SUSTAINABLE PROCESS DEVELOPMENT FOR POLYMER PRECURSOR BASED ON ECONOMIC ANALYSIS AND LIFE CYCLE ASSESSMENT STUDIES

By

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SUSTAINABLE PROCESS DEVELOPMENT FOR POLYMER PRECURSOR BASED ON ECONOMIC ANALYSIS AND LIFE CYCLE ASSESSMENT STUDIES

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Abstract:

Polymer Plastic**s** have been an integral part of our existence for more than a quarter of a century now. The amount of plastic produced every day is becoming a matter of grave concern since most of it is non-biodegradable and originates from non-renewable fuel sources. It not only pollutes the environment over a longer period of time because of the difficulty to dispose it but also increases the carbon footprint. Biodegradable plastics originating from renewable sources, on the other hand, provide distinct advantage in terms of green design. Poly Lactic Acid (PLA) is a potential substitute for presently used plastics. This work presents the development of a sustainable process for the manufacture of highly pure lactic acid (99 wt. % on dry basis) which is used as PLA precursor. The process is based on a process patented by NCL, Pune and is simulated using Aspen Plus® version 8.2. Green Design principles have been used during process development. The process has been optimized using sensitivity analysis and optimization block in Aspen Plus. Detailed process economic analysis and optimization has been carried out using Aspen Integrated Economic Analysis along with a Life Cycle Assessment (LCA) study in SimaPro. SUSTAINABILITY EVALUATOR has been used to assess overall sustainability of the process and to determine economic, environmental and social impacts.

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CHAPTER I

MOTIVATION

1.1 Overview

In today’s world plastic products have become ubiquitous, and therefore rather unavoidable. We come in contact with polymer plastic directly or indirectly every day. Plastics are used in almost every industry; ranging from durable goods like furniture and appliances to nondurable goods like trash bags, cups etc.

A polymer can be defined as a large chain molecule of higher molecular weight, composed of a repeated sequence of monomer molecules **(Roussak and Gesser 2013)**. Plastic is a name derived from the plastic property of a material and is now used commonly for polymer products, even though most of them do not actually possess that property. Thus the term plastic is generally used to refer to polymer products. In this work, the terms plastic and polymer have been used interchangeably. A majority of the polymers are formed on a hydrocarbon backbone along with other elements. The properties of polymers can be modified by adding side-chains of different elements depending on the necessary application.

Michael Tolinski in his book titled *Plastics and Sustainability* talks about some characteristics of today's industrial plastics **(Tolinski 2012).**

- Inexpensive
- Customized properties
- Simple chemical structures
- Lightweight yet strong
- Processed from high energy feedstock (frozen fuel)
- Recyclable but expensive

The annual world plastic production has increased at an astonishing rate over the past six-seven decades. Starting with about 11.5 Megatons (MT) in 1940 to about 27 MT in 1970 and thereafter doubling every decade to more than 150 MT in 1990 to more than a 1000 MT a year currently **(Roussak and Gesser 2013).** With this increase in production there is a subsequent increase in plastic waste as well. According to the Environmental Protection Agency (EPA), in 1960, plastics made up less than 1% of all waste streams. Today we have reached about 13% of plastics all waste streams. This tells us two things: 1) the amount of plastic production has increased rapidly; which is obvious given the extraordinary demand for plastic products. 2) Plastics aren't recycled effectively enough and therefore there is a need to create "new" plastic material.

1.2 Plastic Pollution and the Way Forward

The real challenge confronting us today is the amount of plastics that is being dumped into the environment without consideration for the consequences. Nowadays, we can see increased plastic products dumped in water bodies like ponds and lakes. A once clean pond is now cluttered with various types of plastic products like bags, cups, etc. In the past 25 years, production of plastic bags has risen from zero to 500 billion per year which is roughly a 1 million bags per minute.

From a purely environmental point of view, the concern is that most of these plastic products are non- biodegradable and take hundreds of years to degrade. Table 1.1 lists the types of plastic pollution which affect different animal species.

Table 1.1: Types of plastic pollution affecting different animal species

Type of pollution	Description
Land	Chlorinated plastics release toxic chemicals into the soil which seeps into the groundwater and is harmful to animals that drink this water Landfills contain high amount of non-biodegradable plastics which are harmful for the habitant species
Oceans	Part of the plastic pellets (nurdles) which are shipped for manufacturing other plastic products are spilled into the ocean. In 2012 there was about 165 Mt of plastics released in the ocean **(Knight 2012).** Around 4,00,000 marine mammals have known to perish annually due to plastic pollution **(Chiras 2004)**
Animals	Plastics are a potential poison for animals which can in turn be harmful for humans as well. Marine mammals are highly vulnerable to plastic products and some species have found to contain large amount of plastic products in their stomach.

As observed from Table 1.1, plastics are adversely affecting the balance of the eco-system. Although the effects may not be very obvious to the layman at this moment, it is believed that in the coming decade or so, the situation is going to be alarming. The only way to prevent this from happening is to make conscious efforts to minimize the impact of this pollution. Following are the options that are being considered:

1. Limit the production of plastics. This is the ideal solution; however given our current dependence on plastics it is highly improbable.
2. Plastic Reuse/Recycle – It is being practiced but has its limitations in terms of magnitude and cost. In some cases recycling the plastic may take up more energy, thereby damaging the environment even more. It is very important to identify the situations where recycling is effective. Life Cycle Assessment (LCA) is a tool that can be used for this purpose. A detailed account of LCA will be given in Chapter 7.
3. Increasing use of biodegradable plastics – This is currently the most effective method to reduce plastic pollution without really affecting the unique plastic properties. It is also an economically viable solution. Biodegradable plastics are those which can be decomposed by micro-organisms at a rate which is practically acceptable. Biodegradable plastics must not be confused with plastics being produced from bio-resources. Contrary to popular belief, some biodegradable plastics actually originate from non-renewable sources.

   Plastics derived from non-renewable fossil fuels lock up majority of the carbon in the plastic instead of being utilized in plastic processing. The carbon gets trapped inside the plastic lattice and is seldom recycled. Other biodegradable plastics originate from a renewable source like sugarcane, corn, bagasse etc. as shown in Figure 1.1. Here, although we are not locking up any of the carbon, we are using up a potential food source which might be more important in than the use of the resource for plastics in some cases. This is the prevalent debate about Food vs. Fuel which will be discussed at length later in this chapter.

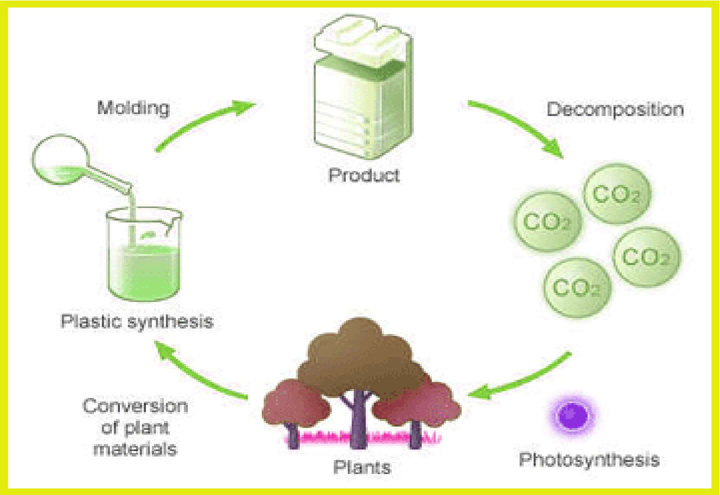


Figure 1.1: This diagram depicts the life cycle of a biodegradable plastic originating from renewable source (Figure reproduced from www.biotechonweb.com)

Table 1.2 describes the type of polymer plastic and its degree of environmental pollution and carbon footprint. It could be argued from this information that biodegradable plastics originating from bio-resources are potentially the most environmental-friendly choice.

Table 1.2: Type of plastic and degree of pollution and carbon footprint

Type of polymer plastic	Degree of Pollution and Carbon Footprint
Non-biodegradable originating from non-renewable resources	High pollution, high carbon footprint
Non-biodegradable originating from renewable resources	High pollution, low carbon footprint
Biodegradable originating from non-renewable resources	Low pollution, high carbon footprint
Biodegradable originating from renewable resources	Low pollution, low carbon footprint

Although biodegradable plastics that come from a renewable source seem to be an excellent solution, they have their own issues. Currently, the processes for manufacturing biodegradable plastics from renewable sources (biofuels etc.) are not economically viable because non-renewable fuel sources have a better competitive price. However, this situation is changing rapidly and it has been predicted that as fuel resources run dry in the coming decade, fuel prices will rise alarmingly. Additionally, biodegradable plastic physical characteristics like tensile strength, density etc. aren't competitive enough with traditional plastics as there has only been limited research and development in this area.

1.3 Food vs. Fuel

Biofuels are energy sources derived from recently living organisms, for example crops like sugarcane, corn or organisms like algae **(Stein 2007).** Crops are the only the raw materials used to generate biofuels and are not biofuels themselves. Different crops are used to produce biofuels in different parts of the world as shown in Table 1.3.

