 1.2: Tools Available for the Assessment of Sustainability Impacts

Sustainability Category	Tools Used for Impact Assessment
Economic	Aspen Process Economic Analyzer, Sustainability Evaluator
Environmental	Life Cycle Assessment using SimaPro, Sustainability Evaluator
Social	Sustainability Evaluator

Atlee (Atlee 2006) provided some basic features that are desirable for sustainability metrics (as listed by Shadiya **(Shadiya 2010)**):

- Simple and easily accessible by any audience
- Predictive and consistent
- Serve as decision making tool
- Economical efficient: data collection should be easily
- Unbiased
- Applicable to several process

Developing a single quantifying scheme by taking all these desirables into account is an enormous task which include multi-criterion decision making process as discussed earlier. The effort made by Shadiya **(Shadiya, 2010)** in the development of the SUSTAINABILITY EVALUATOR (SE) has been discussed in this work**.**

The tool developed by Shadiya required further modification for more effective use in evaluating sustainability of any process. In this work, modification of SUSTAINABILITY EVALUATOR has been done to make it more effective and user friendly. The existing version of SUSTAINABILITY EVALUATOR is excel based tool where inputs are given in an excel worksheet and also the output results are stored in the same worksheet. With the development in technical world there has been an increasing need of making the tool more user friendly and robust. So, an attempt has been made in this work to modify the SUSTAINABILITY EVALUATOR using VBA programming. A user friendly graphical interface has been developed to evaluate sustainability of a process.

1.4 Scope and Objectives

The scope and objectives of this study are mentioned below:

1. Modify the SUSTAINABILITY EVALUATOR tool and develop a program using Excel VBA to make the tool more user friendly and effective.

2. The modified SUSTAINABILITY EVALUATOR tool should allow the user to customize the potency factors of different metrics determining the impacts of the process on economics, environment and social welfare and also change the weight factors of economic, environmental and social index if required.
3. The new sustainability tool should generate ready comparison information for the user as external output files while comparing sustainability index of alternate manufacturing processes.

The background of this study and literature review is discussed in Chapter Two. The working procedure of the previous excel version of the SUSTAINABILITY EVALUATOR is described in Chapter Three. Chapter Four includes different features of modified Excel VBA based SUSTAINABILITY EVALUATOR and the working principles. The results and discussion is included in Chapter Five. Chapter Six provides conclusion and options of future work.

CHAPTER II

LITERATURE REVIEW

The purpose of this chapter is to describe the background of this study. Process design concepts, tools available for designing chemical processes, issues regarding engineering design, and how to address these issues are described briefly in this chapter.

2.1 Process Design Synthesis

Designing new products, new processes and the reconfiguration of processes for more efficient production and or developing of new technology are discussed in process design area of engineering study. The design of process can be very complex because a lot of constraints are required to be considered. The synthesis of the process flowsheet is one of the important steps of chemical process design (Diwekar et al., 1992). The Douglas five step hierarchical approach for process synthesis can be used to develop process flowsheet (Taal et al., 2003). The steps of the Douglas hierarchical approach is given below (Turton et al., 2009):

- Select the process type - batch or continuous
- Design the input - output structure of the process
- Define the recycle structure
- Design the separation scheme
- Design the energy recovery system

2.2 Tools available for designing chemical processes

The advancement of chemical process simulation software has made chemical process design more efficient and robust. Chemical process simulation tools mimic the behavior of an actual process. These tools can be used to design, optimize, test and integrate new or retrofit processes (Casavant and Cote 2004). Simulation tools use mathematical, thermodynamic and process unit models to solve mass and energy balance for processing unit (Motard et al., 1975). The process simulator can predict process conditions for the product, byproduct and waste streams, size equipment and process economics based on material stream inputs. Several process simulation tools such as CHEMCAD, ASPEN PLUS, and ASPEN HYSIS have been developed over the years. For this study, data using ASPEN PLUS and ASPEN HYSIS tools are used.

2.3 Process design issues and optimization

Process design engineers have to consider a lot of constraints while designing chemical processes. The design must ensure profitability of the process. At the same time, the designer needs to consider the impact of the products or process on the environment. Health and safety issues and social concerns are also required to be considered. As a result, to design sustainable processes, process engineers needs to cover the following elements: economic benefit, resource efficiency, environmental impacts and social concerns. The main challenge engineers must address is, how economic, environmental and social aspects of the chemical process can be incorporated into early stages of process design. The implementation of sustainable development should simultaneously maximize the economic and social benefits of the process and minimize adverse impact on the environment. The solution of this problem is not an easy task as engineers have to optimize multiple objectives. Process designers have to deal with not only process design and product development details, but also need to consider environmental regulations, social impacts and economic benefits. So process designers require a well-defined, robust and efficient tools to calculate sustainability index in order to design sustainable chemical processes.

2.4 Methodology

When designing products and processes, engineers must look at the bigger picture, i.e. the economy and environment, instead of merely focusing on the process plant and the economic benefits to the corporation (Bakshi and Fiksel, 2003). Shadiya in 2010 developed a unique tool called the SUSTAIINABILITY EVALUATOR which evaluates the sustainability concerns in the early stages of design. The methodology proposed is given below step by step.

Step 1: Base case process modeling

- Collection of input data from literature
- Simulate process on a process simulator e.g. Aspen Plus

Step 2: Sustainability assessment of the base case using the “SUSTAINABILITY EVALUATOR”

- Evaluate economic impact
- Environmental impact
- Social impact

Step 3: Complete a sensitivity analysis

- Identify process parameters that affect process sustainability
- Re-configuring process structure

Step 4: Optimize process based on the results of the sensitivity analysis

- By maximizing profit, minimizing wastes and minimizing health and safety concerns

Step 5: Evaluate the sustainability of the optimized process using the "SUSTAINABILITY EVALUATOR"

- If the design is acceptable move to step 6, otherwise repeat step 5

Step 6: If process is sustainable based on step 5, ACCEPT

2.4.1 Base Case Model Simulation

ASPEN PLUS simulator is used to simulate the base case chemical process as it is easily available for engineering students at Oklahoma State University. It takes the desired input step by step in a graphical interface and generates results accordingly. This tool is also used for optimization, sensitivity analysis, economic analysis and equipment sizing for a process.

2.4.2 Sustainability Indices Evaluation Using SUSTAINABILITY EVALUATOR

The SUSTAINABILITY EVALUATOR is a Microsoft Excel based tool which takes the values obtained from ASPEN PLUS Simulator for the sustainability concerns as inputs, calculates the individual impacts of three different aspects of sustainability and gives output for them individually and overall sustainability impact for that process as well. Figure 2.1 shows some of the concerns addressed by the tool as summary.

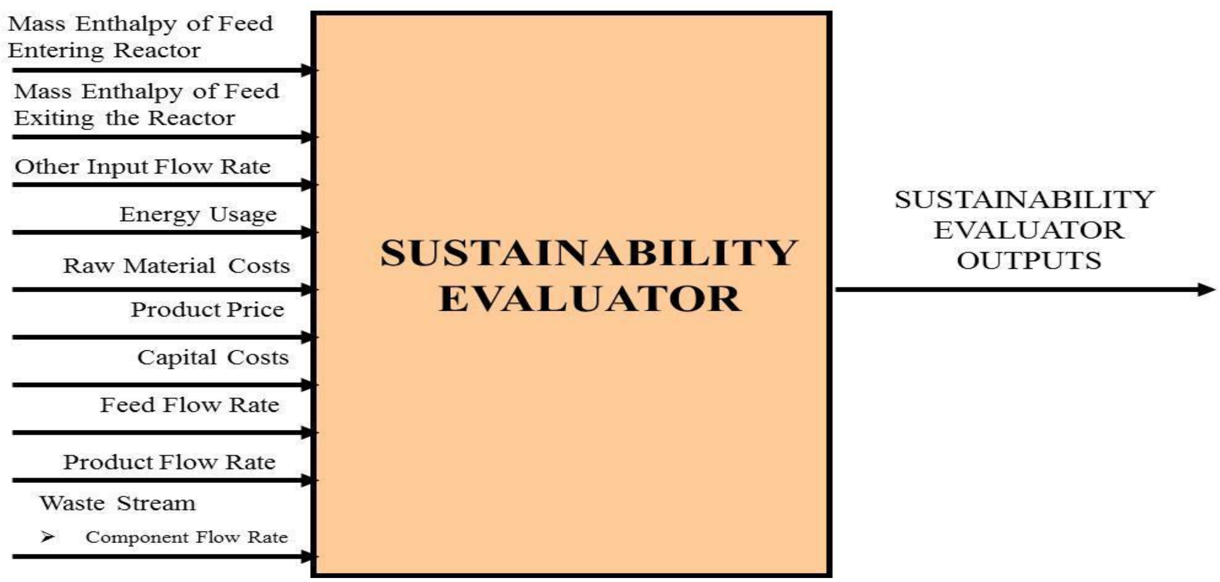


Figure 2.1: Summary of the SUSTAINABILITY EVALUATOR Inputs (Shadiya & High, 2010)

In this figure profit, energy costs, waste treatment costs are the economic concerns; atmospheric acidification, global warming, environmental burdens, ozone depletion, photochemical smog, resource usage etc. are the environmental concerns; health and safety risks such as risk of exposure, explosion, flammability etc. are the health and safety concerns.

The description of the metrics that address economic, environmental, health and safety concerns incorporated into this impact assessment tool are discussed below.

2.4.2.1 Economic Impact Assessment using SUSTAINABILITY EVALUATOR

The final aim in every industrial process is to maximize profits. So, a process has to be economically viable to be economically sustainable. Therefore, a methodology has been presented in the SUSTAINABILITY EVALUATOR which addresses the economic concerns by doing a profitability analysis on the process. Shadiya (2010) introduced the following concerns to evaluate economic sustainability as Table 2.1.

Table 2.1: Table describing all the economic concerns addressed by SUSTAINABILITY EVALUATOR

Concerns	Definitions and calculations	Indicator
Product Revenue	Revenue measurement generated from the desired product and by-products.	Higher the better
Raw Material Costs	Costs of the raw materials used in manufacturing the desired product.	Lower the better
Waste Treatment Costs	The expenses associated with treating wastes generated in a process.	Lower the better
Operating costs	The costs of energy used in manufacturing a particular/desired product.	Lower the better
Material Value Added	The difference between the product revenue and the raw material costs (Carvalho et al., 2008).	Higher the better
Annualized Capital Costs	The capital recovery factor (CRF) is evaluated using equation 2.1, where n is Number of Years and I is Interest Rate $\text{CRF} = \frac{i(1+i)^n}{(1+i)^{n-1}}$ (2.1)	Lower the better
Profit	Profit = Product Revenue + By-product Revenue - (Raw Material Cost + Waste Treatment Cost + Operating Cost +Annualized Capital Cost) (2.2)	Higher the better

2.4.2.2 Environmental Impact Assessment Using SUSTAINABILITY EVALUATOR

Protection of the environmental is a big issue currently and as so in the SUSTAINABILITY

EVALUATOR. The environmental burden impact and resource usage impact are combined together to give the overall Environmental Index.

2.4.2.2.1 Environmental Burden Assessment

There are several concerns that the SUSTAINABILITY EVALUATOR takes into account while assessing environmental impact of a process as per Shadiya (2010) which are included in Table 2.2

Table 2.2: Table describing all the concerns for Environmental Burden Addressed by SUSTAINABILITY EVALUATOR

Concerns	Definitions	Indicator
Global warming	Defined as the increase in the temperature of the earth surface due to activities such as industrial and transportation emissions	Lower the better
Stratospheric ozone depletion	Depletion of Ozone layer which causes cancer from ultraviolet rays.	Lower the better
Photochemical smog	Reaction that occurs when photochemical smog causing chemicals such as petrochemicals are reacted with combustive substances leading to a smog like appearance at the right temperature and sunlight (IChemE Metrics, 2002)	Lower the better
Ecotoxicity to Aquatic Life	Extent of an increase in eco-toxicity to aquatic organisms due to the presence of pollutants in water sources	Lower the better
Aquatic oxygen demand	Extent of the increase in oxygen needed by aerobic microorganism due to the presence of pollutants in water sources	Lower the better
Atmospheric acidification	Extent of the acid increase in the environment when chemicals such as ammonia, sulfuric acid, hydrochloric acid, hydrogen fluoride, nitrogen dioxide and sulfur dioxide are	Lower the better

	emitted into the atmosphere (IChemE Metrics, 2002; da Costa and Pagan, 2006).	
Eutrophication and resource usage	Extent the acid increase in water sources when chemicals such as acetic acid, hydrochloric acid and hydrogen fluoride etc. are discharged (IChemE Metrics, 2002).	Lower the better

Potency Factors for Chemicals that Cause all these 8 impacts are given in appendix (IChemE Metrics, 2002)

2.4.2.2.2 Resource Usage

SUSTAINABILITY EVALUATOR takes the following factors into account for calculating resource usage impact of a chemical process on environment which is represented in Table 2.3 (Shadiya, 2010).

Table 2.3: Table describing all the concerns for Resource Usage Analysis Addressed by SUSTAINABILITY EVALUATOR

Concerns	Definitions	Indicators
E-factor	$E-Factor = \frac{Total\ Waste}{Mass\ of\ Product\ (kg)}$	Lower the better
Reaction Mass Efficiency	$Reaction\ Mass\ Efficiency = \frac{Mass\ of\ Product\ (kg)}{Mass\ of\ Reactant\ (kg)}$	Higher the better
Mass productivity	$Mass\ Productivity = \frac{1}{Mass\ Intensity} \times 100$	Higher the better
Mass Intensity	$Mass\ Intensity = \frac{Total\ Mass\ used\ in\ Process\ Step}{Mass\ of\ Product\ (kg)}$	Higher the better
Energy Intensity	$Energy\ Intensity = \frac{Energy\ Consumed}{Mass\ of\ Product\ (kg)}$	Lower the better
Water Intensity	$Water\ Intensity = \frac{Water\ Consumed}{Mass\ of\ Product\ (kg)}$	Lower the better

2.4.2.3 Social Impact Assessment Using SUSTAINABILITY EVALUATOR

Shadya (2010) focused on safety risk by implementing the index developed by Heikkila (1999) and health risk by using data from the International Agency for Research on Cancer (2009) and Score Card (2005) evaluating process while evaluating overall social impact of a process.

2.4.2.3.1 Assessment of Process Safety Risk

The metrics considered in this regard are discussed below:

1. Heat of main and side reaction index: Defined as amount of heat that is released during a chemical reaction.
2. Flammability index: Measures the probability of chemical burning with air when there is a chemical leak.
3. Explosivity index: Extent the probability for a gas to form an explosive when mixed with air.
4. Corrosive index: Extent of the likelihood of corroding plant equipment by chemicals such as acids, acid anhydrides and bases.
5. Temperature index: Extent of the possible risk in a process due to the temperature range in the process.
6. Pressure index: Extent of the possible risk due to the pressure range in the process.
7. Equipment process safety index: Extent the risk associated with your process based on equipment found in a process.
8. Process safety structure index: Extent the dependability of a process structure based on engineering practice, industry standard and related incidents.
9. Toxic Exposure Index: Extent of the health risk allied with a certain chemical and it is measured by its threshold limit value (TLV).

Table 2.3 represents the index scores of the ten metrics described. As suggested by Heikkila (1999), an overall safety index can be evaluated by summing each of the ten metrics from the table.

Table 2.4: Index Scores for Process Safety Structure Index

Safety Metric	Index Range
Heat of Main Reaction Index	0-8
Heat of Side Reaction Index	0-8
Flammability Index	0-8
Explosiveness Index	0-8
Corrosiveness Index	0-4
Temperature Index	0-8
Pressure Index	0-8
Equipment Safety Index	0-8
Safety Level of Process Structure Index	0-10
Toxic exposure Index	0-30
Overall Safety Index	0-100

2.4.2.3.2. Assessment of Process Health Risk

The metrics considered in this regard are discussed below:

1 Carcinogenic health risk: Degree the carcinogenic risk from the chemicals present in the process.

2 Developmental health risk: Degree of risks for a growing child when a pregnant woman is exposed to toxic chemicals present in the process.

3 Reproductive health risk: Degree of risks posed to the reproductive system when exposed to reproductive toxicants present in the process for an adult

4 Cardiovascular health risk: Degree of risks posed to the circulatory system when exposed to cardiovascular toxicants present in the process for an adult

5 Endocrine system health risk: Degree of risks posed to the endocrine system after exposed to endocrine toxicants present in the process for an adult.

6 Liver damage health risk: Degree of risks posed to the gastrointestinal tract, liver, or gall bladder after exposure to toxicants present in the process for an adult.

7 Immune system damage health risk: Degree of risks posed to the immune system after exposure to immunotoxicants present in the process.

8 Kidney damage health risk: Degree of risks posed to the kidney, ureter and bladder after toxic

exposure.

9 Skeletal system damage health risk: Degree of risks posed to the bones, muscles and joint after toxic exposure.

10 Neurological damage health risk: Degree of risks posed to the nervous system after toxic exposure.

11 Respiratory system health risk: Degree of risks posed to nasal passages, pharynx, trachea, bronchi, and lungs when they are exposed to toxicants present in the process for an adult.

Table 2.4 represents the index scores of the twelve metrics described. Mass flow rates of the substances releasing are to be multiplied by the respective index value from the table for each metric to evaluate the overall health metrics of the system.

Table 2.5: Index Scores for Health Metrics

Health Metric	Index Range
Carcinogenic Risk	0-1
Developmental Damage	0.6 or 1
Reproductive System Damage	0.6
Circulatory System Damage	0.6
Skeletal System Damage	0.6
Endocrine System Damage	0.6
Gastrointestinal and Liver Damage	0.6
Immune System Damage	0.6
Kidney Damage	0.6
Skeletal System Damage	0.6
Nervous System Damage	0.6
Respiratory System Damage	0.6
Sensory System Damage	0.6

2.4.2.4 Overall Sustainability Impact in the SUSTAINABILITY EVALUATOR

As we know by now that evaluating overall sustainability of a process is a multi-objective optimization problem and all three metrics has different units, they must me normalized to a common unit first before combining together. The metrics are normalized by using a ranking system procedure here. After normalizing the metrics are combined together to calculate overall sustainability impact (SUI) given by the equation 2.3 developed by Shadiya (2010).

$$SUI = 0.20 * EI + 0.40 * ENVI + 0.40 * SCI \quad (2.3)$$

Where

EI = Economic Impact

ENVI = Environmental Impact

SCI = Social Impact

Using weights to calculate potential solution for multi-objective optimization problems has been a straight forward approach and has been by several researchers because of its advantage of getting one final solution instead of multiple Pareto solutions (Jin et al., 2001; Yaochu et al., 2001). The main objective here was to derive an overall impact value ranging from 0-1. Processes with overall impact values close to 0 are more sustainable compared to the processes with values close to 1. Hence the lower the overall sustainability impact, the more sustainable the process is. Social and environmental impacts were allotted a higher value of 0.40 where a weight of 0.20 was allotted to the economic impact to calculate the overall impact.

2.4.3 Sensitivity Analysis

A sensitivity analysis is useful in investigating how the variation of one parameter can affect a targeted objective or goal. A sensitivity analysis assists in identifying optimum operating conditions and process configurations. In sensitivity analysis, there are independent and dependent variables. Dependent variables are variables that are being evaluated when independent variables are fluctuated. As the goal of this research is to determine the most sustainable process option, the dependent variables in this work will be the sustainability metrics that were discussed in the previous section, which will change in occasions when different parameters such as operating conditions, mass flow rate, reactor temperature and pressure, number of stages in distillation columns, reflux ratio etc. are changing.

The sensitivity analysis is done using ASPEN PLUS simulator here. The simulator has an inbuilt sensitivity analysis tool and by using that it is very easy to explore how changes in parameters affect the overall sustainability of a process. Here the parameters such as reactor temperature and pressure, mass flow rates, operating conditions, reflux ratio, number of stages in distillation column etc. are the independent variables and overall sustainability of a process is the dependent variable. After conducting the analysis the process needs to be reconfigured as required. Reconfiguration of the process may include adding additional separation equipment, reactor operating condition modification, recycle stream incorporation, changing reflux ratio etc.