Table 1.3: The figure shows the primary plant source used for biofuel production in different parts of the world. Derived from information in **(Stein 2007)**

Country/Region	**Primary plant source of biofuel**
United States and China	Corn and Soybean
Brazil and India	Sugarcane
Europe	Sugar Beet, Wheat, Barley
Asia and Africa	Cassava

As discussed earlier, the interest in biofuels has increased considerably in recent years. The following list is a recap of the reasons why fossil fuel dependency needs to be reduced **(Ajanovic 2011)**:

- Excessive consumption of fossil fuel resources leading to reduction of resources at an alarming rate
- Increased greenhouse gas emissions
- Disproportionate distribution of resources leading to accelerated import from under-developed countries.

Although, prima-fascia biofuels looks like the decisive solution to these problems, there are several difficulties with biofuels as discussed earlier. Those are summarized below.

- Limited crop resources
- Limited available land for harvesting crop
- Market competitive prices
- Production efficiency/ technology advancement

The primary opposition to the production of biofuel comes from the fact that most of the resources currently used as raw materials are also used as food. Since, several regions have shortage of food resources, the question is whether it is really worth using some of these crops to produce biofuels. Although there is no conclusive data to prove that the food resources are directly being used for biofuel production, the debate will rage on. There are currently two solutions that are being considered:

- Considerable increase crop production
- Use of non-edible crops (e.g. switchgrass, jatropha) and organisms (e.g. algae) as biofuel sources.

Biofuel from algae is a burgeoning sector. Several new start-ups companies like Algenol Biofuels and Solazyme are being setup. Established names like Exxon Mobil have invested more than $100 million to develop algae derived biofuel.

The prediction is that once enough technological advances have been developed to manufacture biodegradable polymers from renewable sources, most of the short-comings mentioned above will be overturned.

The current work is based on one such process to manufacture polymer grade lactic acid, a precursor for poly lactic acid (PLA). PLA is a biodegradable plastic which has received a lot of attention in the last decade or so. The fermentation products coming from a biofuel source has been used as one of the raw materials for the lactic acid process. A detailed account of lactic acid and PLA properties and uses is presented in the following section.

CHAPTER II

PROCESS SUSTAINABILITY

2.1 Introduction

The word sustainability has been derived from the Latin word *sustinere* which means *to hold up.* To sustain literally means "to support" or "to maintain." More relevant is the definition provided by the World Commission on Environment and Development in 1987 "*development that meets the needs of the present without compromising the ability of future generations to meet their own needs".* Although a push sustainability has been around since the 1990s, it is only in the 21st century that it came into prominence. The gradual realization that the current rate of human activities cannot continue without significantly and perhaps permanently damaging the environment has led people to consider sustainability more seriously**(Cabezas, Pawlowski et al. 2003)** .

Although sustainability is a generic term, its implication in today's world is based on three important pillars – Environmental, Economic and Social. The environmental aspect of sustainability deals with preserving nature. As the world is driven by money, economics becomes an integral part of any process or product. The social aspect of sustainability is the least researched and often the overlooked factor.

This is partly because it is very difficult to identify and measure social implications. Also, the social sustainability factors are varied and it is difficult to have generic metrics. In most cases, social sustainability will have very specific factors pertinent only to the product or the process. Andrew gives a nice illustrative diagram explaining sustainability (Figure 2.1)

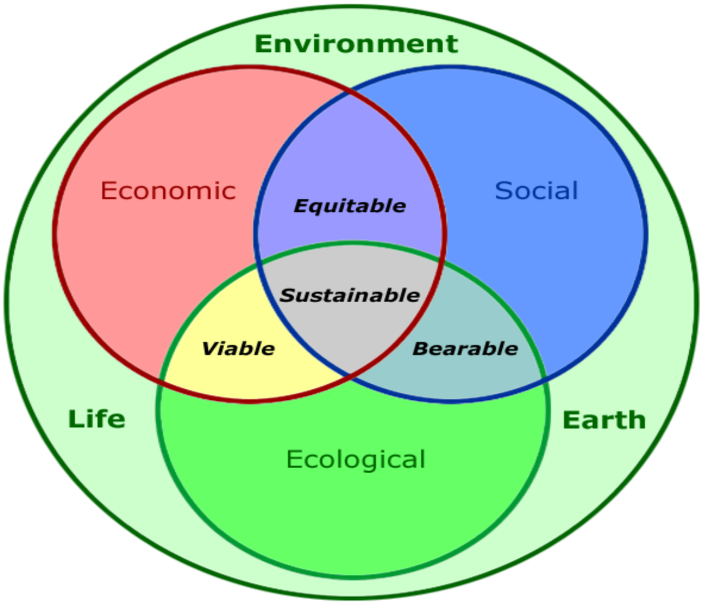


Figure 2.1: This a diagram made by Andrew in Photo Shop, January 14, 2009, released as free content.

The above Venn diagram is comprised of the three building blocks of sustainability as described earlier – Economic, Ecological and Social. If a process is economically and ecologically sustainable then it can be categorized as a viable process. A bearable process is s one which is environmentally and socially sustainable. Lastly, if both economic and social aspects of a process are sustainable then it can be termed as equitable. The ultimate and often elusive goal is to design a process that is sustainable in all three aspects and make it sustainable in the true sense.

It should be noted that these three facets of sustainability are related and inter-dependent. Thus it is often impossible to attain one of those without affecting the other. As such, the three aspects should be considered simultaneously while designing a process. This creates something called a multi-objective optimization problem. To illustrate this fact further, consider a waste-water treatment process. The aim is to minimize the waste in the effluent water stream which will make the process better in terms of environmental and social (health) aspects. However, the treatment comes at a cost. The lower the waste is in the waste stream, the costlier is the process and therefore not sustainable economically. Thus the process designer needs to find the right balance between the three.

Figure 2.2 depicts the current and ideal states of sustainability. It can be seen from the diagram that the most of the sustainability indices are based the use of fossil fuels.

The prime concerns with this dependence on fossil fuels is that they produce CO_2 and other particulate matter on burning which adversely affects both the environment as well as human health. It is also known to be the major contributor towards global warming. Additionally, fossil fuel resources are steadily declining and the concept of sustainability has come to the forefront partly due to this fact. However, merely knowing this is of little help. The challenges lie in formulating alternative fuel resources and making it sustainable. As shown in the diagram the current fuel reserves won’t last long beyond 2025 and therefore a gradual phasing out fossil fuels is necessary. This can be achieved by implementing concept of green design, conducting and utilizing pertinent life cycle analysis studies, steadily shifting to renewable sources for material and energy etc.

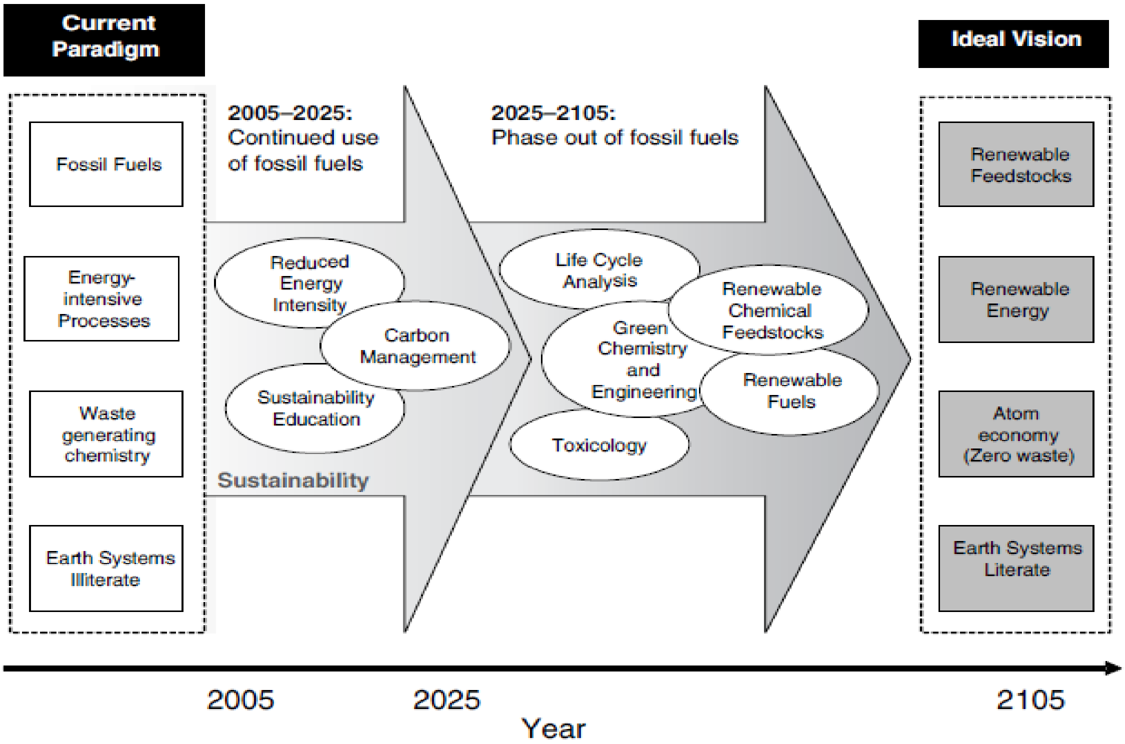


Figure 2.2**:** Diagram indicating the present and future for sustainability (Reproduced from **(Industry and Council 2005))**

2.2 Sustainability Metrics

Ideally, we would like to have environmentally friendly processes giving maximum product output with the use of minimal resources while considering the health and safety of the people likely to get affected. The goals to attain sustainability listed above would not be achievable without having proper measuring schemes to assess progress. As the business adage says "*only what gets measured gets managed"***(Beloff, Lines et al. 2005).** One of the possible solutions is to use metrics or indicators based on specific guidelines. The metrics should capture environmental impacts, economic viability and social concerns. However, designing appropriate sustainability metrics to measure a sustainability index for all three aspects and making them simple enough for generic use yet comprehensive enough to be useful for different types of processes is no easy task. There have been several attempts to quantify economic and ecological sustainability. The challenge lies in integrating them and introducing the social aspect into the metrics.