2.4.4 Process Optimization

The next step is to do the process optimization using ASPEN PLUS simulator again. Here the goal is to maximum profit using equation 2.2 for the process while minimizing wastes flow rates and also including constraints that have been selected based on the results of the sensitivity analysis done in the previous step. The simulator has an inbuilt optimization tool that we can use to find the optimum process criterions. Reduction in waste stream flow rates will reduce adverse environmental impact and also the health risks while improving the safety risks. The optimization of this process will improve the overall sustainability impact of the process.

2.4.5 Sustainability Re-evaluation

After finishing doing the sensitivity analysis and also the optimization analysis, the process is re-evaluated using the SUSTAINABILITY EVALUATOR. Now the user has to check whether the overall impact is more or less than the previous process design. The user can accept the newly optimized process if the design has a low overall sustainability impact than previous non-optimized design and vice versa. The optimization step (Step-4) is repeated and the process is evaluated again and again using the SUSTAINABILITY EVALUATOR until any satisfactory final solution is not obtained.

CHAPTER III

SUSTAINABILITY EVALUATOR: HOW IT WORKS

The SUSTAINABILITY EVALUATOR evaluates sustainability index of a process as an impact assessment tool. The metrics which have been used to evaluate sustainability index are described in chapter two. This chapter represents the impact assessment of production of Lactic acid. The process and simulation data that is used as input for sustainability evaluation are taken from MS thesis work by Susmit Bapat (Susmit 2014). The manufacturing process of Poly Lactic acid and simulation results for base case and two other configurations of the Lactic acid process model are described briefly in following section.

3.1 Process Description

Stage 1: Preparation of Crude Lactic Acid Feed Stock

In this stage, crude lactic acid feed stock is prepared from sugar cane juice. By fermentation process, 10% wt. solution of calcium lactate is obtained from sugar cane juice. Calcium lactate solution reacts with 50% by wt. solution of sulfuric acid to produce crude lactic acid. Figure 3.1 represents process block diagram of stage 1 of the manufacturing process of poly lactic acid and the main reaction involved.

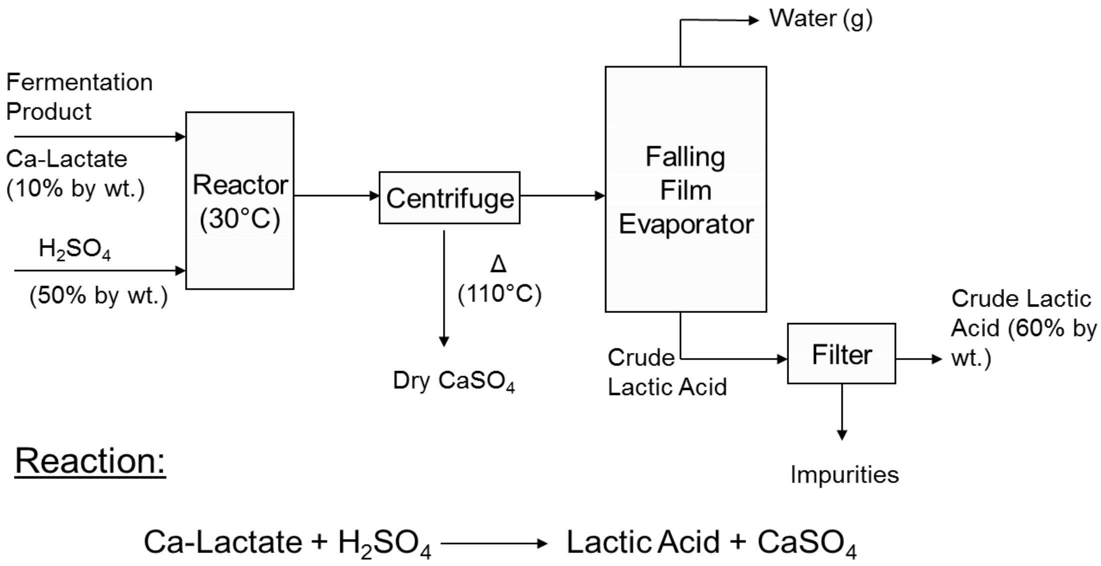


Figure 3.1: Process Block Diagram of First Stage of the Manufacturing Process of Poly Lactic Acid (Susmit, 2014)

Stage 2: Esterification Using Trickle Phase Continuous Counter Current Method with Doping of Known Impurities in Lactic Acid Feed

In this stage, Lactic acid reacts with methanol and produces Methyl Lactate through esterification reaction. Known amount of impurities are added to the crude lactic acid such as oxalic acid, malic acid, acetic acid and fumaric acid continuously and dissolves in 1% methanol.

Detailed process block diagram for stage 2 and the main reaction involved in this stage is given below as figure 3.2.

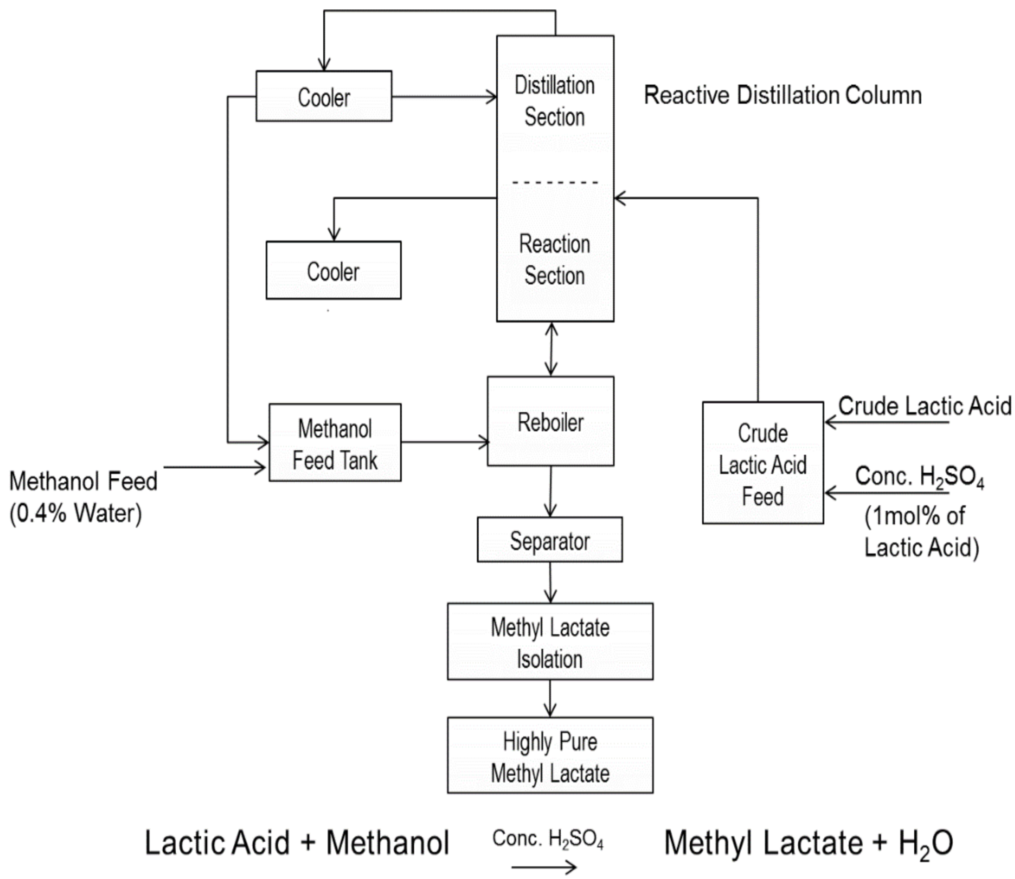


Figure 3.2: Process block Diagram of the Second Stage of the Manufacturing Process of Poly Lactic Acid (Susmit, 2014).

Stage 3: Hydrolysis of Highly Pure methyl Lactate to Produce Highly Pure Lactic Acid

In this stage highly pure methyl lactate (99.8%) from stage 2 is reacts with distilled water to produce acetic acid in presence of pure lactic acid. In this reaction pure lactic acid acts as an auto catalyst increasing the reaction rate and purity of the product. Figure-3.3 represents the process block diagram for stage 3 of manufacturing process of polymer grade lactic acid and the main reaction involved.

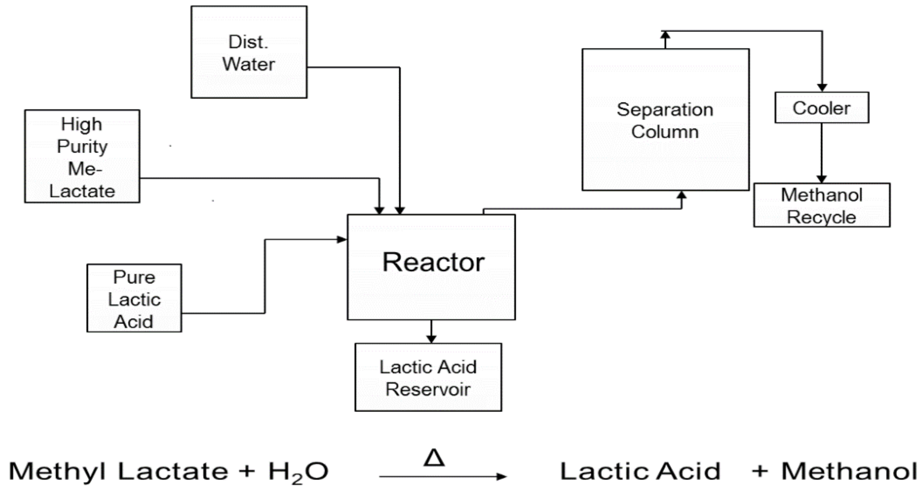


Figure 3.3: Basic Process Flow Diagram for the Third Stage of the Manufacturing Process of Polymer Grade Lactic Acid.

After simulating the process in Aspen plus simulator the data obtained were used to evaluate the overall sustainability evaluator using the tool SUSTAINABILITY EVALUATOR. Detailed process flow diagram for the overall manufacturing process developed in Aspen plus is given below as figure 3.4.

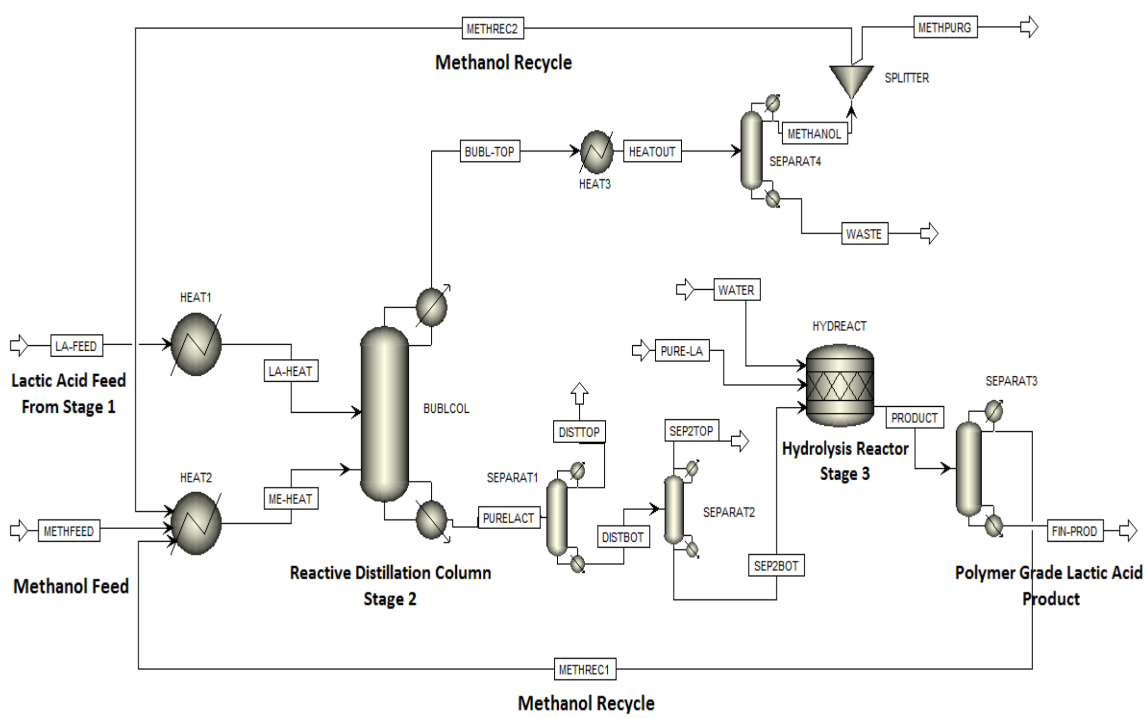


Figure 3.4: Process Flow Diagram Developed in Aspen Plus for the Manufacturing Process of Polymer Grade Lactic Acid (Susmit, 2014)

3.2 Input Section

The input section of sustainability evaluator tool has five different categories to take inputs from the user. The categories are environmental burden, resource usage, economic impact, health impact and safety impact. The user selects the chemicals associated with the impact under evaluation and enters inputs for mass flowrates, product and raw material prices, molecular weight, material of constructions, process temperature and pressure and other information essential for sustainability evaluation in excel spreadsheet.

3.2.1 Environmental Burden

The environmental burden section of sustainability evaluator consists of eight environmental concerns. The chemical(s) associated with the process contributing to each impact category is selected and mass flowrate of the chemical(s) is entered in kg/yr. The waste stream of the process provides the information regarding chemicals responsible for environmental burden. A screen shot of input section for environmental burden category is given as figure 3.5. The steps necessary for environmental burden evaluation are given below:

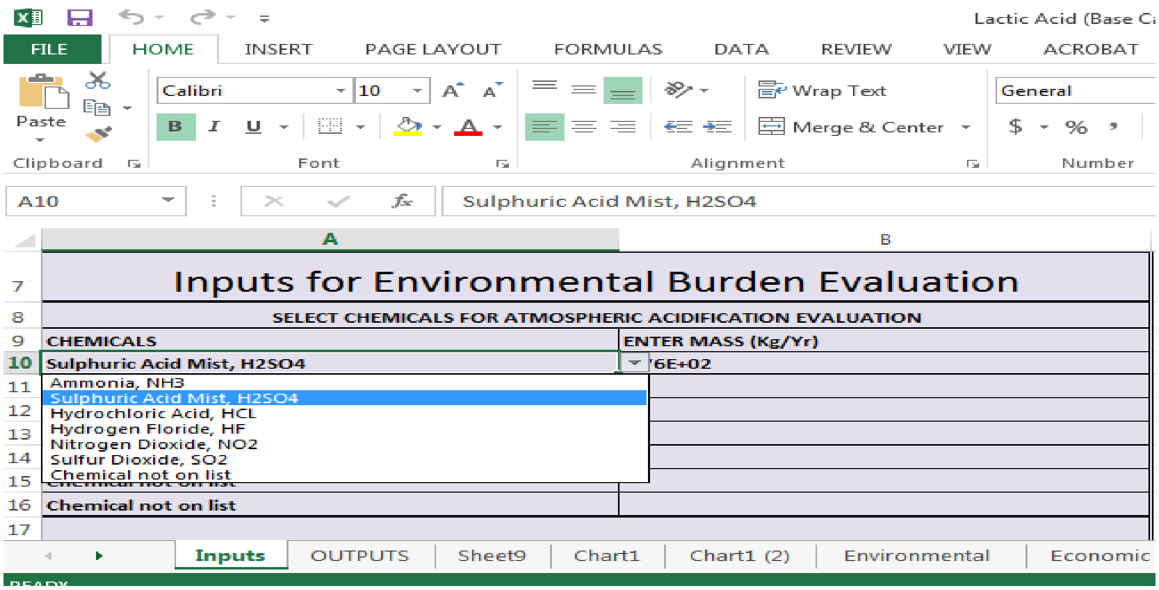


Figure 3.5: Screen Shot Demonstrating Selection of Chemicals from Dropdown Menu

Step 1: Atmospheric acidification is the first impact category for environmental burden evaluation. The chemicals present in the waste stream which are responsible for this impact category is selected from the dropdown menu on the left and mass flow rate is given in the right side. For other chemicals in that list which are not responsible for atmospheric acidification, “chemical not on this list” is selected and mass flow rate is left blank. Figure 3.6 represents the screen shot of entering inputs for Atmospheric acidification.

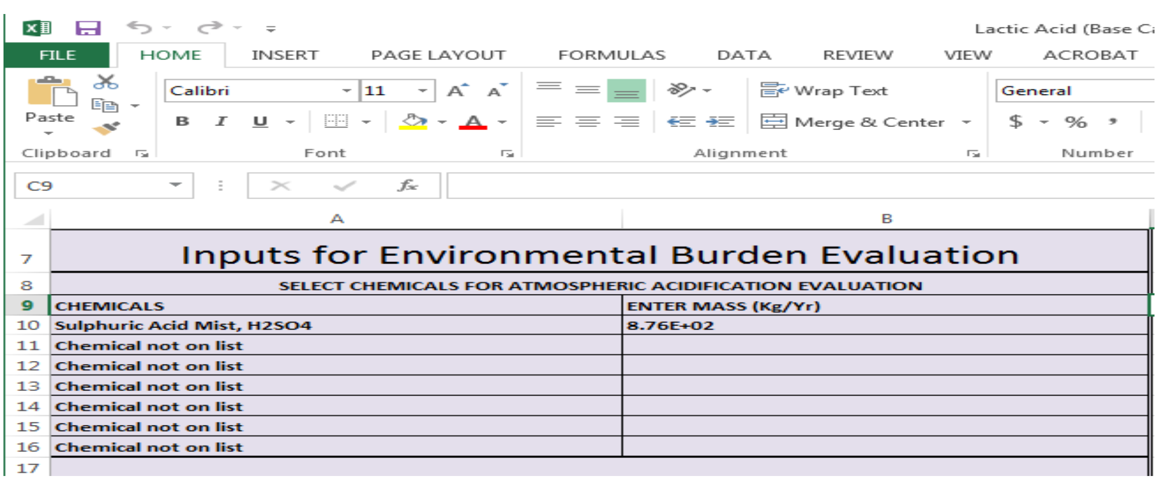


Figure 3.6: Screen Shot Demonstrating Chemicals that Contribute to Atmospheric Acidification

Step 2: Global warming is the second impact category. The chemicals responsible for global warming are selected and mass flow rate in kg/yr for each chemical is entered into the tool. Mass flow rate data are obtained from the waste stream of the process. Figure 3.7 represents the screen shot of entering inputs for global warming impact.

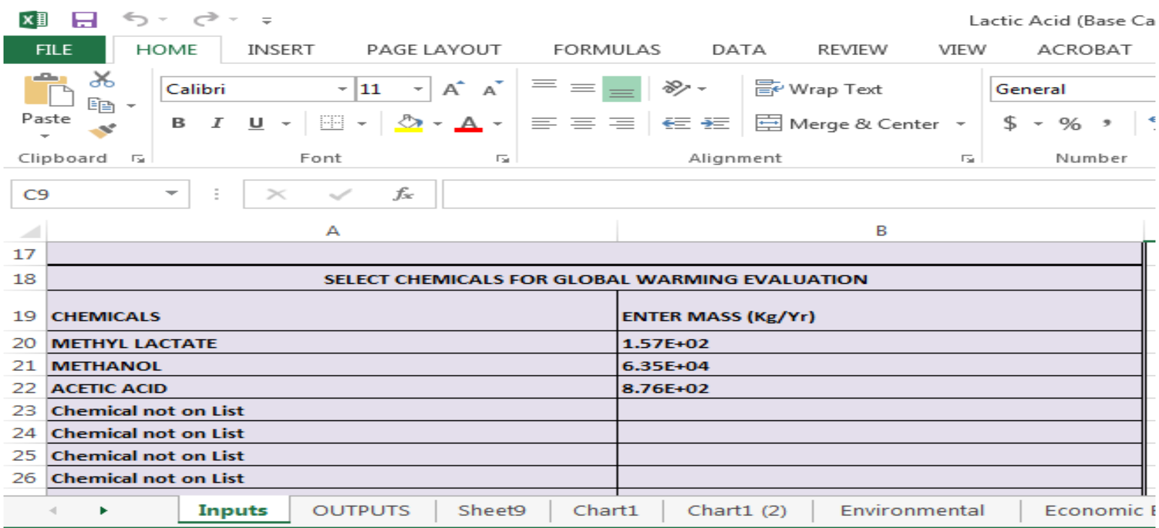


Figure 3.7: Screen Shot Demonstrating Chemicals that Contribute to Global Warming

Step 3: For other six categories step 1 and step 2 are repeated.