According to **Tanzil (Tanzil 2006)** and **Shadiya (Shadiya 2010),** sustainability can be broadly classified into three main categories – Socio-environmental, socio-economic and eco-efficient. Socio—environmental concerns deal with environment impacts that could adversely affect society. Socio-economic metrics measure the economic wellbeing of society. Lastly, eco-efficient indices are used to measure the economic viability of the process with minimal environmental damage.

Atlee (Atlee 2006) provides some generic characteristics 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

As explained earlier, integrating these desirables into a single measuring scheme is a monumental task. One such effort has been made by **Shadiya (Shadiya 2010)** in the development of the SUSTAINABILITY EVALUATOR and has been used in this work**.** Details about the SUSTAINABILITY EVALUATOR and its use are given in Chapter 8.

Several tools could be used to assist in measurement of the parameters. A diagram listing the tools is depicted in Figure 2.3.

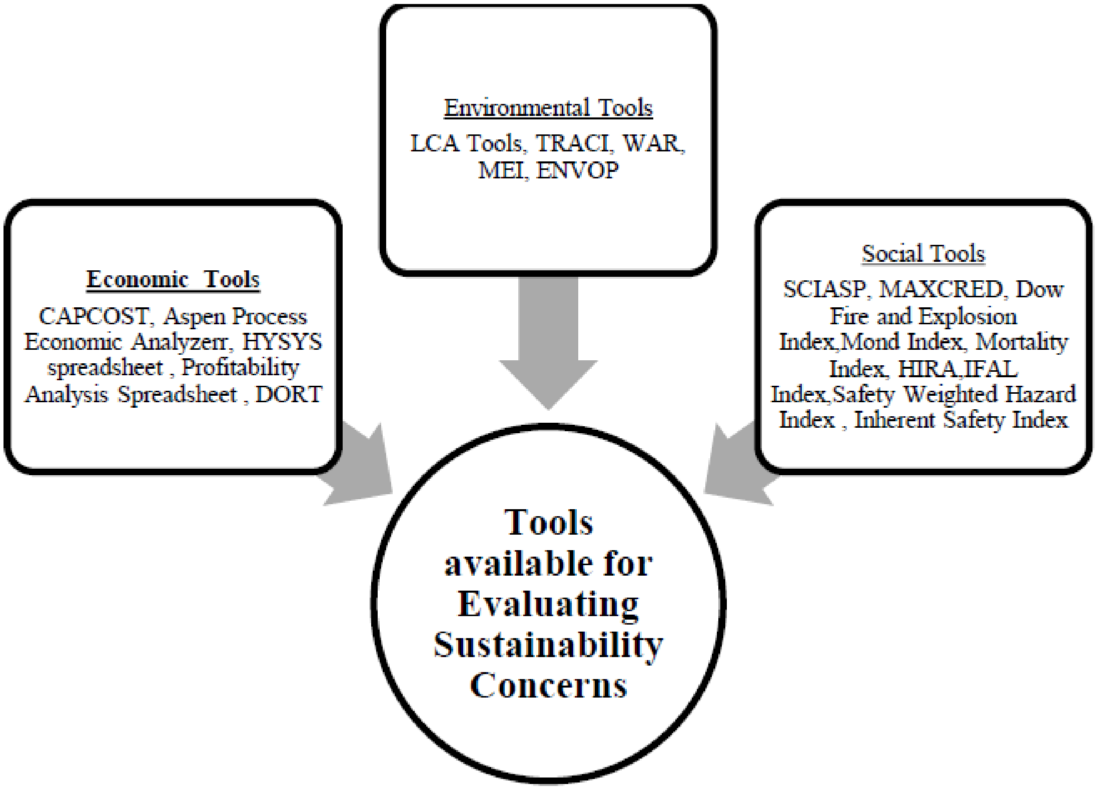


Figure 2.3: Tools available for evaluating sustainability concerns reproduced from **Shadiya (Shadiya 2010)**

The tools listed are used to either to measure the process parameters (e.g. Aspen Process Economic Analyzer) or are used directly as sustainability metrics or indices (e.g. LCA, Sustainability Evaluator). Table 2.1 shows a list of tools used in this work to quantify sustainability for the lactic acid process.

Table 2.1: Tools used for sustainability impact assessment

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

Figure 2.4 provides a systematic outlook utilized for sustainability analysis in this work.

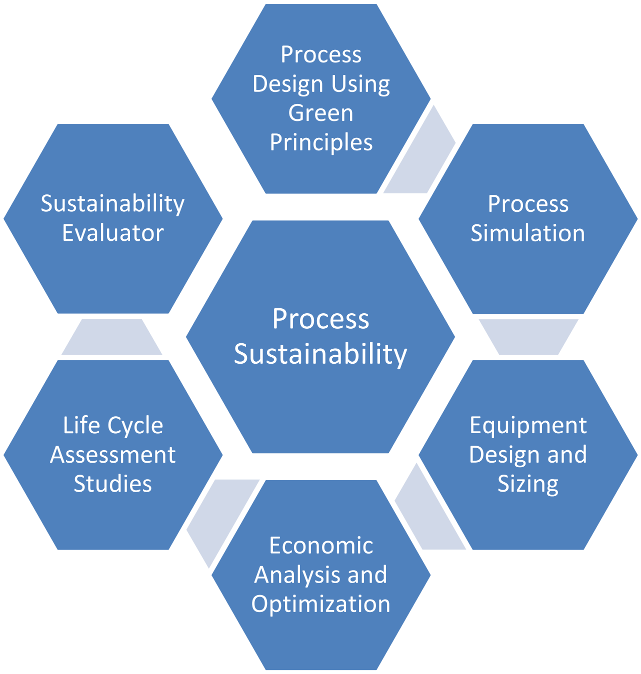


Figure 2.4: Workflow for sustainable process design

The workflow proposed in Figure 2.4 is the framework utilized in this work. As shown in the figure, development of a sustainable process is the guiding factor for this work. The three pillars of sustainability – economy, environment and society have each been analyzed individually as well as a whole. The subsequent chapters will explain in detail how each of the step has been carried out and how the results are eventually utilized for evaluating sustainability of the process.

CHAPTER III

LACTIC ACID BACKGROUND

Lactic acid was first isolated in 1780 by Swedish scientist Carl Wilhelm Scheele by crystallizing its calcium salt **(Datta and Henry 2006)**. It is a weak organic acid with a hydroxyl group and a carboxylic group present on adjacent carbon atoms in the carbon chain. This duality in structure allows it to react either as an acid or as an alcohol.

Traditionally, lactic acid has had applications in the food, chemical, and pharmaceutical industries. In the food industry, lactic acid with a purity of about 85 wt. % is used to introduce a sour taste in food products, for example in pickles and sauerkraut. It is also used as an acidulant in the food industry **(Guilherme, Silveira et al. 2012)**. In addition, it is also used in the textile industry as a caustic **(Al-Shammary, Aziz Mian et al. 1993, Södergård A 2010)**. Around 80-85 wt. % of lactic acid is manufactured for use in the food industry. More recently however, there has been an increased focus on manufacturing lactic acid of high purity (99 wt. % on dry basis) which can be used as the monomer for producing poly-lactic acid (PLA).

PLA can be obtained from lactic acid via two different mechanisms – 1) direct polymerization of lactic acid by poly-condensation or 2) condensation to form lactide (intermediate) and corresponding ring-opening polymerization to obtain PLA **(Guilherme, Silveira et al. 2012)**.

PLA is a biocompatible and biodegradable material that has numerous applications in sustainable plastic products **(Qin, Zhao et al. 2009)**. Along with the ease of disposal, lactic acid polymers also possess high tensile strength and can be used in the packaging industry and for medical and biological applications **(John, Nampoothiri et al. 2007)**. Table 1.4 summarizes the applications of PLA in various industries **(Mehta, Kumar et al. 2005, Södergård A 2010)**.