3.2.2 Resource Usage

Inputs required for resource usage impact evaluation are entered under resource usage category. The steps are described below:

Step 1: Total mass flow rate of the desired product is entered in kg/yr.

Step 2: Total mass flow rate of non-benign reactant is entered.

Step 3: Molecular weight of the desired product is entered.

Step 4: Molecular weights of the reactants are entered.

Step 5: Total waste produced in the process is entered.

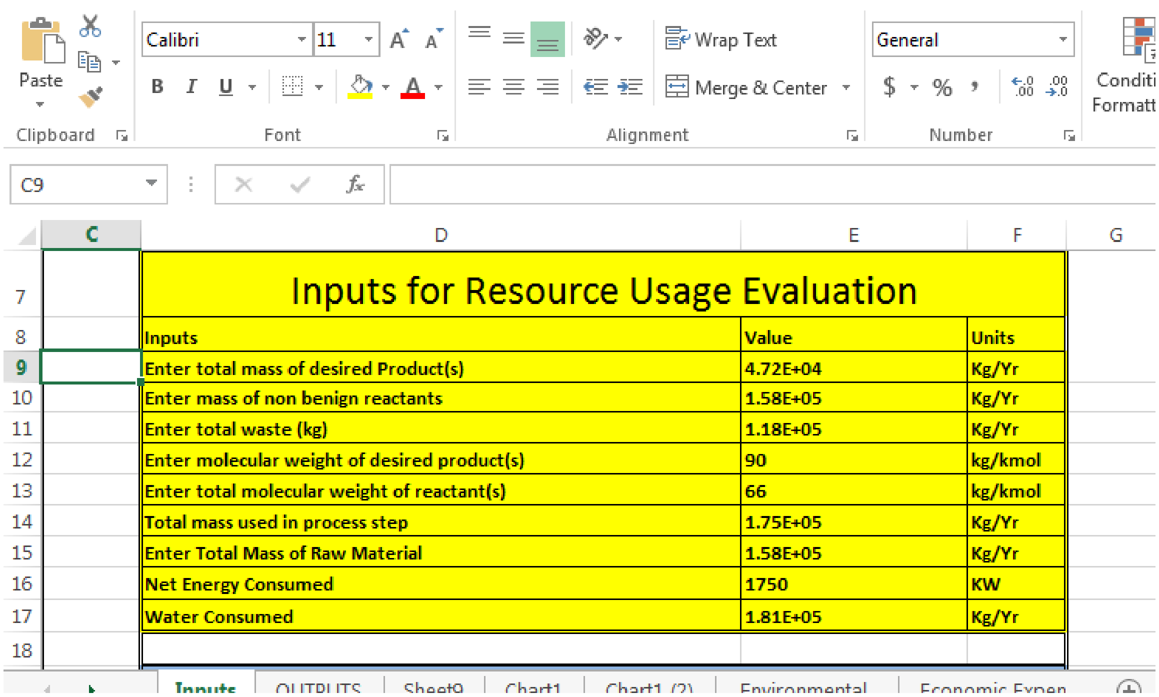
Step 6: Total mass used in process steps is entered. Mass of reactants, solvents or side streams introduced into the process for separation of products are included into flow rate of total mass used in the process.

Step 7: Total mass of raw materials is entered.

Step 8: Net energy consumed by the process is entered which includes sum of the energy used by different process equipment. Net energy consumed can be obtained from process simulator software directly.

Step 9: Total water consumed by the process is entered.

After completing all steps, the inputs section for resource usage evaluation should look like screen shot in figure 3.8



Inputs for Resource Usage Evaluation		
Inputs	Value	Units
Enter total mass of desired Product(s)	4.72E+04	Kg/Yr
Enter mass of non benign reactants	1.58E+05	Kg/Yr
Enter total waste (kg)	1.18E+05	Kg/Yr
Enter molecular weight of desired product(s)	90	kg/kmol
Enter total molecular weight of reactant(s)	66	kg/kmol
Total mass used in process step	1.75E+05	Kg/Yr
Enter Total Mass of Raw Material	1.58E+05	Kg/Yr
Net Energy Consumed	1750	KW
Water Consumed	1.81E+05	Kg/Yr

Figure 3.8: Screen Shot Demonstrating Inputs for Resource Usage

3.2.3 Economic Evaluation

In economics category, necessary inputs for economic impact evaluation are entered. The steps for economic impact evaluation is described below.

Step 1: Total mass flow rate of the primary product is entered. For multiple products, mass flow rates of all the products needs to be entered separately.

Step 2: Selling price of the primary product is entered. For multiple products, selling prices of all the products needs to be entered separately.

Step 3: Mass flow rate of primary raw materials is entered. For multiple raw materials, mass flow rates of all the raw materials needs to be entered.

Step 4: Selling price of primary raw materials is entered. For multiple raw materials, selling prices of all other raw materials needs be entered also.

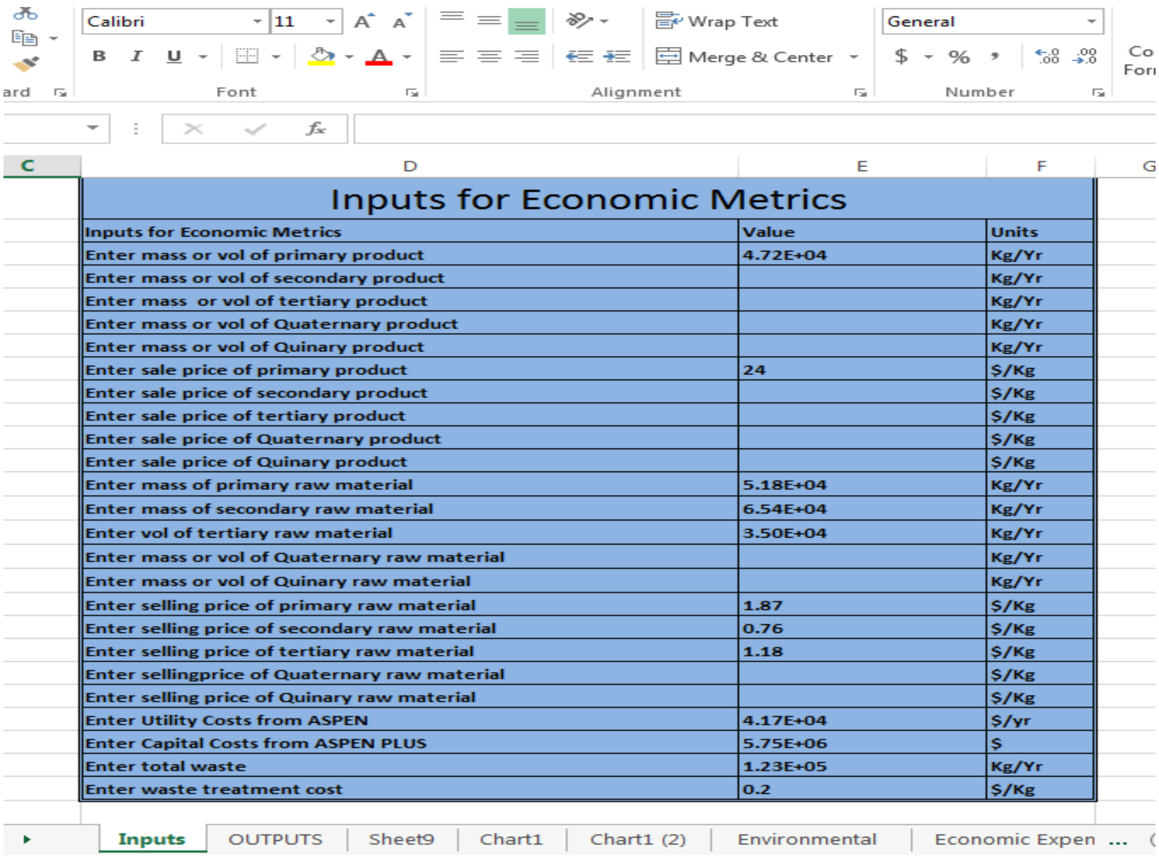
Step 5: Operating costs is entered.

Step 6: Capital costs is entered.

Step 7: Total waste management costs is entered.

Step 8: Waste treatment costs is entered.

After completing all steps the inputs section for economic impact evaluation should look like the screen shot in Figure 3.9.



Inputs for Economic Metrics		
Inputs for Economic Metrics	Value	Units
Enter mass or vol of primary product	4.72E+04	Kg/Yr
Enter mass or vol of secondary product		Kg/Yr
Enter mass or vol of tertiary product		Kg/Yr
Enter mass or vol of Quaternary product		Kg/Yr
Enter mass or vol of Quinary product		Kg/Yr
Enter sale price of primary product	24	$/Kg
Enter sale price of secondary product		$/Kg
Enter sale price of tertiary product		$/Kg
Enter sale price of Quaternary product		$/Kg
Enter sale price of Quinary product		$/Kg
Enter mass of primary raw material	5.18E+04	Kg/Yr
Enter mass of secondary raw material	6.54E+04	Kg/Yr
Enter vol of tertiary raw material	3.50E+04	Kg/Yr
Enter mass or vol of Quaternary raw material		Kg/Yr
Enter mass or vol of Quinary raw material		Kg/Yr
Enter selling price of primary raw material	1.87	$/Kg
Enter selling price of secondary raw material	0.76	$/Kg
Enter selling price of tertiary raw material	1.18	$/Kg
Enter sellingprice of Quaternary raw material		$/Kg
Enter selling price of Quinary raw material		$/Kg
Enter Utility Costs from ASPEN	4.17E+04	$/yr
Enter Capital Costs from ASPEN PLUS	5.75E+06	$
Enter total waste	1.23E+05	Kg/Yr
Enter waste treatment cost	0.2	$/Kg

Figure 3.9: Screen Shot Demonstrating Inputs for Economic Evaluation

3.2.4 Safety Impact Evaluation

For safety impact assessment for the process, the necessary inputs for safety are entered and the step are described below.

Step 1: Mass enthalpy of the reactants obtained from the streams entering the reactor are entered.

Step 2: Mass enthalpy of the product obtained from the stream coming out from the reactor is entered.

If there are other reactors, Step 1 and 2 are repeated and data ate entered in the side reaction section of the SUSTAINABILITY EVALUATOR.

Step 3: The user selects the chemicals responsible for Flammability impact. The chemicals are selected from the drop down menu as demonstrated earlier. Once the user has selected the flammable chemicals, the flash point temperatures will be supplied by SE tool. Chemical not on the list is selected if any chemical is not found in the drop down menu.

Step 4: The user selects the chemicals responsible for Explosivity Impact. The chemicals are selected from the drop down menu as demonstrated earlier. Once the user has selected the explosive chemicals the explosive limit will be supplied by SE tool. Then again chemical not on the list is selected if any chemical is not found in the drop down menu.

Step 5: The user selects chemicals responsible for Exposure impact. The chemicals are selected in the drop down menu as demonstrated earlier. Once the user has selected the chemicals harmful for human health the toxic limit value will be supplied by SE tool. Chemical not on the list is selected if any chemical is not found in the drop down menu.

Step 6: The user selects the material for Corrosion impact evaluation. In the dropdown there are only three options which are stainless steel, carbon steel and better material needed. If there is no corrosive chemical of concern, any one of these is selected. As there could be various chemicals that are considered corrosive such as nitric acid, for those cases strong material of construction might be needed instead of other two materials in the list. So, better material needed option is selected for that case.

Step 7: The user selects the inputs for Inventory Index in tones/hr.

Step 8: The user selects inputs for Temperature Index where the highest operating temperature of the process is selected.

Step 9: The user selects inputs for Pressure Index where the highest operating pressure of the process is selected.

Step 10: The user selects inputs for Equipment Index where the highest risk equipment present in the process is selected.

Step 11: The user provides Inputs for Safety Level of Process Structure Index where the safety level is selected. If there is no safety incident data available for the process, No data or neutral is selected.

After completing all steps, the inputs section for safety metrics impact evaluation should look like screen shot in figure 3.10.

Inputs for Safety Metrics		
Inputs for Safety Metrics	Value	Units
Inputs for Heat of Main Reaction		
Enter enthalpy of reactants	-6.02E+03	J/g
Enter enthalpy of products	-5.97E+03	J/g
Inputs for Heat of Side Reaction		
Enter enthalpy of reactants		J/g
Enter enthalpy of products		J/g
Enter extent of reaction		
Inputs for Flammability Index		
Chemical	Flash point temperature	Units
dimethyl ether	-45	°C
methanol	10	°C
Chemical not on list	NA	°C
Chemical not on list	NA	°C
Chemical not on list	NA	°C
Chemical not on list	NA	°C
Chemical not on list	NA	°C
Chemical not on list	NA	°C
Chemical not on list	NA	°C
Chemical not on list	NA	°C
Chemical not on list	NA	°C
Inputs for Explosiveness Index		
Chemical	Explosive Limit	Units
methanol	30	
dimethyl ether	23.6	
Chemical not on list	NA	
Chemical not on list	NA	
Chemical not on list	NA	
Chemical not on list	NA	
Chemical not on list	NA	
Chemical not on list	NA	
Chemical not on list	NA	
Chemical not on list	NA	
Chemical not on list	NA	
Inputs for Toxic Exposure Index		
Chemical	Toxic value limit	PPM
dimethyl ether	1000	
Methyl Alcohol, Methanol	200	
Chemical not on list	NA	
Chemical not on list	NA	
Chemical not on list	NA	
Chemical not on list	NA	
Chemical not on list	NA	
Chemical not on list	NA	
Chemical not on list	NA	
Chemical not on list	NA	
Chemical not on list	NA	
Inputs for Corrosion Index		
Carbon steel		
Inputs for Inventory Index		
1–10 tonnes/hr		
Inputs for Temperature Index		
300–600 °C		
Inputs for Pressure Index		
0–0.5 or 5–25 bar		
Inputs for Equipment Safety Index		
Air coolers, reactors, high hazard pumps		

Figure 3.10: Screen Shot Demonstrating Inputs for Safety Impact

3.2.5 Health Impact Evaluation

There are 11 different sub divisions in the input section of Health impact assessment according to the impact categories. The chemical(s) responsible for each health concern for each category is selected by the user and the mass flow rate in kg/yr is entered. The waste stream provides the information on the chemicals. The steps are described below to assess the health impact from SE.

Step 1: Neurological Damage Evaluation is the first impact category. The user selects the chemical(s) that are responsible for Health risk associated with neurological damage from the waste stream. The selection is done from the dropdown menu as explained earlier. After completing this step, the input section for safety metrics neurological impact evaluation should look like screen shot as figure 3.11

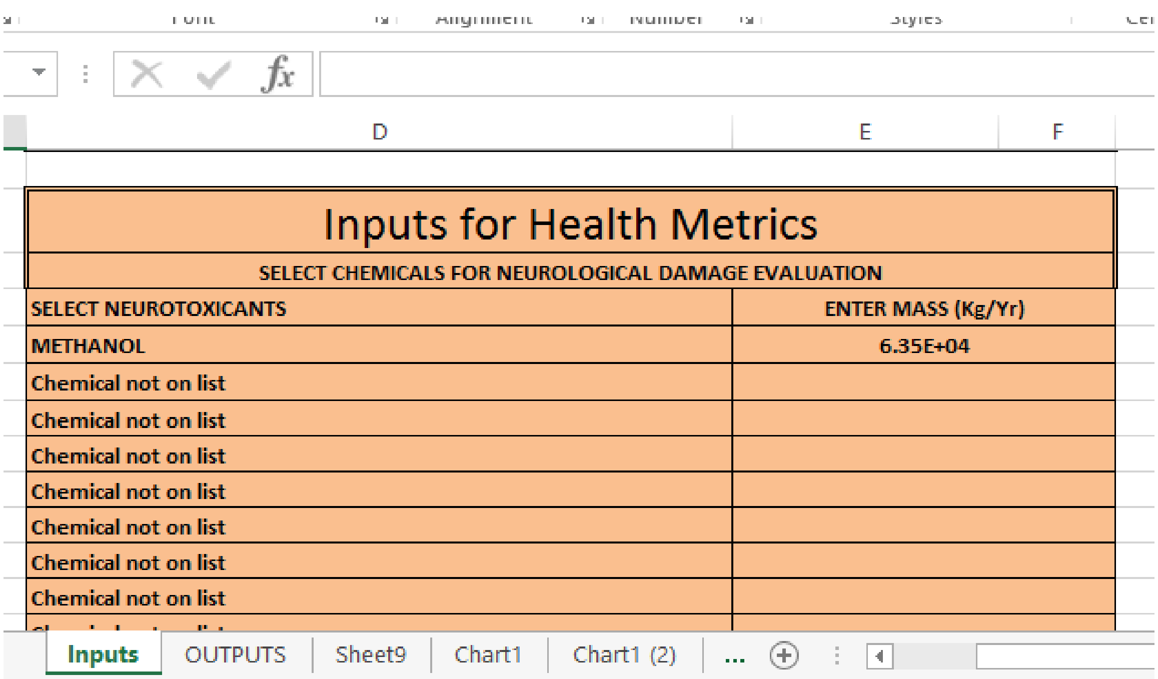


Figure 3.11: Screen Shot Demonstrating Inputs for Health Impact

Step 2: The procedure explained in Step 1 is repeated for the other 10 health impact categories which are Sensory Organ Damage Evaluation, Carcinogenic Evaluation, Immunotoxicity Evaluation, Musculoskeletal Damage Evaluation, Developmental Tissue Damage Evaluation, Productive System Damage Evaluation, Kidney Damage Evaluation, Respiratory Evaluation, Cardiovascular Damage Evaluation, Endocrine System Damage Evaluation, Liver Damage Evaluation one by one. Chemical not on the list is selected if any chemical is not on the list for any impact category.

3.3 Output Section

The impact assessment results are presented in six tabs named as: Output, Economic Impact Economic expense, Environmental Impact and Health Impact in the excel worksheet. The output tab provides the results of all the five categories discussed earlier. Figures 3.12 to 3.17 represents the results as screen shots.