Table 3.1: Summary of polymer grade lactic acid applications

Industry	Property	Application
Medical	Non-toxic, relatively strong, bio-compatible, sterilizable	Medical Implants; clinical applications – sutures; meshes, bone fixation devices
Packaging	High tensile strength, thermal resistance, impact resistance, transparency	Flexible Films, thermoforming, lamination
Textile	bacteriostatic, flame-retardant, and weathering resistance	Geo-textiles, Industrial Fabrics, Fibers, Home Furnishings
Environmental	Bio-compatible	As sorbent in wastewater treatment; As a substrate for nitrogen removal; as a bioremediation agent
Other	Biodegradability, flame-retardant, thermal resistance	To manufacture sandbags, weed prevention nets, vegetation nets, vegetation pots, ropes, binding tape for use in the agriculture industry

PLA competes with traditional plastics like poly-ethylene terephthalate (PET) and poly propylene (PP) in terms of sustainability **(Tolinski 2012)** and applicability. PLA is a biodegradable polymer and decomposes at composting conditions and temperatures above 60 °C. PLA production requires less energy per kg as compared to PET and PP (42 MJ/kg for PLA as compared to 73 MJ/kg for PP and 80 MJ/kg for PET) **(Tolinski 2012)**. Recycling PLA, however, is difficult using traditional mechanical or melt-recycling methods because of its temperature and water sensitivity. To accomplish this, chemical processes which can hydrolyze PLA to lactic acid are being developed.

According to a comparison study performed by Tabone, Cregg et al. PLA is the top ranked polymer in terms of rankings based on green design principles and ranks sixth according to Life Cycle Assessment studies **(Tabone, Cregg et al. 2010)**. It is therefore considered as one of the more sustainable alternatives to plastics being used currently.

To obtain high quality PLA, polymer grade lactic acid (~99 wt. % purity) is the starting point. Several efforts have been made previously to obtain high purity lactic acid. Those methods generally have the following limitations.

1. High pressure and temperature required to achieve the intended purity which increases cost.
2. High pressure and temperature also lead to formation of by-products (unwanted methyl esters) during the esterification reaction which are difficult to separate.
3. Use of acid catalyst in the hydrolysis reaction hampers lactic acid purity.
4. Limited conversion for the esterification reaction due to product build-up.

Background information about lactic acid and Poly Lactic Acid (PLA) has been provided in this chapter. A detailed process description for the lactic acid process in question is provided in Chapter 4 and the other details about process development have been provided in subsequent chapters.

CHAPTER IV

PROCESS DESCRIPTION

This process development is based on a laboratory scale patented process by the National Chemical Laboratory (Pune) to manufacture polymer grade lactic acid **(Barve 2010)**. The process can be roughly divided into three stages as described below:

Part of the following chapter has been adapted from previous work **(Susmit S Bapat 2014)** and from the patent **(Barve 2010).**

Stage 1 Preparation of Crude Lactic Acid Feed Stock

Figure 4.1 provides a basic process flow diagram for stage 1 of the process.

A glass lined stirred reactor was charged with a 10% by wt. solution of calcium lactate in water that had been obtained from fermentation of sugar cane juice. A 50% by wt. sulfuric acid in water was charged added to the calcium lactate solution in water in a stoichiometric ratio to release free lactic acid. The reaction mixture was then stirred for 60 minutes and then filtered on the centrifuge. The wet cake of calcium sulfate was washed with water to remove adhered acidity. The wet cake of calcium sulfate was dried at 110° C to give white calcium sulfate.

The filtrate and washing were concentrated on the falling film evaporator under vacuum to get crude lactic acid. The crude lactic acid that was obtained was a viscous, dark reddish brown liquid and contained impurities of fermentation. It was treated with activated charcoal and filtered to get transparent and clear crude lactic acid in water having concentration of 60%.

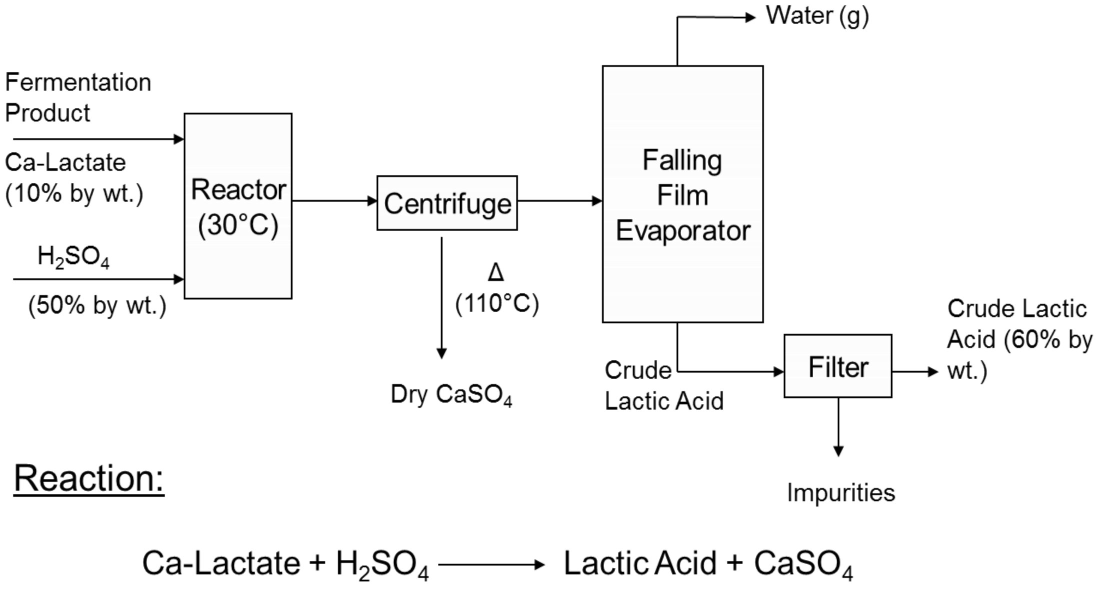


Figure 4.1: Basic process flow diagram for the first stage of polymer grade lactic acid production.

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

Figure 4.2 provides a basic process flow diagram for stage 2 of the process.

The crude lactic acid prepared in Stage 1 was pre-mixed with concentrated sulfuric acid (1 mole % of lactic acid) and different impurities were added to is, such as oxalic acid, malic acid, acetic acid and fumaric acid all put together by dissolving in small amount of methanol (1% each of the impurity by wt. lactic acid was added) was charged and stored in a/the tank. This crude lactic acid mixture containing known impurities was continuously pumped through a pre-heater at 1000 g/h. The temperature of the pre-heater was maintained by a hot oil circulator so as to continuously maintain crude lactic acid temperature at 96° C. The heated crude lactic acid was fed continuously to the middle of the trickle phase column section 1, fixed just above the re-boiler. Fresh methanol feedstock containing 0.4% water was stored in the tank. This methanol was continuously pumped through pre-heater at 750 g/h. The superheated methanol vapors were bubbled through a sparger at the bottom of the reboiler containing crude methyl lactate steady state feed stock obtained from Stage 1. The heated lactic acid obtained from lactic acid pre-heater was allowed to trickle down continuously through a packed column section and was allowed to react continuously with the superheated methanol vapors obtained from the methanol pre-heater through the re-boiler which rises through a trickle phase column. The methyl lactate formed and unconverted crude lactic acid was allowed to trickle down continuously through the trickle phase column section to the re-boiler. The crude methyl lactate formed along with the impurities was removed continuously in the form of over-flow from the reboiler through the cooler. The water rich layer containing some traces of methyl lactate was continuously recovered at the bottom, whereas the methanol rich fraction was collected continuously throughout the cooler.

It should be noted that the eventual product purity is greatly influenced by the reactive distillation described above. A reactive distillation operation consists of simultaneous reaction and separation processes **(Stichlmair and Frey 1999)**. In this case, methanol reacts with crude lactic acid to produce methyl lactate. As per the patented process, water and methanol are being simultaneously separated in the same column. However, while simulating this process it was observed that an additional separation column (Separat 4) was more effective for carrying out the separation of methanol and water than having a side-draw from the RadFrac column. It can therefore be said that the Bubble Column Reactor and Separat 4 together represent the Reactive Distillation Column. However, it should be noted that the more significant separation of methyl lactate and water + methanol is still occurring in the Bubble Column Reactor. As the product (i.e. methyl lactate) is being continuously removed from the reactor the reaction equilibrium shifts towards the product side, thereby increasing maximum conversion according to Le-Chatelier's principle.