OUTPUTS for Environmental Burden Evaluation		
Atmospheric Acidification	5.69E-01	Ton/y Sulfur Dioxide Equivalent
Global Warming	7.10E+02	Ton/y Sulfur Carbon Dioxide Equivalent
Stratospheric Ozone Depletion	0.00E+00	Ton/y Trichlorofluoromethane Equivalent
Photochemical Smog Formation	1.32E+01	Ton/y Ethylene Equivalent
Aquatic Acidification	3.50E-02	Ton/y H+ Ions Equivalent
Aquatic Oxygen Demand	9.62E+01	Ton/y Oxygen Equivalent
Ecotoxicity to Aquatic Life	0.00E+00	Ton/y Copper Equivalent
Eutrophication	0.00E+00	Ton/y Phosphate Equivalent

Figure 3.12: Screen Shot Demonstrating Output for Environmental Burden Analysis

OUTPUTS for Resource Usage Evaluation		
Effective Mass Yield	30%	
E-Factor	2.5	Kg/Kg
Atom Economy	137%	
Mass Intensity	3.71	Kg/Kg
Mass Productivity	27%	
Reaction Mass Efficiency	30%	
Material Intensity	2.3	Kg/Kg
Energy Intensity/ Fossil Fuel Usage	0.03706	KW/Kg
Water Intensity	3.8	Kg/Kg

Figure 3.13: Screen Shot Demonstrating Output for Resource Usage Analysis

OUTPUTS for Process Safety Evaluation		
	Results	Maximum Value
Heat of main reaction index	2	25%
Heat of side reaction index	0	0%
Flammability index	6	75%
Explosiveness index	4	50%
Toxic Exposure Index	24	80%
Corrosiveness index	0	0%
Temperature index	6	75%
Pressure index	0	0%
Equipment safety index	4	50%
Safety Level of Process Structure index	4	40%
Total Inherent Safety index	50	

Figure 3.14: Screen Shot Demonstrating Output for Process Safety Analysis

OUTPUTS for Health Evaluation		
Carcinogenic Risk	0.00E+00	Tons/yr
Immune System Damage	0.00E+00	Tons/yr
Skeletal System Damage	5.26E-01	Tons/yr
Developmental Damage	3.81E+01	Tons/yr
Reproductive System Damage	0.00E+00	Tons/yr
Kidney System Damage	0.00E+00	Tons/yr
Respiratory System Damage	3.92E+01	Tons/yr
Cardiovascular System Damage	5.26E-01	Tons/yr
Endocrine System Damage	0.00E+00	Tons/yr
Liver Damage	3.86E+01	Tons/yr
Nervous System Damage	3.81E+01	Tons/yr
Sensory System Damage	6.20E-01	Tons/yr

Figure 3.15: Screen Shot Demonstrating Output for Health Impact Analysis

OUTPUTS for Economic Evaluation	
Revenue	$1,133,403.84
Operating Costs	$41,659.30
Waste Treatment Costs	$24,629.62
Raw Material Costs	$188,020.27
Capital Costs	$5,753,800.00
Annualized Capital Cost	$676,071.5
Material Value Added	$945,383.57
Profit	$203,023.15

Figure 3.16: Screen Shot Demonstrating Output for Economic Impact Analysis

OUTPUTS for OVERALL SUSTAINABILITY IMPACT	
Economic Impact	0.25
Environmental Impact	0.10
Social Impact	0.25
Sustainability Index	**0.19**

Figure 3.17: Screen Shot Demonstrating Output for Overall Sustainability Impact Analysis

Graphical representation of these results are given as Figures 3.18 to 3.21.

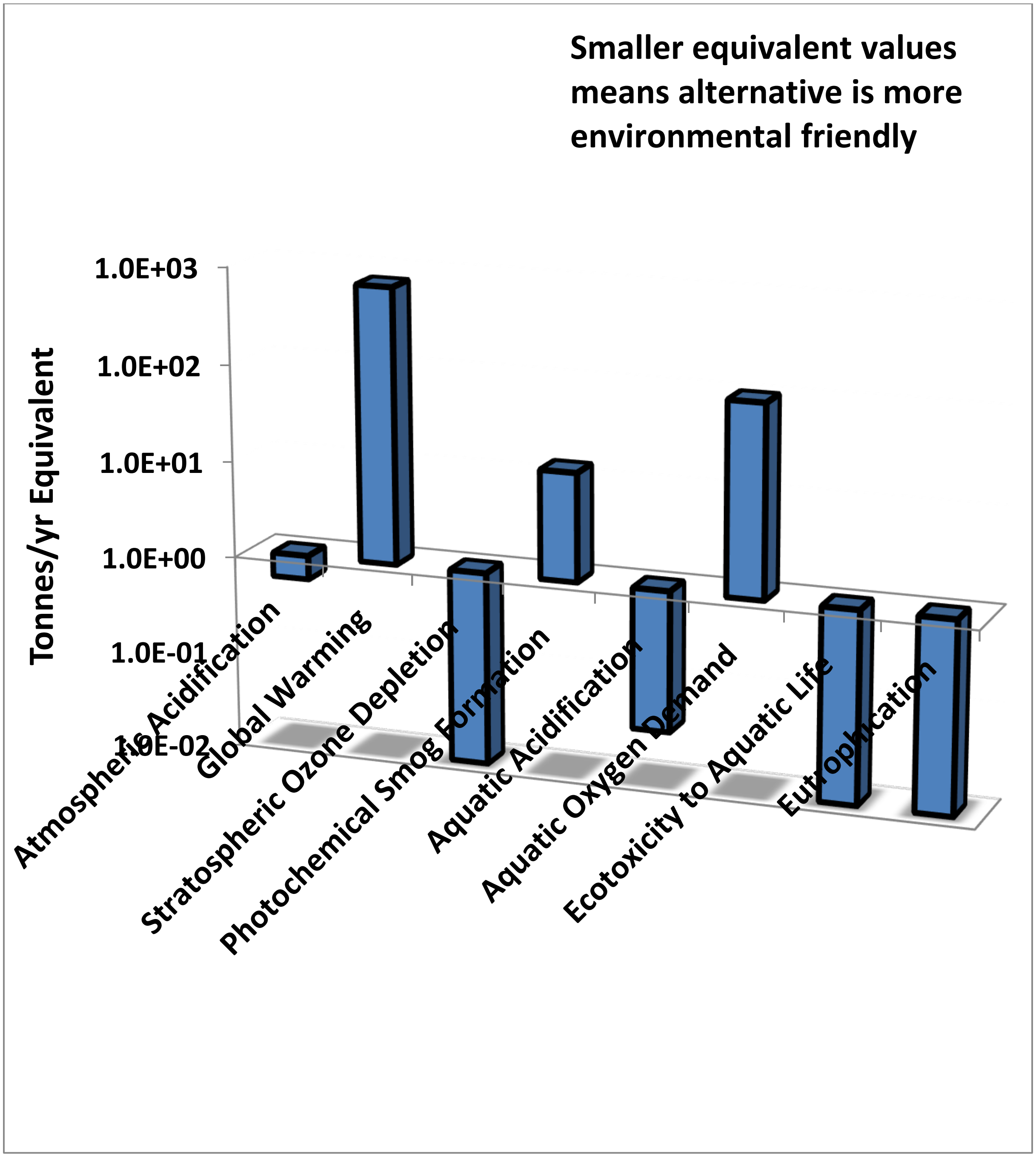


Figure 3.18: Graphical Representation of Environmental Burden Analysis Results

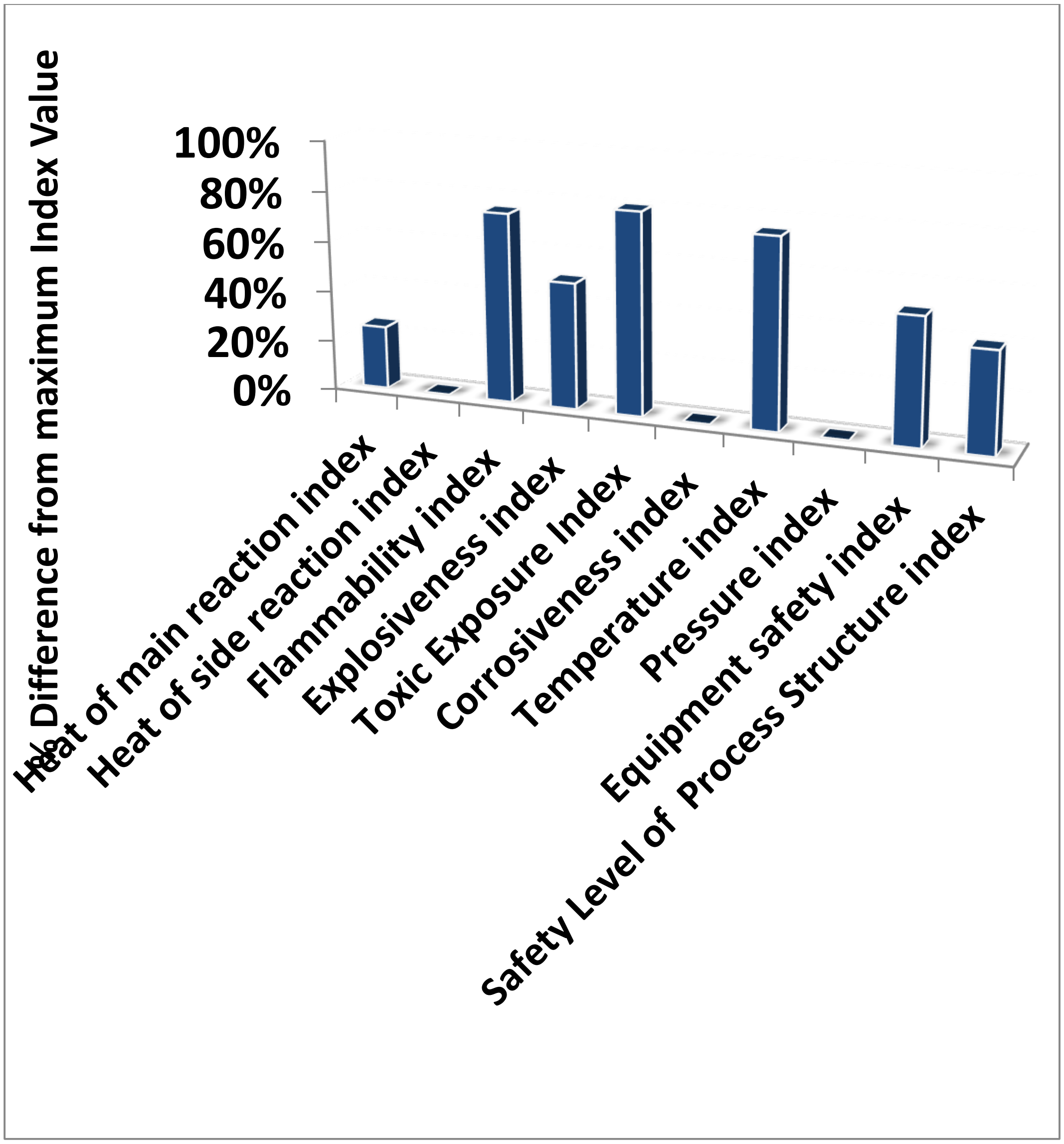


Figure 3.19: Graphical Representation of Process Safety Analysis Results

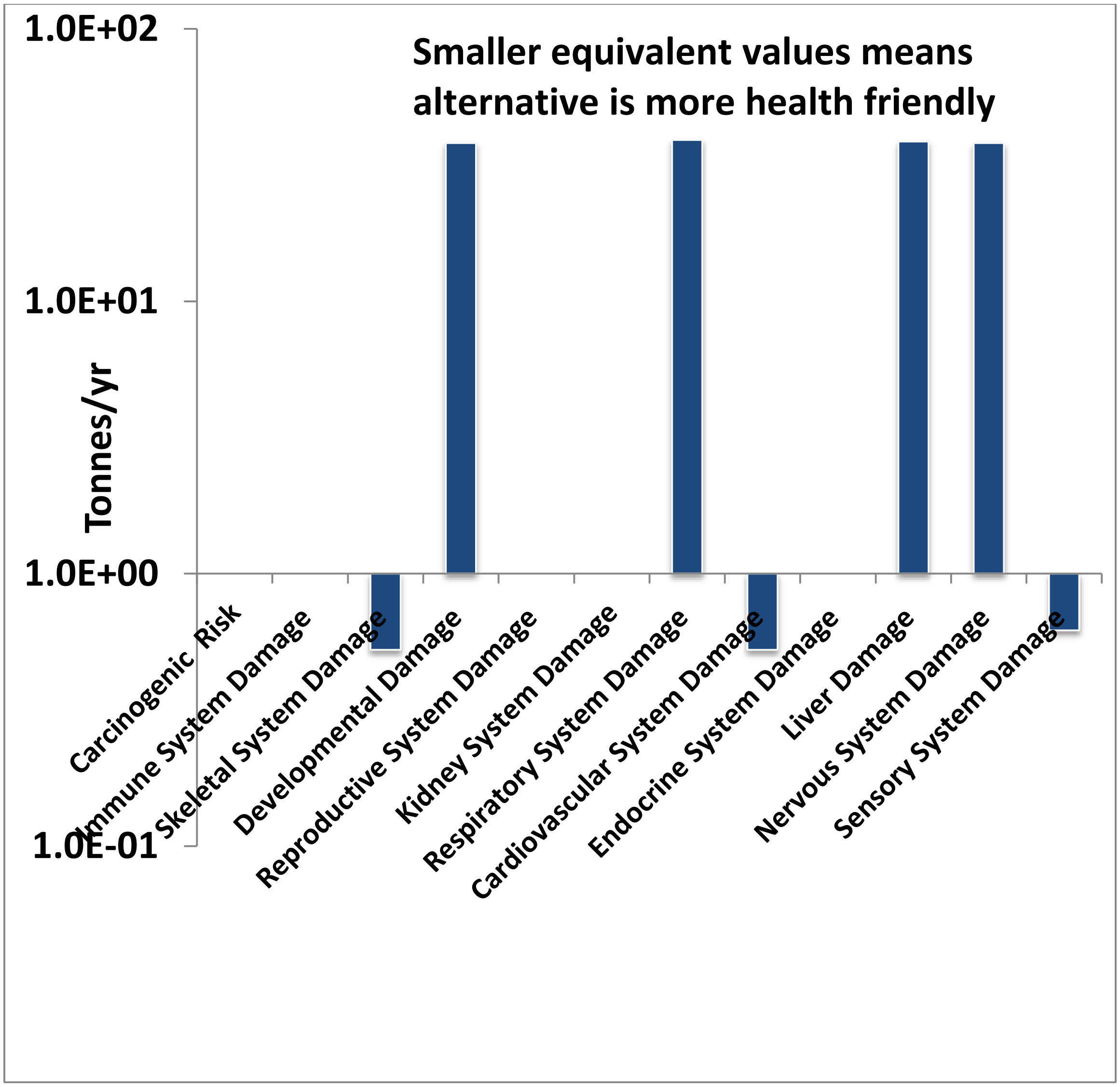


Figure 3.20: Graphical Representation of Health Analysis Results

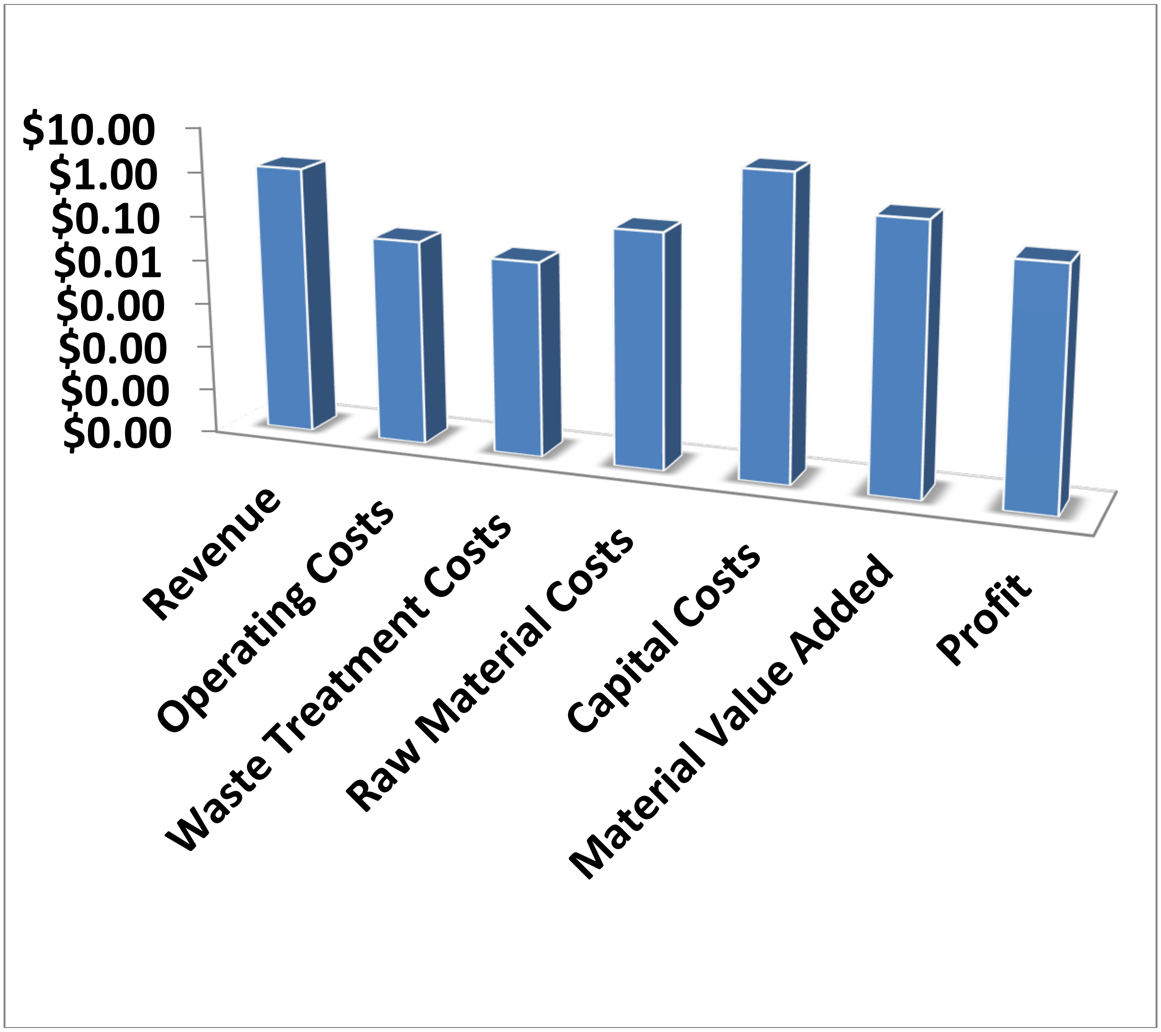


Figure 3.21: Graphical Representation of Economic Impact Analysis Results

CHAPTER IV

MODIFIED SUSTAINABILITY EVALUATOR: HOW IT WORKS

4.1 Input Section

The input section of the modified SUSTAINABILITY EVALUATOR starts with a window where the user can choose from the options whether to evaluate either Environmental Index or Economic Index or Social Index or the Overall Sustainability Index of a process. The starting window looks like Figure 4.1. Here the user has selected the option to evaluate Overall Sustainability Index.

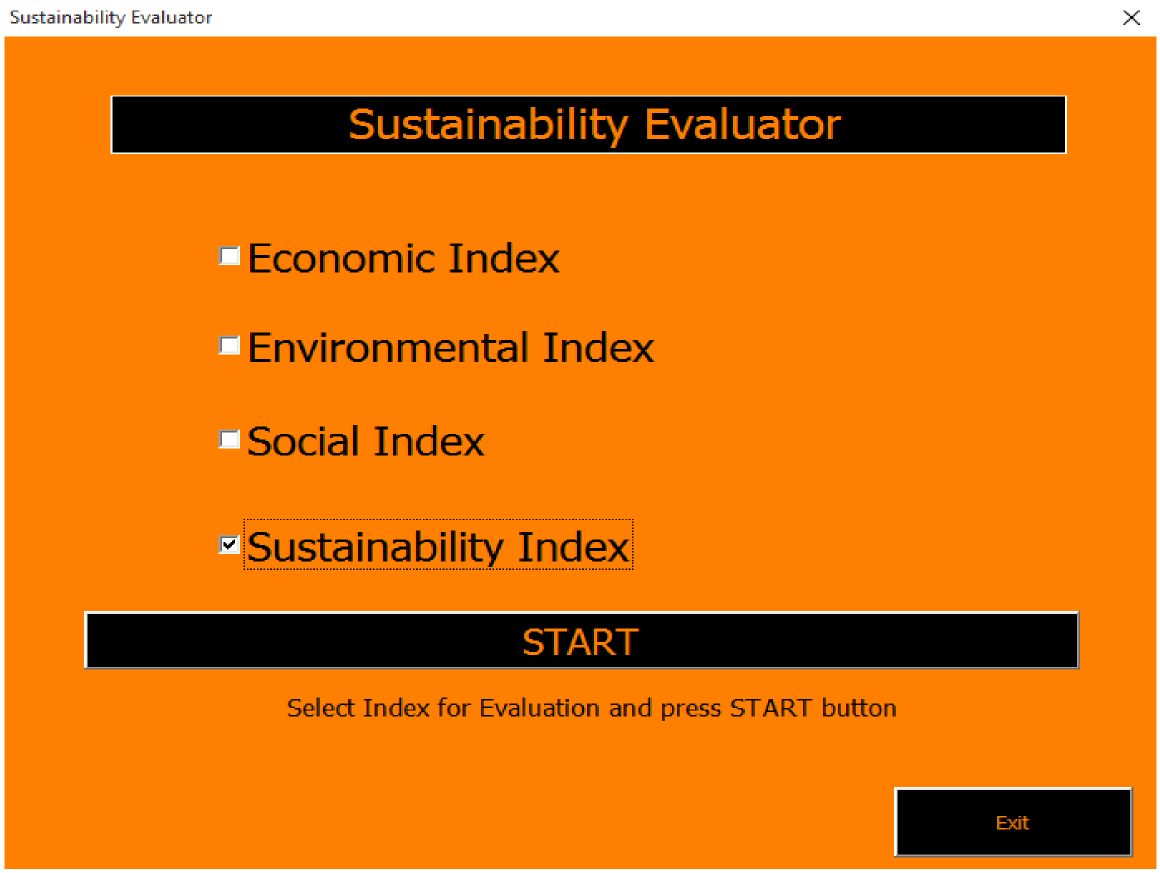


Figure 4.1: Screen Shot Demonstrating Data Input in Modified SUATAINABILITY EVALUATOR

When the user presses start, the window associated with the selected index will appear. Figure 4.2 represents the window if Sustainability Index is selected which is for taking economic input data. Mandatory fields will be marked red. Values to the mandatory fields are entered and press next.

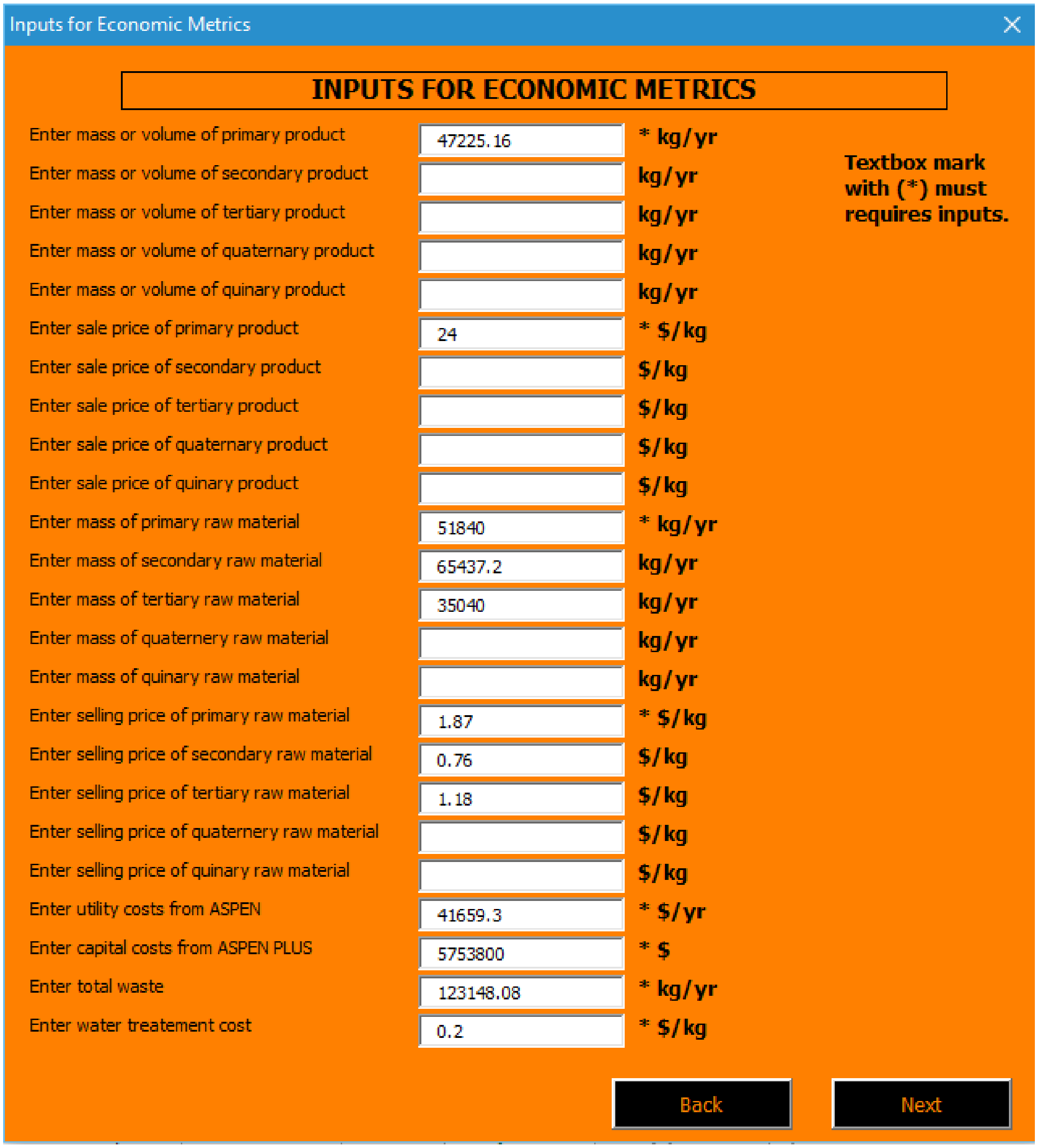


Figure 4.2: Screen Shot Demonstrating Economic Data Input

Then the output for Economic Index will appear as the next window. Figure 4.3 represents the window for Economic Index output. Press next to show the next input window.

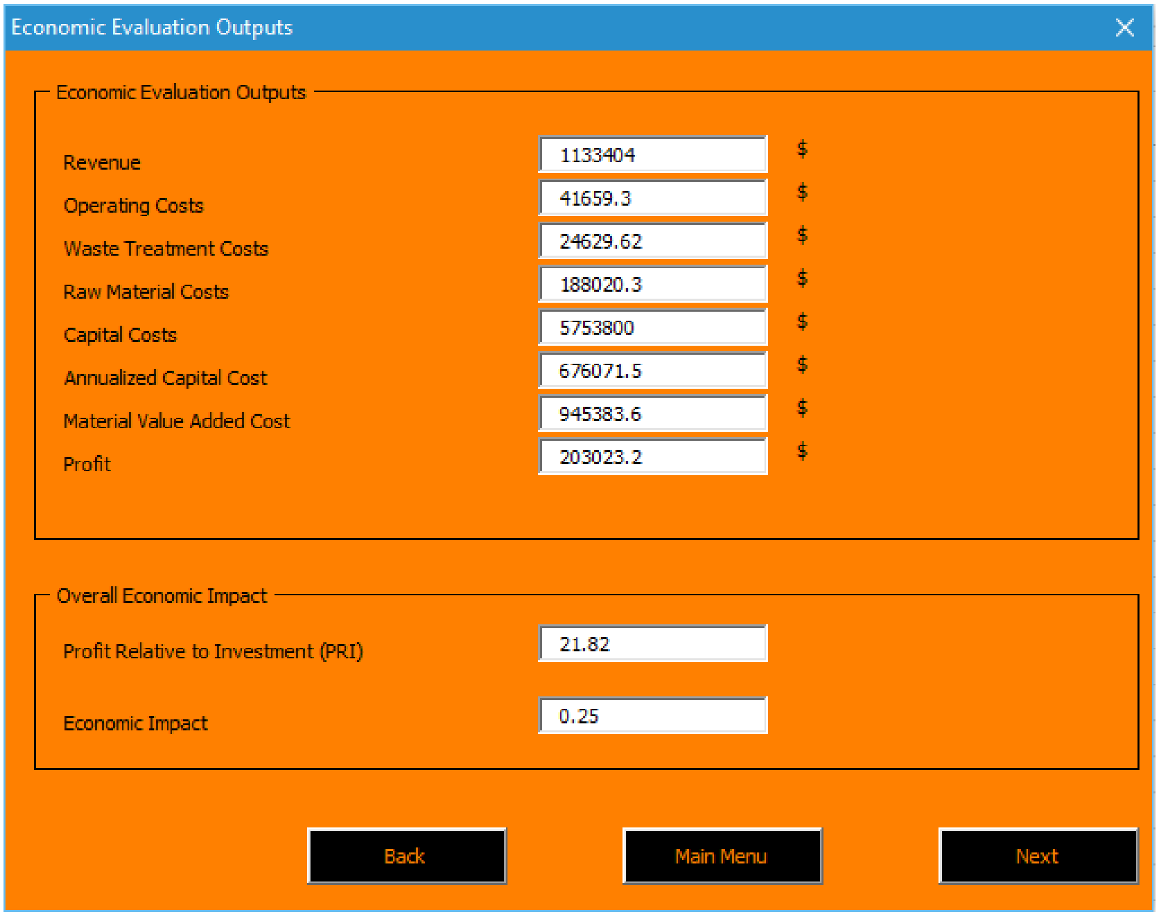


Figure 4.3: Screen Shot Demonstrating Economic Index Output Data

The next window will take input for resource usage evaluation. Figure 4.4 represents the window for resource usage input. After putting the inputs in the fields the user needs to press next.

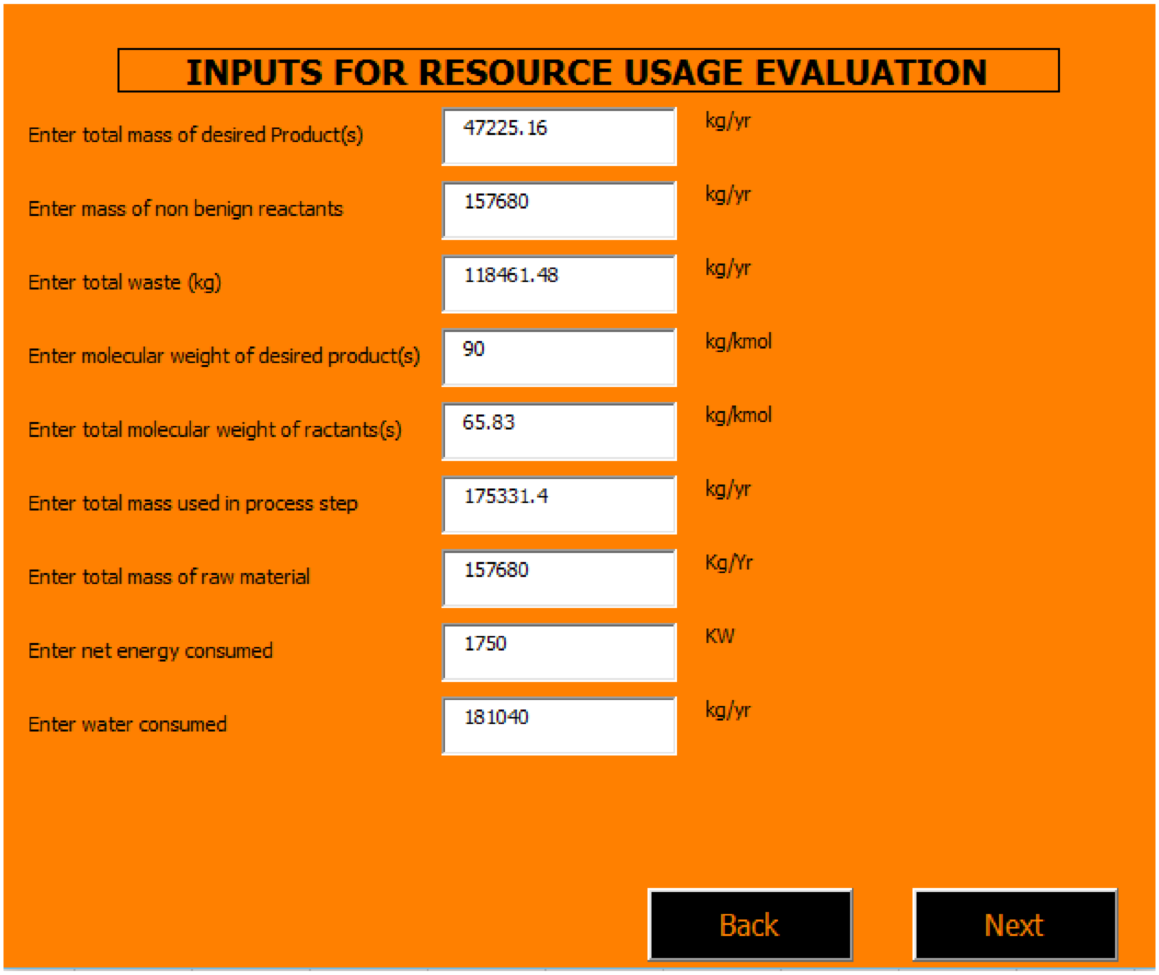


Figure 4.4: Screen Shot Demonstrating input for Resource Usage

The next window will show the output results for resource usage. Figure 4.5 represents the window showing output data for resource usage. Then press next.

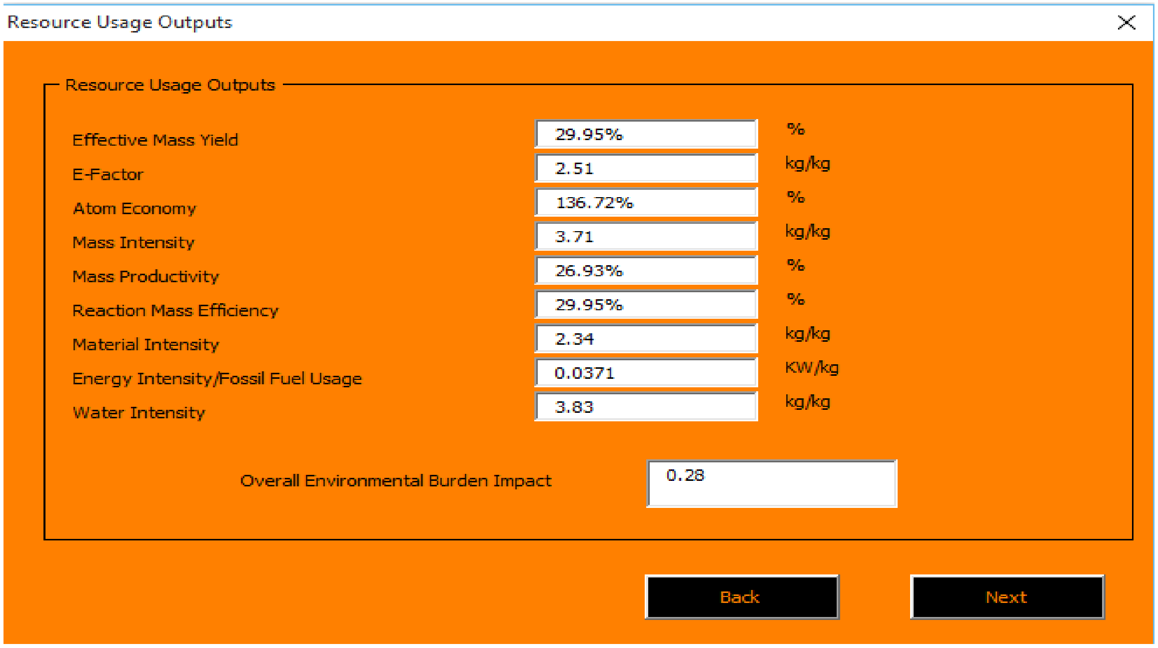


Figure 4.5: Screen Shot Demonstrating Output for Resource Usage

From the next window the tool will start taking input for evaluating Environmental Burden evaluation. The first category is Global Warming. The used needs to select the chemicals from the list on the left side of the window and move it to the right side by clicking the arrow provided in between. The user will now be able to enter the values for the selected chemicals. Default potential factors are being taken for the respective chemicals in the background. If the user wants to give potential factor different from the default value they can do that too in the specific field on the right side of the window. Then press next. Figure 4.6 represents the window showing data input for Global warming evaluation.

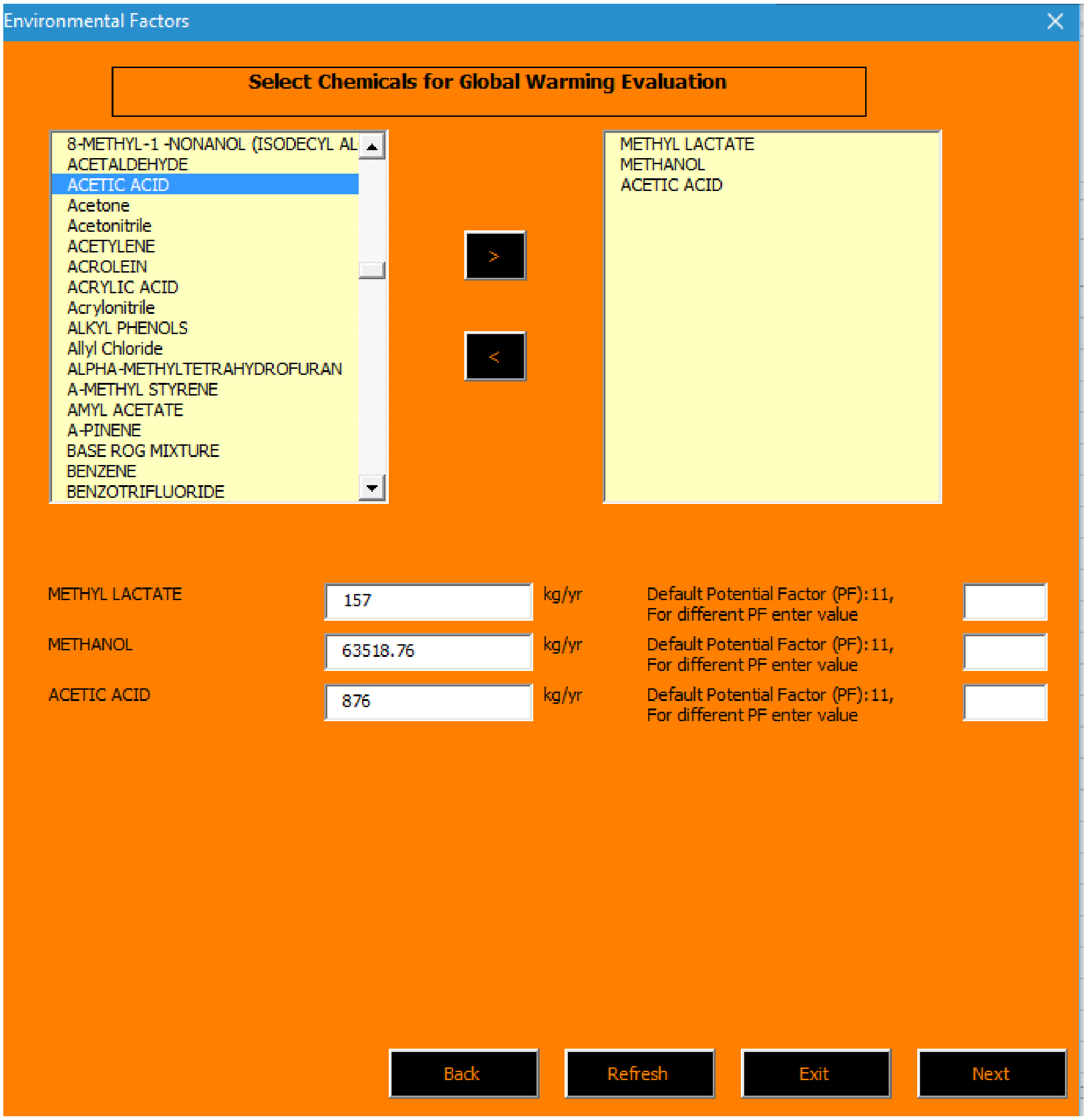


Figure 4.6: Screen Shot Demonstrating Input for Global Warming Impact

Then the next windows will take inputs for evaluating other six categories one by one and previous step is repeated for each of the six categories. The windows will be similar to figure 4.6 for each cases.

After completing all the categories for environmental burden analysis, the next window will show the output for overall Environmental Index by combining both Environmental Burden and Resource Usage impact. Then press next. Figure 4.7 represents the window showing output for Environmental Index.