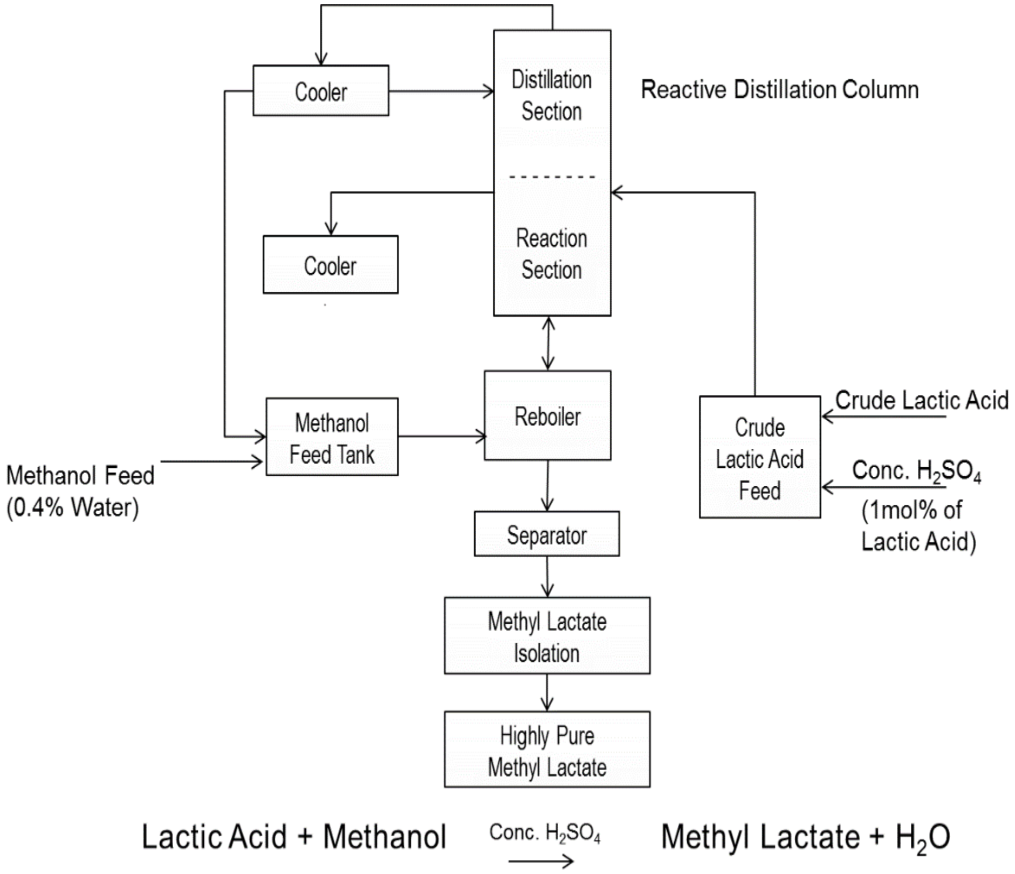


Figure 4.2: Basic process flow diagram for the second stage of polymer grade lactic acid production.

Stage – 3 Hydrolysis of Highly Pure S-(-)-methyl Lactate to Get Highly Pure L-(+)-lactic Acid.

Figure 4.3 provides a basic process flow diagram for stage 3 of the process.

Highly pure methyl lactate obtained from Stage 2, having 99.8% purity by wt. was charged to the glass lined stirred reactor and was further charged with distilled water, along with pure lactic to facilitate the hydrolysis reaction. The methanol vapors formed during the hydrolysis reaction were allowed to rise through the column and condensed in the cooler and was fractionated with reflux to get to top temperature at 65° C. Any trace amount of methanol or unconverted methyl lactate was recovered and recycled.

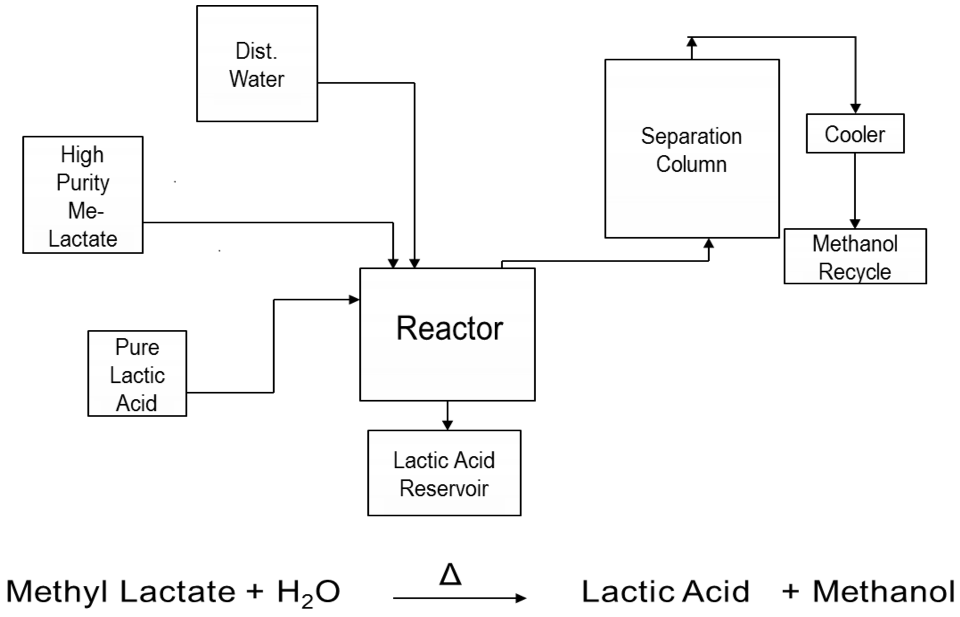


Figure 4.3: Basic process flow diagram for the third stage of polymer grade lactic acid production.

The ingenuity of stage 3 lies in the fact that pure lactic acid is used as an auto-catalyst to avoid impurities. The use of an auto-catalyst facilitates achieving high lactic acid purity (99 wt. % on dry basis) and also increases the reaction rate. Also, methanol which is a by-product of the hydrolysis reaction is recycled back to the bubble column, thereby reducing the inventory cost and energy.

It should be noted that the process flow diagrams depicted in Figure 4.1, Figure 4.2 and Figure 4.3 have been retained as per the process described in the patent and should be used for reference purpose only. While performing the simulations certain changes have been made to the process for either simplicity or improved productivity.

Since it is evident that Stage 2 and Stage 3 are the key stages of the process, the focus of this work is Stage 2 and Stage 3. Therefore, this work is based on starting with crude lactic acid and obtaining polymer grade lactic acid at the end of the process.

CHAPTER V

MODEL DEVELOPMENT

Some part of the following chapter has been reproduced from previous work **(Susmit S Bapat 2014)**

5.1 Introduction to Aspen Plus

Aspen Plus v8.2 **(AspenTech 2000)** has been used for model development. Aspen Plus is one of the most widely used chemical process simulation software packages used in industry as well as for academic purpose. It is short for Advanced System for Process Engineering and was developed in the 1970s by researchers at MIT's Energy Laboratory **(H. Scott Fogler 2001)** . It was then commercialized in the 1980s during the startup of the company AspenTech. Aspen Plus is a multi-purpose software for process engineers and can be used for flow simulation, equipment design, costing. The Aspen Plus built-in library has the capability to model chemical processing equipment like reactors, separators, pumps, columns and can handle single phase as well as multiphase systems including solids. Additionally it also has an extensive thermodynamic and physical parameter database.

5.2 Methodology

The following step-wise methodology was adopted while developing the model and simulating the lactic acid process in Aspen Plus that was described in Chapter 4.

5.2.1 Thermodynamic Model Selection

The majority of the process deals with highly polar components like lactic acid and methyl lactate, so the model must be based on activity coefficients. In addition, lactic acid and methyl lactate both display non-ideal behavior and the activity coefficient method is the best way to represent highly non-ideal liquid mixtures at low pressures which again indicates the requirement of an activity coefficient model. Therefore, initially the NRTL thermodynamic model was used as the thermodynamic property model for this process. But, the NRTL property model works well only for the vapor phase predictions. Hence, the NRTL-Hayden O'Connell property model was selected which provides accurate predictions for both phases in VLE. Following are the binary parameters used from the Aspen Plus database:

Table 5.1: Binary parameters for the methanol, water and methyl lactate system obtained from Aspen Plus database

Component i Component j Temperature units Source	METHANOL WATER K VLE-HOC	METHANOL Me-LACT K VLE-HOC	WATER Me-Lact K VLE-HOC
AIJ	-2.6311	-3.8591	3.3293
AJI	4.8683	7.4858	-1.9763
BIJ	838.5936	975.377	-723.8881
BJI	-1347.527	-2151.8792	609.8886

5.2.2 Unit Operation Model Selection in Aspen Plus

The next step in model development was to select the appropriate unit operation model based on the equipment information available and the required output. The unit operation models in Aspen Plus are used to mimic actual pieces of equipment like reactors, distillation columns or pumps **(AspenTech 2000)** . Major equipment details are briefly discussed in section 5.2.1 and unit operation model selection is described in section 5.2.2. The equipment information is useful in selecting the appropriate unit operation model in Aspen Plus.

5.2.2.1 Major Equipment Used

5.2.2.1.1 Bubble Column Reactor (Reactive Distillation Column)

In the lactic acid process, the reactive distillation column which facilitates the production of methyl lactate has been modelled as bubble column reactor. It is basically a cylindrical tray column having a sparger/ gas distributor at the bottom **(Kantarci, Borak et al. 2005)** . As this reactive distillation process is based on the efficient reaction between the liquid and gaseous phases, the gaseous phase is sparged in the form of bubbles from the bottom of the column and the liquid phase is distributed from the top. As such the bubble column reactor could be termed as a continuous counter current trickle phase reactor.

Bubble columns are extensively used as multiphase contactors and reactors in chemical and petrochemical industries. This is primarily because of their excellent heat and mass transfer properties leading to higher heat and mass transfer coefficients which in turn leads to reduction in cost. There are no moving parts as such and therefore the maintenance cost is minimal. Also, because of their compactness, the operating and maintenance cost decreases.