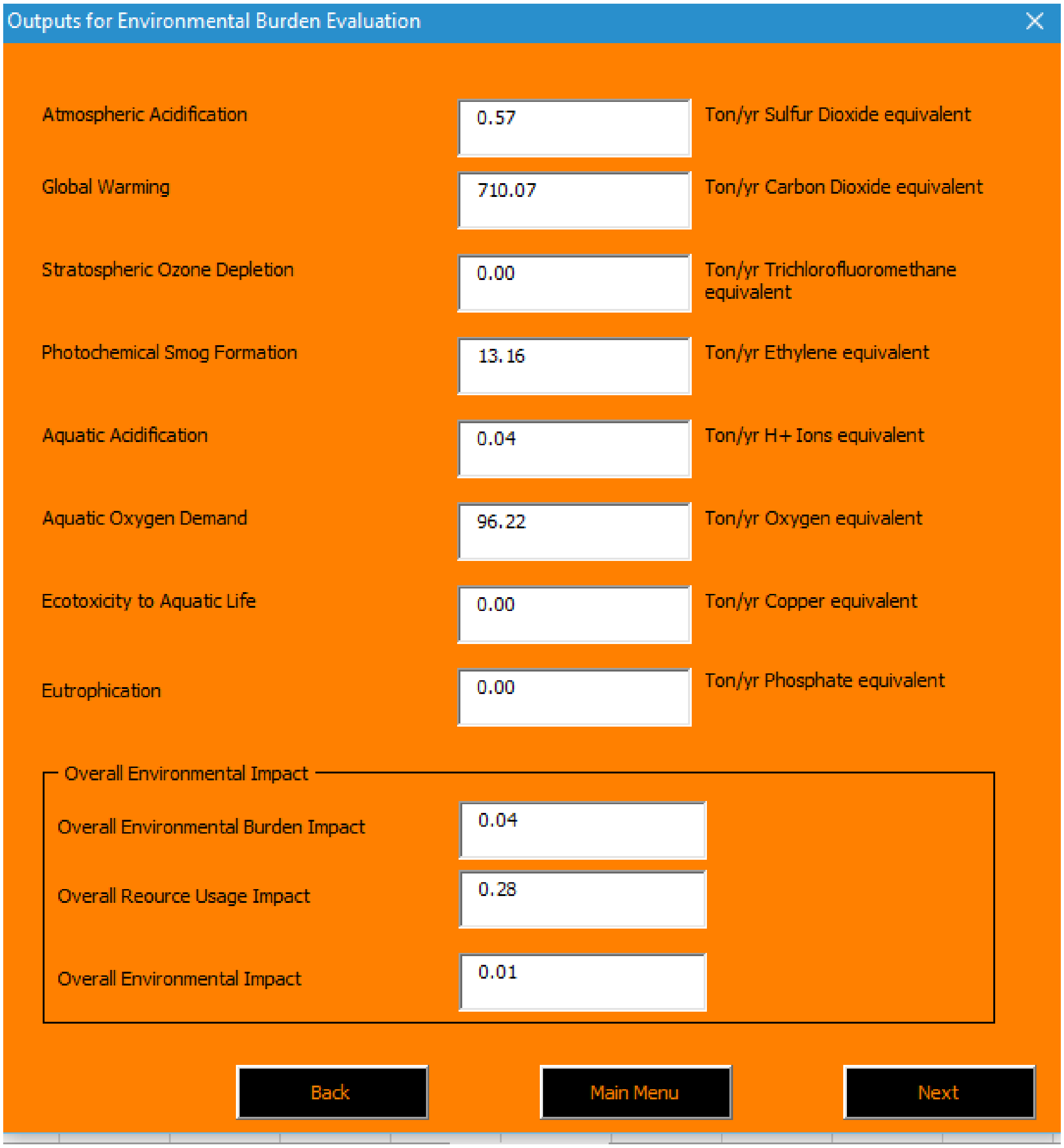


Figure 4.7: Screen Shot Demonstrating Output Result for Overall Environmental Impact

Then the next window will start taking inputs from the user for safety metrics. The first category is heat of main reaction. In this window the user needs to enter the enthalpy of reactants and product to calculate the heat of main reaction. To calculate the heat of side reactions enter the enthalpy of reactants and products from side reaction (if any). Then press next. Figure 4.8 represents the window showing data input for heat of main reaction.

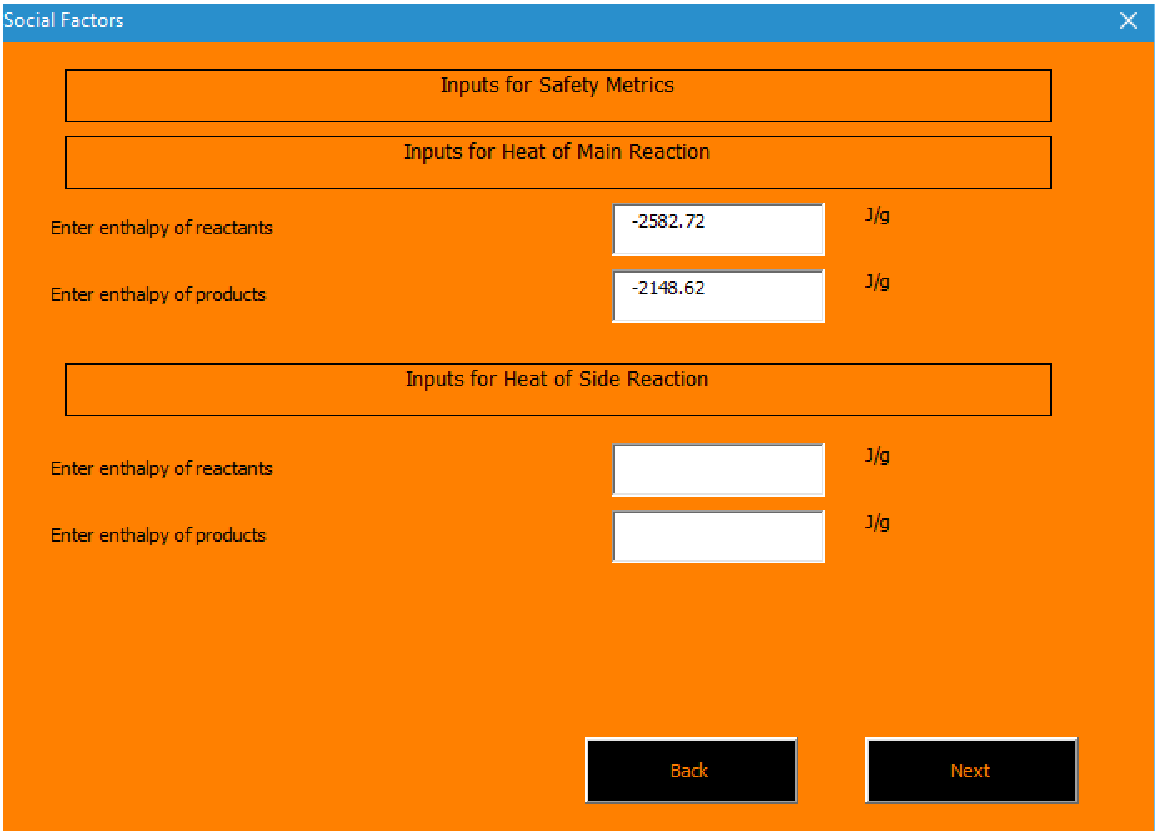


Figure 4.8: Screen Shot Demonstrating Input for Heat of Reaction Calculation

The next window will take input for evaluating flammability impact. Select the chemical responsible for flammability impact from the list on the left side of the window and move it to the right side. Then press next. Figure 4.9 represents the window showing data input for calculating flammability index.

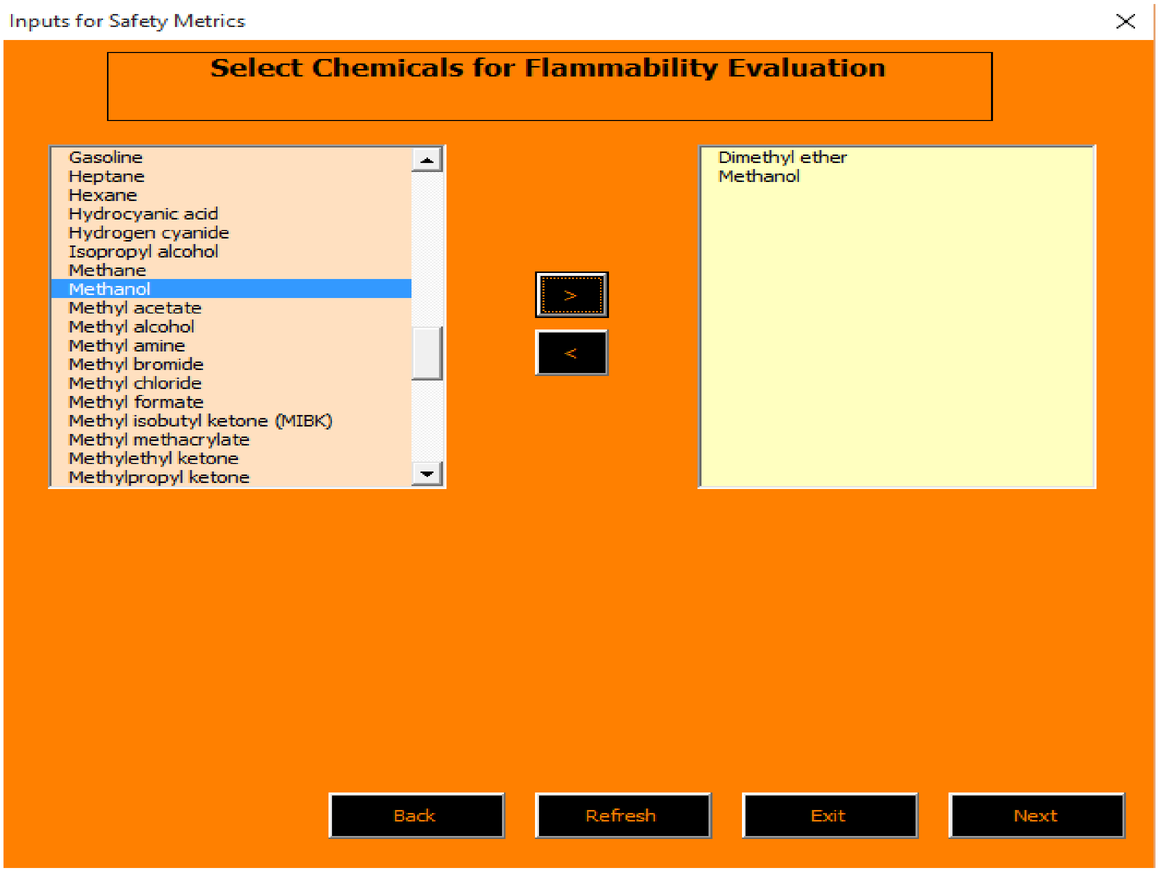


Figure 4.9: Screen Shot Demonstrating Input for Calculating Flammability Index

Then the next windows will take input for evaluating Explosivity Index, Exposure Index, Corrosion Index, Temperature Index, Pressure Index, Equipment Index, Process Structure Index one by one. Then press next. The windows for safety inputs will be similar to Figure 4.9.

Now this is the part where user gives the inputs for different categories for calculating health impact. The window will now take input for evaluating neurological damage index at first. The user needs to select the chemicals responsible for neurological damage impact from the list on the left side of the window and move it to the right side. The user will now be able to enter the values for the selected chemicals. Default Potency factors are being taken for the respective chemicals in the background. If the user wants to give potential factor different from the default value they can do that too in the specific field on the right side of the window. Then press next.

Figure 4.10 represents the window showing data input for calculating neurological damage evaluation.

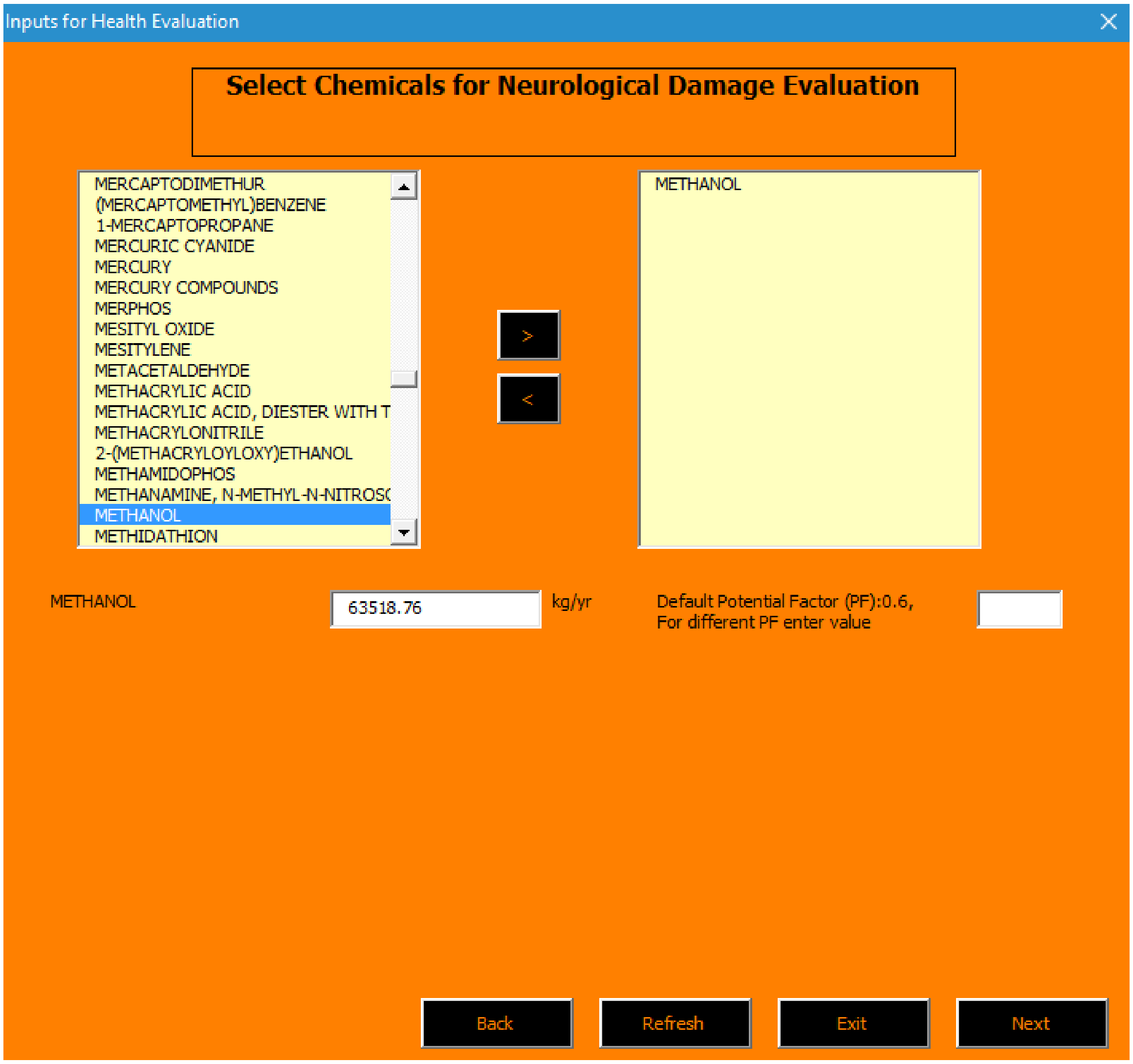


Figure 4.10: Screen Shot Demonstrating Input for Calculating Neurological Damage Impact

The next 11 windows will take input for 11 categories for health impact evaluation. The windows will be similar to Figure 4.10. The user needs to press next every time after giving input for each category.

After finishing giving inputs for all the categories of Health impact, the next window will show the output for overall Social Index by combining both process safety impact and health impact. Then the user needs to press next. Figure 4.11 represents the window showing output result for process safety index and health index and also overall Social Index.

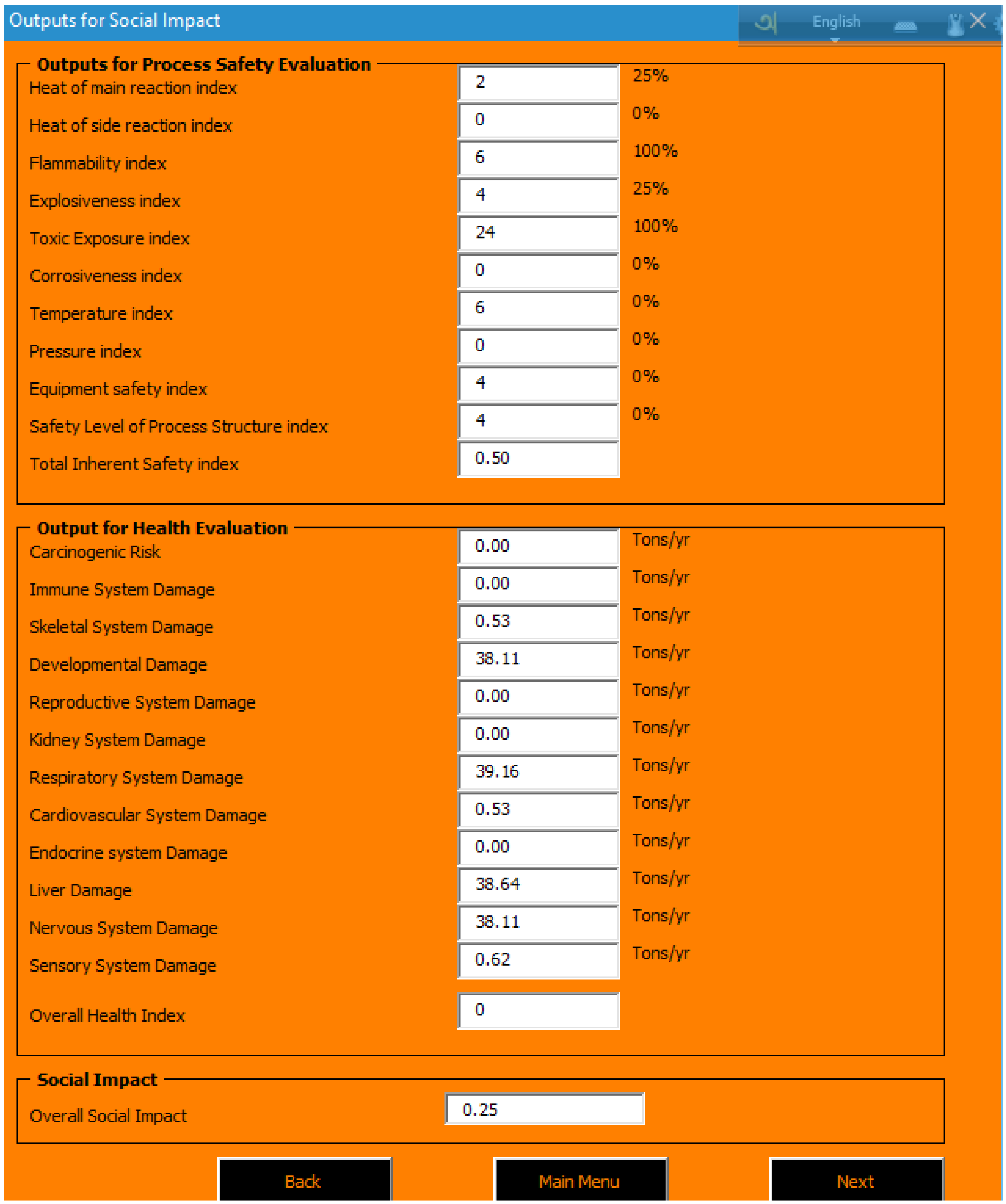


Figure 4.11: Screen Shot Demonstrating Output Results for Overall Social Metric

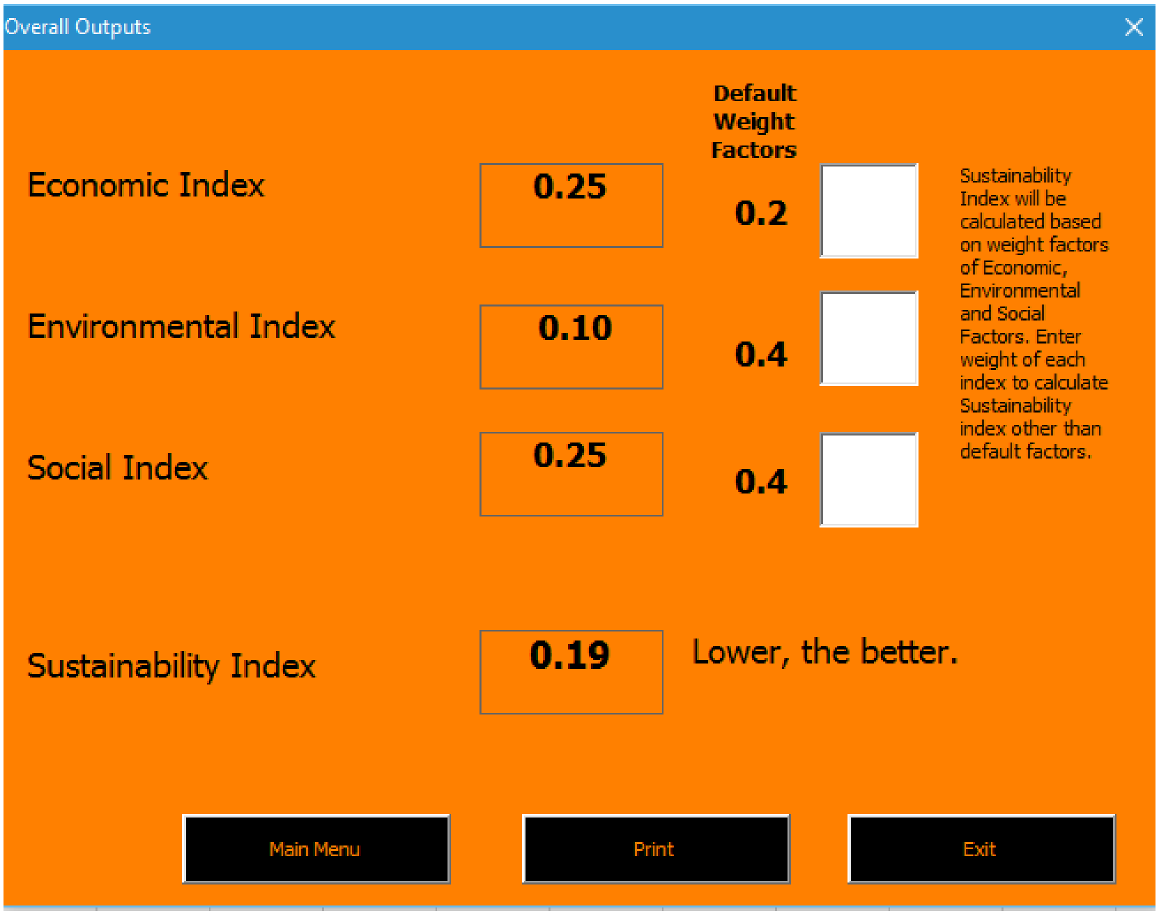


Figure 4.12: Screen Shot Demonstrating Final Results of Sustainability Index

Graphical representations of the output results will be generated automatically in the assigned excel file. Figures 4.12 to 4.15 are showing those graphs.

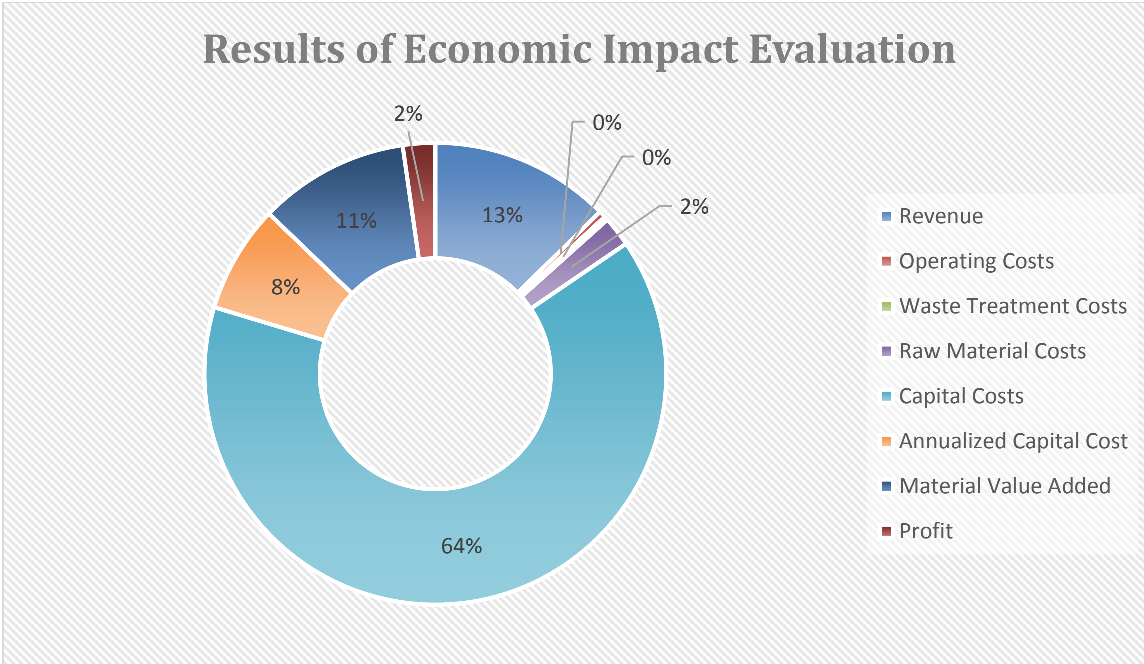


Figure 4.13: Graphical Representation of Output Result for Economic Impact Evaluation

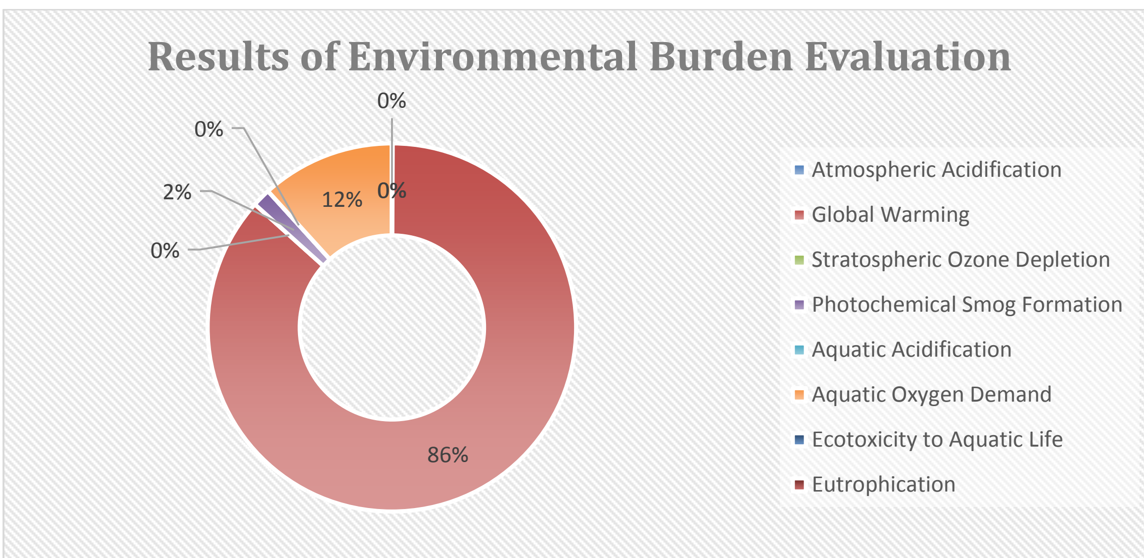


Figure 4.14: Graphical Representation of Output Result for Environmental Burden Evaluation

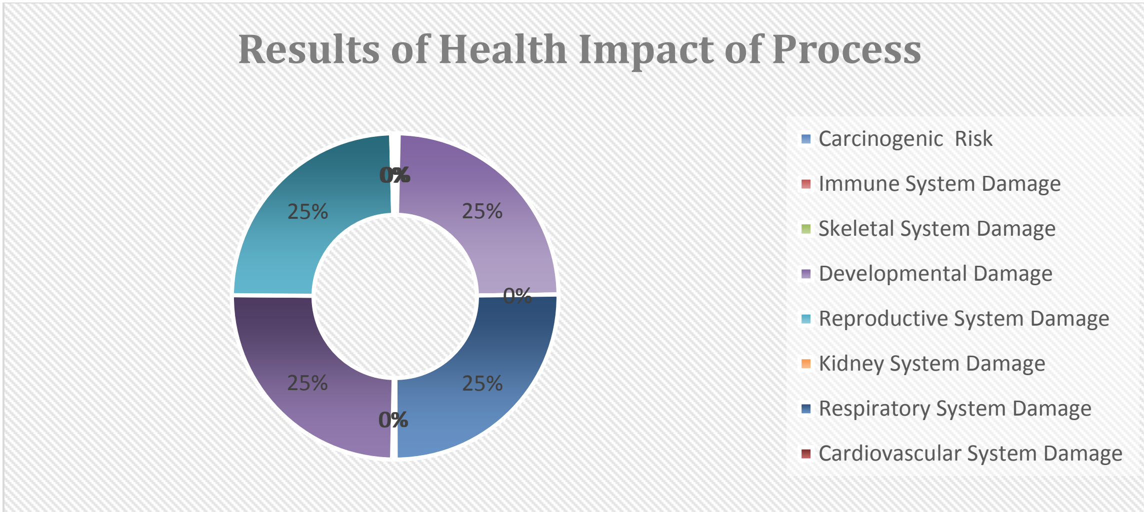


Figure 4.15: Graphical Representation of Output Result for Health Impact Evaluation

CHAPTER V

RESULTS AND DISCUSSION

In this chapter, the results of this study is presented and discussed to validate the new sustainability evaluator developed using Excel VBA and also the modifications done.

5.1 Validation of the New SUSTAINABILITY EVALUATOR

To validate the results obtained from new sustainability evaluator, sustainability index for the same process has been calculated by previous Excel version of SUSTAINABILITY EVALUATOR (SE) and new modified SE and then the results has been compared. In this study, overall sustainability index of manufacturing process of Poly Lactic Acid (PLA) (Bapat, 2014) has been calculated by both SE and modified SE. The results obtained for different metrics are mentioned below:

5.1.1 Economic Index

The input values for Lactic Acid manufacturing process are taken from MS thesis of Susmit Bapat (2014). The results obtained for impacts of different metrics to calculate Economic Index from both SE and modified SE are mentioned as Table 5.1.

Table 5.1: Economic Index Result Comparison

Economic Metrics	Excel Based SE	Modified SE
Revenue	**$ 1,133,403.84**	**$ 1,133,404.00**
Operating Costs	**$ 41,659.30**	**$ 41,659.30**
Waste Treatment Costs	**$ 24,629.62**	**$ 24,629.62**
Raw material Costs	**$ 188,020.27**	**$ 188,020.30**
Capital Cost	**$ 5,753,800.00**	**$ 5,753,800.00**
Annualized Capital Cost	**$ 676,071.50**	**$ 676,071.50**
Material Value Added	**$ 945,383.57**	**$ 945,383.60**
Profit	**$ 203,023.15**	**$ 203,023.20**
Overall Index	**0.25**	**0.25**

From Table 5.1, it is found that, new modified Sustainability Evaluator provides same results for economic index calculation as obtained from previous SUSTAINABILITY EVALUATOR.

5.1.2 Environmental Index

Overall Environmental Index is calculated by combining Environmental Burden Evaluation results and Resource Usage Evaluation results. The results obtained for impact of different metrics to calculate Environmental Burden by both SE and modified SE are mentioned as Table 5.2:

Table 5.2 Environmental Burden Results Comparison

Environmental Metrics	Excel Based SE	Modified SE
Atmospheric Acidification	**0.569**	**0.569**
Global Warming	**710.00**	**710.00**
Stratospheric Ozone Depletion	**0.00**	**0.00**
Photochemical Smog Formation	**13.20**	**13.20**
Aquatic Acidification	**0.035**	**0.035**
Aquatic Oxygen Demand	**96.20**	**96.20**
Eco-toxicity to Aquatic Demand	**0.00**	**0.00**
Eutrophication	**0.00**	**0.00**

The results obtained for impact of different metrics to calculate Resource Usage by both SE and modified SE are mentioned as Table 5.3:

Table 5.3 Resource Usage Results Comparison

Resource Usage Metrics	Excel Based SE	Modified SE
Effective Mass Yield	**30%**	**29.95%**
E-Factor	**2.50**	**2.51**
Atom Economy	**137%**	**136.72%**
Mass Intensity	**3.71**	**3.71**
Mass Productivity	**27%**	**26.93%**
Reaction Mass Efficiency	**30%**	**29.95%**
Material Intensity	**2.30**	**2.34**
Energy Intensity	**0.03706**	**0.0371**
Water Intensity	**3.80**	**3.83**

Table 5.2 and 5.3 represents that the new modified Sustainability Evaluator and excel based Sustainability Evaluator provide same results for Environmental Burden analysis and Resource Usage analysis.

5.1.3 Social Index

Overall Social Index is calculated from Process Safety Evaluation and Health Evaluation. The results obtained for impact of different metrics to calculate Process Safety Evaluation by both SE and modified SE are mentioned as Table 5.4:

Table 5.4 Process Safety Evaluation Comparison

Safety Indices	Excel Based SE	Modified SE
Heat of main reaction	**2**	**2**
Heat of side reaction	**0**	**0**
Flammability	**6**	**6**
Explosiveness	**4**	**4**
Toxic Exposure	**24**	**24**
Corrosiveness	**0**	**0**
Temperature	**6**	**6**
Pressure	**0**	**0**
Equipment Safety	**4**	**4**
Safety Level of Process Structure	**4**	**4**
Total Inherent Safety Index	50	50

The results obtained for impact of different metrics to calculate Health Impact Evaluation by both SE and modified SE are mentioned as Table 5.5.

Table 5.5 Health Evaluation Comparison

Health Indices	Excel Based SE	Modified SE
Carcinogenic Risk	**0.00**	**0.00**
Immune System Damage	**0.00**	**0.00**
Skeletal System Damage	**0.526**	**0.526**
Developmental Damage	**38.10**	**38.10**
Reproductive System Damage	**0.00**	**0.00**
Kidney System Damage	**0.00**	**0.00**
Respiratory System Damage	**39.20**	**39.20**
Cardiovascular System Damage	**0.526**	**0.526**
Endocrine System Damage	**0.00**	**0.00**
Liver Damage	**38.60**	**38.60**
Nervous System Damage	**38.10**	**38.10**
Sensory System Damage	**0.620**	**0.620**

Table 5.4 and 5.5 shows that the new modified Sustainability Evaluator and excel based SUSTAINABILITY EVALUATOR provided same results for process safety index evaluation and health index evaluation.

5.1.4 Overall Sustainability Index

The results obtained for Overall Sustainability Index from combining Economic Index, Environmental Index and Social Index by both SE and modified SE are mentioned as Table 5.6.

Table 5.6 Overall Sustainability Index Comparison

Sustainability Indices	Excel Based SE	Modified SE
Economic	**0.25**	**0.25**
Environmental	**0.10**	**0.10**
Social	**0.25**	**0.25**
Overall Sustainability Index	**0.19**	**0.19**

From Table 5.6 we can conclude, Modified SUSTAINABILITY EVALUATOR calculates the same overall Sustainability Index as obtained from excel based Sustainability Evaluator. So, the results obtained from Modified SUSTAINABILITY EVALUATOR is valid.

5.2 Improvements and Modifications in Modified SUSTAINABILITY EVALUATOR

There has been some modifications or improvements done on the existing SUSTAINABILITY EVALUATOR to make it robust and easy to use the tool. Followings are the improvements:

- More user friendly interface
- Allow user to customize potential factors and weight factors of different impacts
- Auto generated comparison charts for 2 or 3 process evaluations.
- Report generation of results for overall sustainability evaluator for analysis

5.2.1 User Friendly Interface

A more user friendly interface has been developed using Excel VBA where the interface guides the user to give inputs and generates the results accordingly. The user has the option to calculate overall sustainability index or any individual index such as economic index, environmental index or social index using modified sustainability tool. This tool will guide the user to enter inputs according to their requirement and generate outputs for the required index. The report and graphs generated by the tool will allow the user to do primary analysis of impacts of different metrics.

5.2.2 Customization of Potential Factors and Weight Factors for Different Index

The modified SUSTAINABILITY EVALUATOR tool allows the user to change the potency factors of different chemicals responsible for environmental burden or Health effects. The SUSTAINABILITY EVALUATOR uses data from particular sources (mentioned in appendices) for potential impacts calculation of chemicals involved in the process using built in potency factors. If the user want to use data from different source to calculate the potential impacts, this tool allow the user to enter the potency factor and use this potency factor to calculate the impact of the chemicals. This will enable the user to determine the sustainability index for different locations and following different regulations for process design.

Again if there is a need to change the weighting factors assigned by default to Environmental Index, Economic Index and Social Index the user can do that too using modified Sustainability Evaluator. For example, if economic output of different alternatives are similar but the environmental issues are more important for any particular process design, environmental Index needs to be given more weight than Economic Index.

5.2.3 Generation of graphs

The modified SUSTAINABILITY EVALUATOR generates comparison graphs of two or three different cases evaluated. For the previous excel based SUSTAINABILITY EVALUATOR the user had to plot the graphs separately to see the comparison results obtained for different processes. The cases can be base case and one or two more optimized processes done to improve overall sustainability index. The cases can also be two different process types (Batch or Continuous) for the same product. In this study two different configurations of Lactic Acid production have been compared with the base case process. Configuration 1 is the optimized process which uses the data from sensitivity analysis done in Aspen plus simulator in SUSTAINABILITY EVALUATOR. Configuration 2 represents the output from the SUSTAINABILITY EVALUATOR after analyzing the data obtained from the economic analyzer in Aspen plus for doing economic optimization. Figures 5.1 to 5.3 represents the comparison plots generated from the Modified SUSTAINABILITY EVALUATOR.