The most important advantage that the bubble column reactor offers is in terms of cost. It combines the functionality of a reactor and a separator column, thereby significantly reducing fixed cost as well as maintenance cost.

5.2.2.1.2 Hydrolysis Reactor

For the hydrolysis reaction, a glass lined stirred reactor with tori-spherical head was used. A turbine agitator with 6 flat blades was used for continuous stirring.

A continuous stirred tank reactor (CSTR) is basically a tank fitted with a mechanical agitator and some cooling mechanism **(Sinnott 2005)** . The CSTR is a versatile type of reactor and could range from a few liters to several thousand liters. They can handle both homogeneous as well as heterogeneous liquid-liquid and gas-liquid type of reactions. In a CSTR, the mass transfer and heat transfer can be very well controlled because the degree of agitation can be maneuvered to suit the requirement. Therefore, it is specially used when high heat and mass transfer rates are desired. Ideally, the composition in a CSTR remains constant throughout the reactor. However, the composition may not be the same if the reactor is not a well-mixed one.

5.2.2.2 Unit Operation Model Selection

5.2.2.2.1 RadFrac

RadFrac was used to model the bubble column reactor which facilitates the reactive distillation process. The RadFrac model is used for rigorous fractionation, mainly for two or three phase vapor-liquid fractionation. Another advantage of RadFrac is the fact that it can handle chemical reactions, which is the case for reactive distillation column and also RadFrac can deal with strong liquid phase non-ideality.

5.2.2.2.2 RStoich

The hydrolysis reactor is modeled using the RStoich reactor.

RStoic is generally used to model a reactor when:

1) Reaction kinetics data is unavailable or is insignificant.
2) Reaction stoichiometry is known.
3) Extent or conversion of the reaction can be specified

As both conversion as well as stoichiometry was known for the hydrolysis reaction, RStoich was selected to simulate the hydrolysis reactor.

5.2.2.2.3 Distl

Distl is essentially a shortcut distillation model which utilizes the Edmister approach (reference) to model the separation of inlet stream into two products. The following details need to be specified:

- Number of theoretical stages
- Reflux ratio
- Overhead product rate

Distl was used to simulate the methyl lactate purifier (Separat 1)

5.2.2.2.4 Sep 2

Sep2 separates the inlet stream into two outlet streams with specific split fraction. It can be used specially when component purity or recovery is known but the details of the separation are either unknown or unimportant. In the lactic acid process the separator used to isolate pure methyl lactate (Separat 2) and the separator used to separate out pure lactic acid has been simulated using Sep2.

5.2.3 Process Flow Diagram (PFD) Generation

Based on the unit operation model selection, a basic process flow diagram (PFD) is generated in Aspen Plus$^{®}$ (Figure 5.1). It can be noted that this is the configuration devised during the initial synthesis phase. After LCA studies and economic analysis, a revised, more efficient process flow configuration has been developed which is described in later chapters.

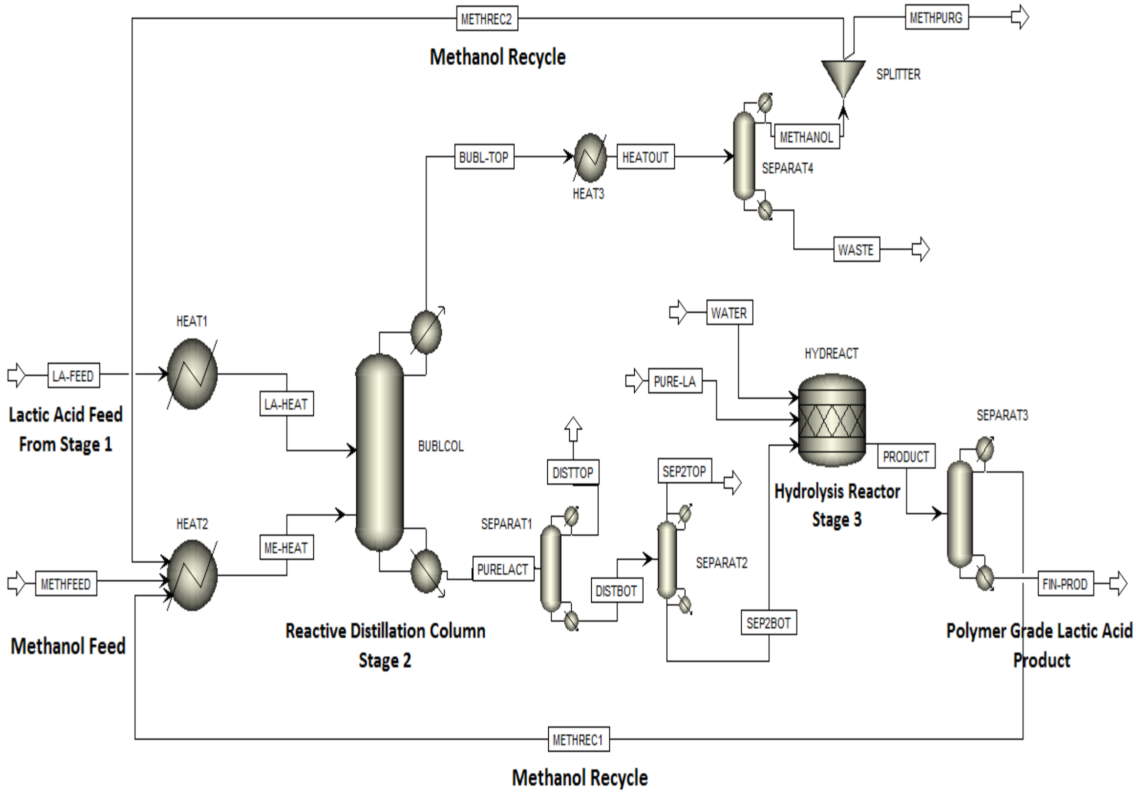


Figure 5.1: Process flow diagram developed in Aspen Plus for the manufacture of polymer grade lactic acid

5.2.4 Sensitivity Analysis

A sensitivity analysis is a technique available in the Aspen Plus software which can be used to ascertain the effects of certain parameters on significant process variables. Alternatively, it can be described as a tool for determining how a process reacts to varying key operating and design variables. Thus, it can be used to obtain optimum process conditions. In this technique different process parameters can be varied independently or simultaneously to study their effect on process variables like mass/mole fraction of desired product (mass/mole purity). Sensitivity analysis is also useful for the following:

1) To perform "what if" studies without actually affecting the simulation

2) To verify whether the solution to a design specification lies within the range of the manipulated variable
3) To perform simple process optimization. It should be noted that sensitivity analysis cannot be used only for multi-objective optimization.

In this work, a sensitivity analyses has been performed for several objective variables including the bubble column reactor (reactive distillation column) and separator parameters- number of stages, distillate to feed ratio, reflux ratio, feed stage; hydrolysis reactor parameters – temperature, pure lactic acid flow, distilled water flow; methanol recycle split ratio as shown in Table 5.2. As can be observed from the table, methyl lactate and lactic acid purity (mass fraction) are the main objective variables. The sensitivity analyses were performed in a systematic manner for each of the major equipment – Bubble Column Reactor, Hydrolysis Reactor, Lactic Acid Separator (Separator 3), Methyl Lactate Separator (Separator 1), Methanol Recycle Splitter, Heater 1, and Heater 2. The process variables were varied to study their effect on objective variables. Table 5.2 also illustrates the summary of the sensitivity analyses conducted and their results. The detailed tabulated results of the sensitivity analyses are provided in Table 5.5 through 5.10.

It can be noted from Table 5.2 that the distillate to feed ratio has a significant effect on purity in the bubble column reactor as well as in both of the separators (Separator 1 and Separator 3). On the other hand, the reflux ratio and number of stages do not have any significant change on purity in any of the three units. Purity is sensitive towards methanol feed location in the bubble column reactor but is not affected by the feed location in either of the two separators.

It was observed that methyl lactate purity increases with an increase in methanol feed stage up to stage no. 15 after which it marginally decreases (Figure 5.2). This observation was expected because as the methanol feed stage increases (column stage number increases from top to bottom), the contact time for methanol and lactic acid increases, thereby increasing mass transfer, subsequently resulting in higher purity of methyl lactate. Along with the sensitivity analysis, the bubble column temperature profile was obtained. The study of profile variations helped in determining the optimum feed stage for the methanol feed stream (Figure 5.3).

Table 5.2: Summary of sensitivity analyses performed

No.	Equipment	Process Variables	Objective Variables (Sensitivity)	Base Case Process Variable	Process Variable Variation Range	Objective Variable Variation Range	Optimum Process Variable Value
1	Lactic Acid Separator (Separator 3)	No. of stages	Lactic Acid Purity (Mass Fraction)	9	9 - 11	0.99 – 0.99	9
2		Distillate to feed		*0.5*	*0.5 - 0.7*	*0.83 – 0.99*	*0.65*
3		Reflux Ratio		1	1 - 1.3	0.99 – 0.99	1
4		Feed Location		5	4 - 5	0.99 – 0.99	5
5	Hydrolysis Reactor	Temperature (K)		373	313 - 413	0.62 – 0.62	373
6		Pure Lactic Acid Flow (kg/hr)		0.015	0.01 – 0.05	0.62 – 0.62	0.01
7		Distilled Water Flow (kg/hr)		2	1.8 – 2.2	0.65 – 0.59	2
8	Bubble Column Reactor	No. of stages	Methyl Lactate Purity (Mass Fraction)	17	5 - 17	0.63 – 0.64	17
9		Distillate to feed		*0.7*	*0.4 – 0.81*	*0.47 - 0.74*	*0.8*
10		Reflux Ratio		2	1 - 4	0.64 – 0.64	1

11		Methanol Feed Stage		*15*	*13 - 17*	*0.59 – 0.64*	*15*
12	Heater 1	Temperature (K)		376	323 - 413	0.64 – 0.64	376
13	Heater 2	Temperature (K)		392	343 - 433	0.64 – 0.64	392
14	Splitter	Methanol Recycle Split Fraction		1	0.15 - 1	0.74 – 0.64	1
15	Methyl Lactate Separator (Separator 1)	No. of stages		10	10 - 12	0.87 – 0.87	10
16		Distillate to feed		*0.6*	*0.1 – 0.6*	*0.67 – 0.87*	*0.6*
17		Reflux Ratio		1.5	1 - 3	0.87 – 0.87	1
18		Feed Location		5	3 - 8	0.86 – 0.87	6

5.2.5 Process Parameter Optimization

Using the data from sensitivity studies, optimum process conditions were determined for each major unit. The optimum was based on achieving the maximum purity for methyl lactate and lactic acid with minimum chemical inventory. In case of temperatures, if no significant change in purity was observed, the base case values from the patent have been used. In all other cases where no significant change in purity was observed, process conditions understandably leading to least costs (capital and operating) and energy consumption, were used.

Stream results tables listing important streams with their process parameters for both the base case and optimized case have been illustrated in Table 5.3 and Table 5.4. Comparing the two tables the improvements in product purity in the optimum case becomes evident. Note that the stream names used are as specified in the process flow diagram.

Table 5.3: Stream results table (Base Case)

Parameter(↓) / Stream(→)	**LA-FEED**	**METHFEED**	**PURELACT**	**DISTBOT**	**SEP2BOT**	**METHREC1**	**PRODUCT**	**FIN-PROD**
Temperature (K)	298.1	298.1	379	393.4	393.4	343.2	373.1	413.7
Pressure (atm.)	1	1	1	1	1	1	1	1
Mass Flow (kg/hr)	10.5	7.5	11.29	8.171	6.921	2.445	8.936	6.491
Mass Fraction (Mass Purity)								
Lactic Acid	0.571		0.001	0.001		trace	0.603	*0.83*
Methyl Lactate			0.613	*0.845*	*0.997*	147 PPM	0.077	0.106
Methanol		0.996	0.003	62 PPB		0.782	0.214	165 PPM
Water	0.381	0.004	0.339	0.093	0.003	0.218	0.106	0.063
Others	0.05		0.045	0.059				

Note: 1) Italicized numbers depict variables with significant variations over the range.
2) Listed row headers depict streams and column headers depict parameters (As shown by arrows)

Table 5.4: Stream results table (Optimized Case) (Later referred to as Configuration 1)

Parameter(↓) / Stream(→)	**LA-FEED**	**METHFEED**	**PURELACT**	**DISTBOT**	**SEP2BOT**	**METHREC1**	**PRODUCT**	**FIN-PROD**
Temperature (K)	298.1	298.1	382.4	414.6	414.6	346.6	373.1	489.8
Pressure (atm)	1	1	1	1	1	1	1	1
Mass Flow (kg/hr)	10.5	7.5	11.056	8.625	8.072	4.129	10.122	5.993
Mass Fraction (Mass Purity)								
Lactic Acid	0.571		730 PPM	935 PPM		0.079	0.624	*1*
Methyl Lactate			0.733	*0.933*	*0.997*	0.195	0.08	41 PPM
Methanol		0.996	0.005	302 PPB		0.54	0.22	4 PPB
Water	0.381	0.004	0.216	0.009	0.003	0.186	0.076	57 PPB
Others	0.05		0.045	0.059				

Note: 1) Italicized numbers depict variables with significant variations over the range.
2) Listed row headers depict streams and column headers depict parameters (As shown by arrows)

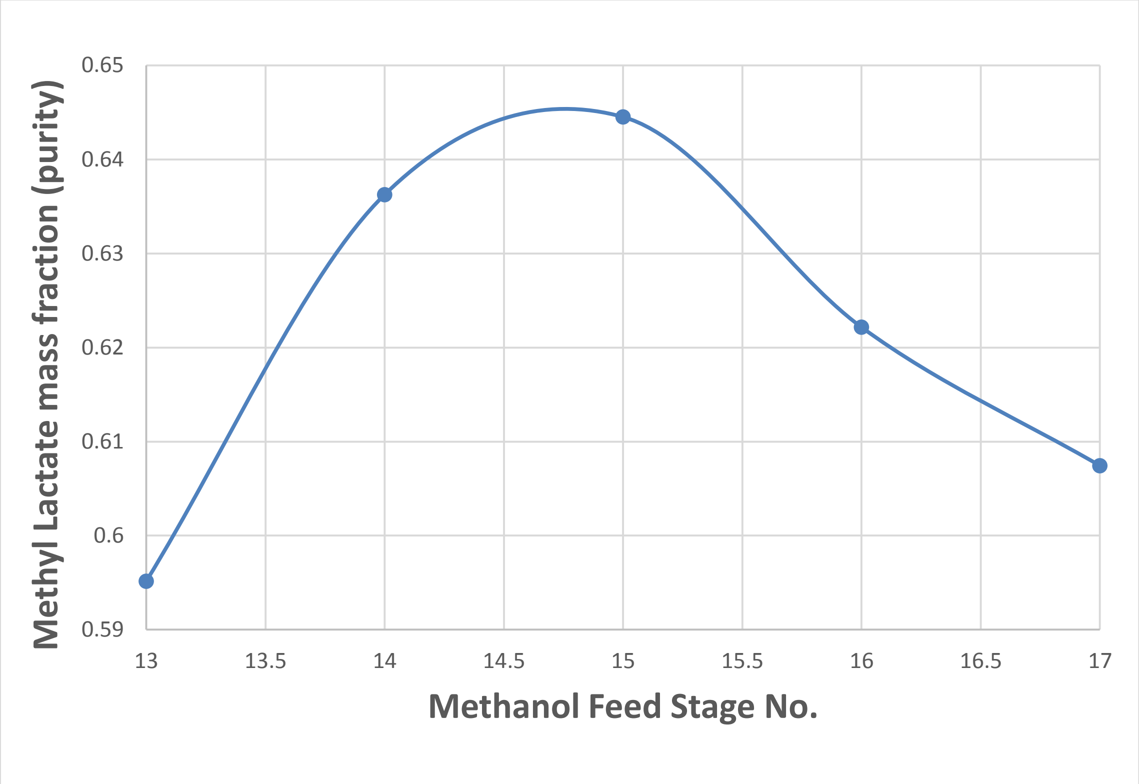


Figure 5.2: Sensitivity analysis results illustrating the effect of methanol feed stage variance in the bubble column reactor.

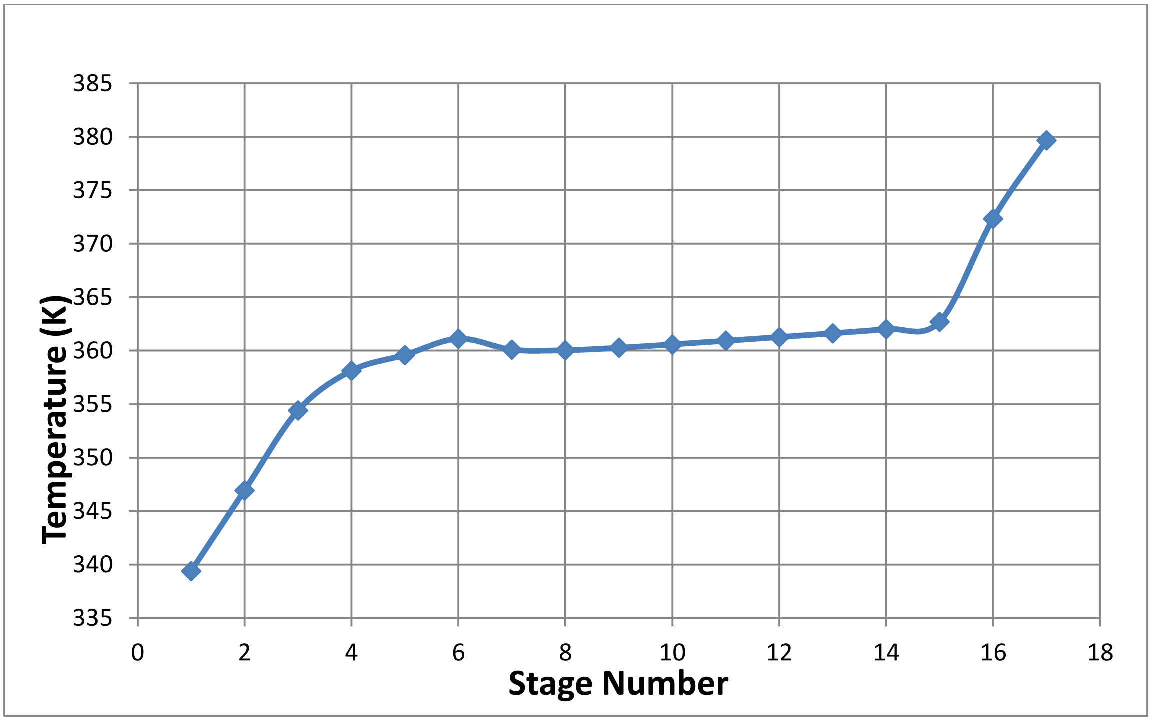


Figure 5.3: Temperature profile for the bubble column reactor (base case).