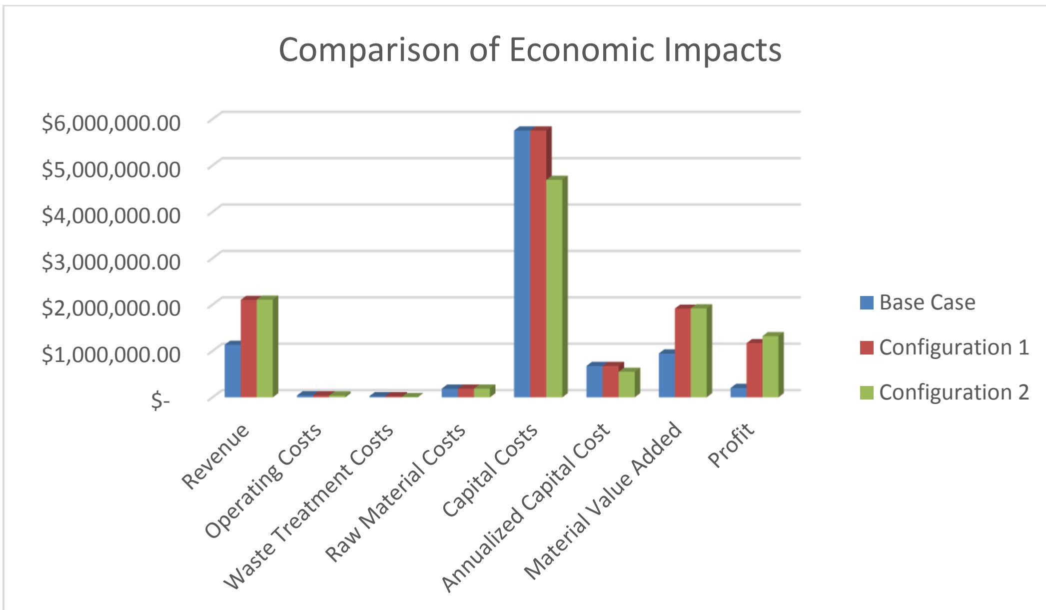


Figure 5.1: Comparison Plot Generated Automatically from Modified SUSTAINABILITY EVALUATOR for Economic Impact Assessment

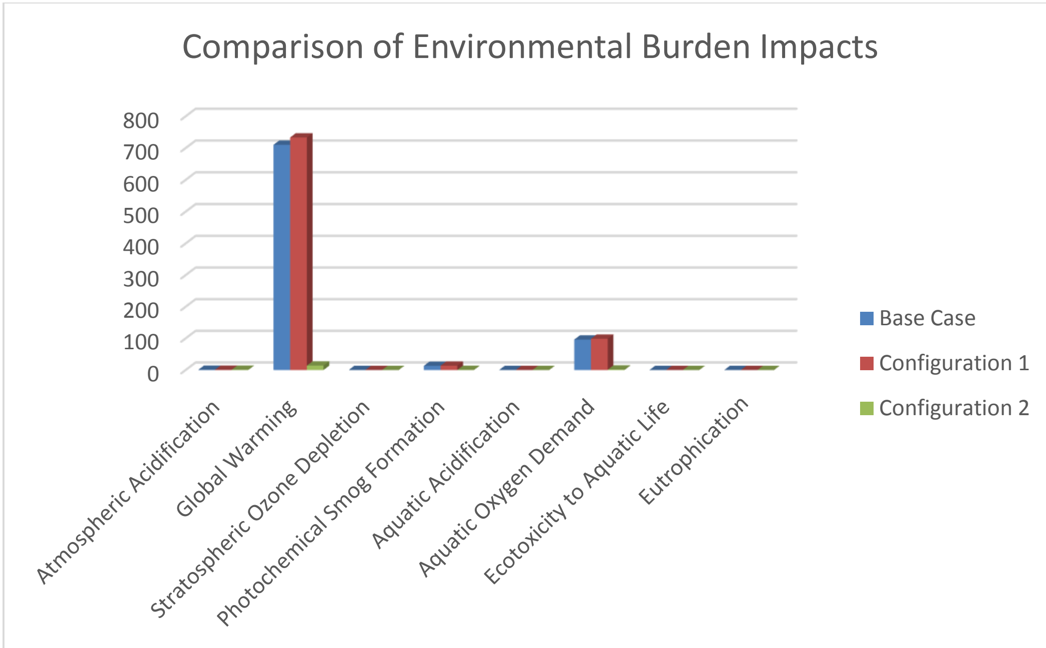


Figure 5.2: Comparison Plot Generated Automatically from Modified SUSTAINABILITY EVALUATOR for Environmental Burden Assessment

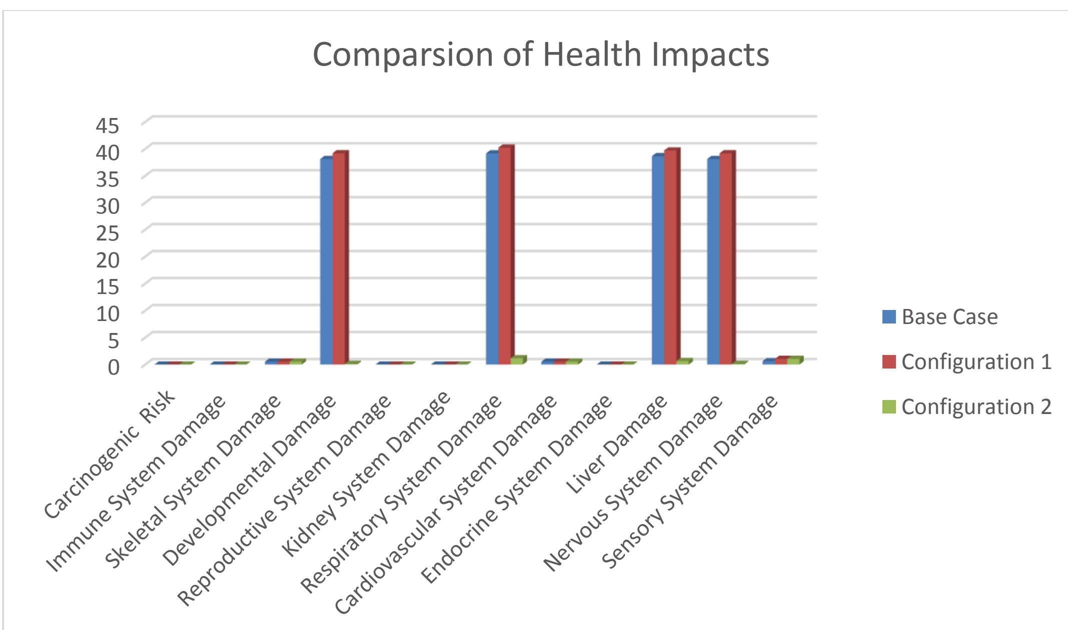


Figure 5.3: Comparison Plot Generated Automatically from Modified SUSTAINABILITY EVALUATOR for Health Impact Assessment

5.2.4 Report Generation

The modified SUSTAINABILITY EVALUATOR creates an easily readable .doc file to show the individual impacts and also the overall sustainability of a process. If there are more than one process evaluations, the values for different processes for different indices are also printed in the external file so that the user can compare easily by looking at the values. Figure 5.4 represents the external file output from Modified SE.

```
Sustainability Evaluation Results



Outputs for Economic Evaluation

Revenue       $1,133,404.00
Operating Costs             $41,659.30
Waste Treatment Costs       $24,629.62
Raw Material Costs          $188,020.30
Capital Costs $5,753,800.00
Annualized Capital Cost     $676,071.50
Material Value Added Cost   $945,383.60
Profit        $203,023.20

Profit Relative to Investment (PRI)       21.82

Economic Impact                           0.25


Outputs for Resource Usage Evaluation

Effective Mass Yield        29.95%
E-Factor                    2.51
Atom Economy                136.72%
Mass Intensity              3.71
Mass Productivity           26.93%
Reaction Mass Efficiency    29.95%
Material Intensity          2.34
Energy Intensity/Fossil Fuel Usage        0.0371
Water Intensity             3.83
Resource Usage Impact       0.28

Environment Burden Evaluation

Atmospheric Acidification               0.569
Global Warming                          710.00
Stratospheric Ozone Depletion           0.00
Photochemical Smog Formation            13.20
```

```
Aquatic Acidifiction                       0.035
Aquatic Oxygen Demand                      96.20
Ecotoxicity to Aquatic Life                0.00
Eutrophication                             0.00
Overall Environmental Burden Impact        0.04
Environmental Index                        0.10

Safety Index

Heat of main reaction index 2
Heat of side reaction index 0
Flammability index          6
Explosiveness Index         4
Toxic Exposure index        24
Corrosiveness index         0
Temperature index           6
Pressure index              0
Equipment safety index      4
Safety Level of Process Structure index   4
Total inherent safety index            0.5

Health index

Carcinogenic Risk           0.00
Immune System Damage        0.00
Skeletal system Damage      0.526
Developmental Damage        38.10
Reproductive System Damage  0.00
Kidney System Damage        0.00
Respiratory System Damage   39.20
Cardiovascular System Damage 0.526
Endocrine System Damage    0.00
Liver Damage                38.60
Nervous System Damage       38.10
Sensory System Damage       0.620
Health Impact               0.25

Overall Sustainability Index 0.19
```

Figure 5.4: External Output File Showing All the Results from modified SUSTAINABILITY EVALUATOR

CHAPTER VI

CONCLUSIONS AND RECOMMENDATIONS

6.1 Conclusions

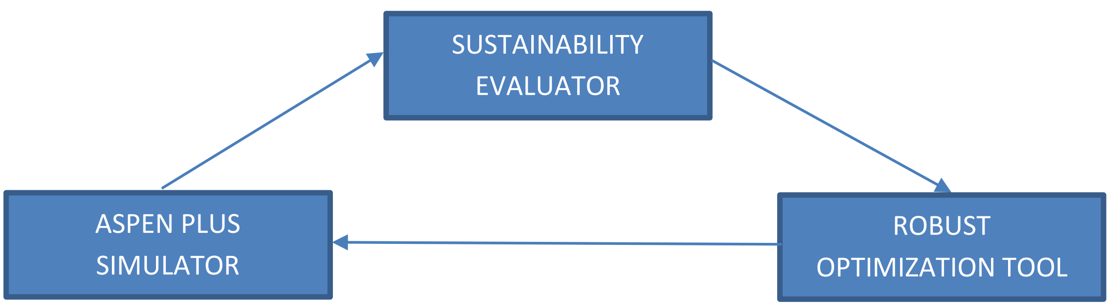
In this study, a modified Sustainability Evaluator tool has been developed using Excel VBA program to make the tool more effective and user friendly. This sustainability tool can be used to calculate individual index value such as economic index, environmental index and social index and also the overall sustainability index. The modified evaluator facilitates the user to customize the potency factors of different metrics as per requirement of the sustainability analysis. The weight factors of the three index to calculate the overall sustainability index can also be customized. The new interface provide guidelines about entering inputs and generate external output files enabling the user to get some ready data to compare the alternatives processes.

In order to validate the modified sustainability tools, the sustainability index of Poly Lactic Acid process has been calculated using previous sustainability tools and modified sustainability tools. The results provides the evidence of the validity of this new modified sustainability evaluator. The modified tool can provide comparison data to determine the best process among alternative processes. An external report can also be generated using the modified SUSTAINABILITY EVALUATOR tool.

6.2 Future Work

Although this work modified the SUSTAINABILITY EVALUATOR into more user friendly tool, there is still scope of improvements. The followings are some suggested research direction to consider:

- Sustainability evaluator can be linked with process simulation software such as Aspen Plus to update the sustainability index automatically if the inputs are changed for simulation software.
- A robust and multi-objective optimization tool can be incorporated with sustainability evaluator to investigate the sensitivity of different metrics or index.
- SUSTAINABILITY EVALUATOR, Aspen plus Simulator and a Robust Optimization Tool can be integrated together to have better results.



- SUSTAINABILITY EVALUATOR can be modified in such a way so that it should enable the user to calculate the sustainability index as different stages of the process or product life.
- SUSTAINABILITY EVALUATOR can be modified so that the process design engineers can have ideas about the sustainability of the process at very early stage of design where data availability is limited.

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APPENDIX

Table 1: Potency Factors for Chemicals that Cause Global Warming (IChemE Metrics, 2002)

Substances	Potency Factor
Carbon dioxide	1
Carbon monoxide	3
Carbon tetrachloride	1400
Chlorodifluoromethane, R22	1700
Chloroform	4
Chloropentafluoroethane, R115	9300
Dichlorodifluoromethane, R12	8500
Dichlorotetrafluoroethane, R114	9300
Difluoroethane	140
Hexafluoroethane	9200
Methane	21
Methylene chloride	9
Nitrogen oxides (NOx)	40
Nitrous oxide	310
Pentafluoroethane, R125	2800
Perfluoromethane	6500
Tetrafluoroethane	1300
Trichloroethane (1,1,1)	110
Trichlorofluoromethane, R11	4000
Trichlorotrifluoroethane, R113	5000
Trifluoroethane, R143a	3800
Trifluoromethane, R23	11700
Volatile organic compounds	11

Table 2: Potency Factors for Chemicals that Cause Stratospheric Ozone Depletion (IChemE Metrics, 2002)

Substances	Potency Factor
Carbon dioxide	1
Carbon monoxide	3
Carbon tetrachloride	1400
Chlorodifluoromethane, R22	1700
Chloroform	4
Chloropentafluoroethane, R115	9300
Dichlorodifluoromethane, R12	8500
Dichlorotetrafluoroethane, R114	9300
Difluoroethane	140
Hexafluoroethane	9200
Methane	21
Methylene chloride	9
Nitrogen oxides (NOx)	40
Nitrous oxide	310
Pentafluoroethane, R125	2800
Perfluoromethane	6500
Tetrafluoroethane	1300
Trichloroethane (1,1,1)	110
Trichlorofluoromethane, R11	4000
Trichlorotrifluoroethane, R113	5000
Trifluoroethane, R143a	3800
Trifluoromethane, R23	11700

Table 3: Potency Factors for Chemicals that Result in the Formation of Photochemical Smog (IChemE Metrics, 2002)

Substances	Potency Factor
1,1-Dichloroethylene	0.232
1,2,3-Trimethylbenzene	1.245
1,2,4- Trimethylbenzene	1.324
1,3,5- Trimethylbenzene	1.299
1-Butene	1.130
1-Pentene	1.040
2,2-Dimethylbutane	0.321
2,3-Dimethylbutane	0.943
2-Butene	0.990
2-Methylbut-1-ene	0.830
2-Methylbut-2-ene	0.770
2-Methylheptane	0.694
2-Methylhexane	0.719
2-Methylnonane	0.657

2-Methyloctane	0.706
2-Methylpentane	0.778
2-Pentene	0.950
3,5-Diethyltoluene	1.195
3,5-Dimethylethylbenzene	1.242
3-Methylbut-1-ene	1.180
3-Methylhexane	0.730
3-Methylpentane	0.661
Acetaldehyde	0.650
Acetic acid	0.156
Acetone	0.182

Table 4: Potency Factors for Chemicals that Cause Eutrophication (IChemE Metrics, 2002)

Dichloroethane (EDC)	0.50
Ammonia	0.24
Arsenic	0.20
Benzene	0.17
Cadmium	2.00
Carbon tetrachloride	0.42
Chloride	0.50
Chlorobenzene	1.00
Chloroform	0.42
Chromium	0.33
Copper	1.00
Cyanide	1.00
Formaldehyde	1.00
Hexachlorobenzene	166.67
Hexachlorobutadiene	50.00
Iron	0.005
Lead	0.20
Manganese	0.10
Mercury	16.67
Methylene chloride	0.50
Nickel	0.17
Nitrobenzene	0.25
Nitrophenol	0.50
Tetrachloroethylene (PER)	0.50
Toluene	0.13
Trichloroethylene (TRI)	0.50
Vanadium	0.05
Xylenes	0.17

Zinc	0.13

Table 5: Potency Factors for Chemicals that Cause Aquatic Oxygen Demand (IChemE Metrics, 2002)

Substances	Potency Factor
Acetic acid	1.07
Acetone	2.09
Ammonium nitrate in solution	0.80
Ammonium sulphate in solution	1.00
Chlorotrifluoroethane	0.54
1,2 – Dichloroethane (EDC)	0.81
Ethylene	1.00
Ethylene glycol	1.29
Ferrous ion	0.14
Methanol	1.50
Methyl methacrylate	1.50
Methylene Chloride	0.47
Phenol	2.38
Vinyl chloride	1.28

Table 6: Potency Factors for Chemicals that Cause Atmospheric Acidification (IChemE Metrics, 2002)

Substances	Potency Factor
Ammonia, NH3	1.88
Sulfuric acid mist, H2SO4	0.65
Hydrochloric acid, HCL	0.88
Hydrogen fluoride, HF	1.60
Nitrogen dioxide, NO2	0.70
Sulfur dioxide, SO2	1.00

Table 7: Potency Factors for Chemicals that Cause Aquatic Acidification (IChemE Metrics, 2002)

Substances	Potency Factor
Acetic acid	0.020
Hydrochloric acid, HCL	0.027

Hydrogen fluoride, HF	0.050
Sulfuric acid	0.020

Table 8: Potency Factors for Chemicals that Cause Eutrophication (IChemE Metrics, 2002)

Substances	Potency Factor
Ammonia	0.33
COD	0.02
Nitrogen	0.42
Nitrogen dioxide, NO2	0.20
Nitrogen oxide, NO	0.13
NOx	0.13
Phosphorus	3.06
PO4 (III-)	1.00

Table 9: Index Score for Heat of Reaction

Mass Enthalpy(Hf) (J/g)	Score
≤ 200	0
<600	2
< 1200	4
< 3000	6
3000	8

Table 10: Index Score for Flammability Index

Flammability Limits (oC)	Score
Not Flammable	0
Flash Point > 55	2
Flash Point ≤ 55	4
Flash Point < 21	6
Flash point < 0 & boiling point ≤ 35	8

Table 11: Index Score for Explosivity Index

Explosivenes s Limit	Score
Not Explosive	0
0-20	2

20-45	4
45-70	6
70-100	8

Table 12: Index Score for Corrosive Index

Material of Construction	Score
Carbon Steel	0
Stainless Steel	2
Better Material Needed	4

Table 13: Index Score for Temperature Index

Temperature (oC)	Score
< 0	2
0-70	0
70-150	2
150-300	4
300-600	6
>600	8

Table 14: Index Score for Pressure Index

Pressure (bar)	Score
0.5 – 5	0
0-0.5 or 5-25	2
20-25	4
50-200	6
200-1000	8

Table 15: Index Score for Equipment Process Safety Index

Type of Equipment	Score
Equipment handling nonflammable, nontoxic materials	0
Heat exchangers, pumps, towers, drums	2
Air coolers, reactors, high hazard pumps	4
Compressors, high hazard	6

reactors	
Furnaces, fired heaters	8

Table 16: Index Score for Process Safety Structure Index

Process Reliability	Score
Safe	0
Sound Engineering Practice	2
No data	4
Probably Unsafe	6
Minor Accidents	8
Major Accidents	10

Table 17: Index Score for Toxic Exposure Index

Toxic Exposure Limit (ppm)	Score
TLV > 10000	0
TLV ≥ 10000	4
TLV ≤ 1000	8
TLV ≤ 100	12
TLV ≤ 10	16
TLV ≤ 1	20
TLV ≤ 0.1	24
TLV ≤ 0.01	30

Table 18: Index Score for Process Safety Structure Index

Safety Metric	Index Range
Heat of Main Reaction Index	0-8
Heat of Side Reaction Index	0-8
Flammability Index	0-8
Explosiveness Index	0-8
Corrosiveness Index	0-4
Temperature Index	0-8
Pressure Index	0-8
Equipment Safety Index	0-8
Safety Level of Process Structure Index	0-10
Toxic exposure Index	0-30
Overall Safety Index	0-100

Table 19: Index Score for Carcinogenic Risk

Type of Carcinogen	Group	Score
Not Carcinogenic	N/A	0
Probably not carcinogenic to humans	4	0.2
Not classifiable as to its carcinogenicity to humans	3	0.4
Possibly carcinogenic	2B	0.6
Probably carcinogenic to humans	2A	0.8
Carcinogenic to humans	1	1

Table 20: Index Score for Health Metrics

Health Metric	Index Range
Carcinogenic Risk	0-1
Developmental Damage	0.6 or 1
Reproductive System Damage	0.6
Circulatory System Damage	0.6
Skeletal System Damage	0.6
Endocrine System Damage	0.6
Gastrointestinal and Liver Damage	0.6
Immune System Damage	0.6
Kidney Damage	0.6
Skeletal System Damage	0.6
Nervous System Damage	0.6
Respiratory System Damage	0.6
Sensory System Damage	0.6

Table 21: Score for Economic Impact

PRI	Economic Impact
0	1
5%	0.75
15%	0.5
20%	0.25

>25%	0

Table 22: Resource Usage Metric Impact Value for Metrics Expressed in percentages

Resource Usage metric (%)	Score
0	0.20
20	0.10
40	0.07
60	0.05
80	0.04
100	0.00

Table 23: Resource Usage Metric Impact Value for metrics expressed in Kilogram

Resource Usage Metrics (kg)	Score
0	0.00
0.5	0.03
1	0.04
5	0.05
10	0.07
50	0.10
200	0.20

Table 24: Environmental Burden Impact Value

Equivalent Impact (Tonnes/year)	Score
0	0
100	0.041
10000	0.0625
100000	0.125

Table 25: Weights for Overall Safety Impact Value

Process Safety Index Value	Score
0	0
25	0.25
50	0.50
75	0.75
100	1.00

Table 26: Weights for Carcinogenic Risk

Tonnes/Year Equivalent	Score
0	0
100	0.083
1000	0.125
10000	0.25

Table 27: Weights for other Health Risks

Tonnes/Year Equivalent	Score
0	0
100	0.025
10000	0.05
100000	0.068

VITA

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