Table 5.5: Overall results table (Optimized Case)

Parameter / Stream→ ↓	LA-FEED	METHFEED	PURELACT	DISTBOT	SEP2BOT	METHREC1	PRODUCT	FIN-PROD
Temperature K	298.1	298.1	379.7	396.4	396.4	346.5	373.1	489.8
Pressure atm	1	1	1	1	1	1	1	1
Vapor Frac	0	0	0	0	0	0	0.293	0
Mole Flow kmol/hr	0.294	0.235	0.301	0.12	0.079	0.123	0.19	0.066
Mass Flow kg/hr	10.5	7.5	12.533	9.241	8.078	4.111	10.093	5.983
Enthalpy Gcal/hr	-0.027	-0.013	-0.027	-0.015	-0.012	-0.008	-0.019	-0.01
Mass Fraction								
LACTIC ACID	0.571		0.001	0.002		0.075	0.623	1
METHYL LACTATE			0.645	0.872	0.997	0.196	0.08	41 PPM
METHANOL		0.996	0.003	53 PPB		0.543	0.221	4 PPB
WATER	0.381	0.004	0.312	0.073	0.003	0.186	0.076	57 PPB
SULFURIC ACID	0.01		0.008	0.011				
C2H4O-01	0.01		0.008	0.01				
C2H2O-01	0.01		0.008	0.011				
C4H6O-01	0.01		0.008	0.011				
C4H4O-01	0.01		0.008	0.011				
Mass Flow kg/hr								
LACTIC ACID	6		0.015	0.015		0.307	6.289	5.982
METHYL LACTATE			8.077	8.057	8.057	0.805	0.806	< 0.001
METHANOL		7.47	0.036	trace		2.232	2.232	trace
WATER	4	0.03	3.904	0.677	0.021	0.766	0.766	trace
SULFURIC ACID	0.1		0.1	0.1				
C2H4O-01	0.1		0.1	0.093				
C2H2O-01	0.1		0.1	0.1				
C4H6O-01	0.1		0.1	0.1				
C4H4O-01	0.1		0.1	0.1				

Table 5.6: Sensitivity analyses results over **Separator 3** for **Lactic acid (LA) mass fraction** by varying Distillate to feed ratio, Reflux Ratio, Feed Location and No. of Stages.

Sensitivity Analyses - Separator 3 (Aspen Model: Distl)							
Distillate to Feed(D:F)		**Reflux Ratio (RR)**		**Feed Location (F-LOC)**		**No. of Stages (NSTAGE)**	
D:F	LA Mass Frac	RR	LA Mass Frac	F-LOC	LA Mass Frac	N-STAGE	LA Mass Frac
0.5	0.830	1	0.999	4	0.999	9	0.999
0.55	0.851	1.1	0.999	5	0.999	10	0.999
0.6	0.873	1.2	0.999			11	1.000
0.65	0.999	1.3	0.999				
0.7	0.999						

Table 5.7: Sensitivity analyses results over **Hydrolysis Reactor** for **Lactic acid (LA) mass fraction** by varying Reactor Temperature, Pure Lactic Acid Inlet Flow Rate and Distilled Water Flow rate

Sensitivity Analyses - Hydrolysis Reactor (Aspen Model: RStoich)					
Reactor Temperature		**Pure Lactic Acid Inlet Flow Rate**		**Water Flow Rate**	
Temperature (K)	LA Mass Frac	Pure Lactic Acid Mass Flow Rate (KG/HR)	LA Mass Frac	Water Mass Flow Rate (KG/HR)	LA Mass Frac
313	0.623	0	0.622	1.8	0.650
323	0.623	0.01	0.622	1.85	0.644
333	0.623	0.015	0.623	1.9	0.637
343	0.623	0.02	0.623	1.95	0.630
353	0.623	0.03	0.624	2	0.623
363	0.623	0.04	0.624	2.05	0.615
373	0.623	0.05	0.625	2.1	0.607
373.15	0.623			2.15	0.599
383	0.623			2.2	0.590
393	0.623				
403	0.623				
413	0.623				

Table 5.8: Sensitivity analyses results over **Bubble Column Reactor** for **Methyl Lactate (Me-La) mass fraction** by varying No. of Stages, Distillate to feed ratio, Reflux Ratio and Methanol Feed Location

Sensitivity Analyses - Bubble Column Reactor (Aspen Model: RadFrac)							
No. of Stages (NSTAGE)		**Distillate to Feed(D:F)**		**Reflux Ratio (RR)**		**Methanol Feed Location (F-LOC)**	
NSTAGE	Me-La Mass Fraction	D:F	Me-La Mass Fraction	RR	Me-La Mass Fraction	F-LOC	Me-La Mass Fraction
5	0.630	0.4	0.473	1	0.641	13	0.595
6	0.631	0.45	0.501	1.2	0.644	14	0.636
7	0.628	0.5	0.531	1.4	0.645	15	0.645
8	0.628	0.55	0.559	1.6	0.645	16	0.622
9	0.627	0.6	0.584	1.8	0.645	17	0.607
10	0.627	0.65	0.612	2	0.645		
11	0.627	0.7	0.645	2.2	0.644		
12	0.627	0.75	0.684	2.4	0.644		
13	0.627	0.8	0.731	2.6	0.644		
14	0.627	0.81	0.740	2.8	0.643		
15	0.627			3	0.643		
16	0.640			3.2	0.643		
17	0.645			3.4	0.642		
				3.6	0.642		
				3.8	0.642		
				4	0.641		

Table 5.9: Sensitivity analyses results over **Bubble Column Reactor** for **Methyl Lactate (Me-La) mass fraction** by varying Heater 1 (Lactic Acid Feed) Temperature, Heater 2 (Methanol Feed) Temperature

Sensitivity Analyses - Bubble Column Reactor (Aspen Model: RadFrac)				
Heater 1 (Lactic Acid Feed) Temperature			**Heater 2 (Methanol Feed) Temperature**	
Heat 1 Temp (K)	Me-La Mass Fraction		Heat 2 Temp (K)	Me-La Mass Fraction
323	0.644		343	0.644
333	0.644		353	0.645
343	0.644		363	0.645
353	0.644		373	0.645
363	0.644		383	0.645
373	0.645		392.15	0.645
376.15	0.645		393	0.645
383	0.645		403	0.645
393	0.645		413	0.645
403	0.645		423	0.645
413	0.645		433	0.645

Table 5.10: Sensitivity analyses results over **Splitter** for **Methyl Lactate (Me-La) mass fraction** by varying methanol split fraction

Sensitivity Analyses - Splitter (Aspen Model: FSplit)	
Methanol Split fraction	**Me-La Mass Fraction**
0.15	0.741
0.2	0.738
0.25	0.734
0.3	0.729
0.35	0.725
0.4	0.720
0.45	0.714
0.5	0.709
0.55	0.703
0.6	0.698
0.65	0.692
0.7	0.685
0.75	0.679
0.8	0.673
0.85	0.666
0.9	0.659
0.95	0.652
1	0.645

Table 5.11: Sensitivity analyses results over **Separator 1** for **Methyl Lactate (Me-La) mass fraction** by varying Distillate to feed ratio, Reflux Ratio, Feed Location and No. of Stages

Sensitivity Analyses - Separator 1 (Aspen Model: Distl)							
Distillate to Feed(D:F)		**Reflux Ratio (RR)**		**Feed Location (F-LOC)**		**No. of Stages (NSTAGE)**	
D:F	Me-La Mass Frac	RR	Me-La Mass Frac	F-LOC	Me-La Mass Frac	N-STAGE	Me-La Mass Frac
0.1	0.675	1	0.870	3	0.861	10	0.872
0.15	0.690	1.1	0.871	4	0.869	11	0.872
0.2	0.706	1.2	0.871	5	0.872	12	0.872
0.25	0.723	1.3	0.871	6	0.873		
0.3	0.741	1.4	0.872	7	0.873		
0.35	0.760	1.5	0.872	8	0.873		
0.4	0.780	1.6	0.872				
0.45	0.801	1.7	0.872				
0.5	0.823	1.8	0.872				
0.55	0.847	1.9	0.872				
0.6	0.872	2	0.872				
		2.1	0.872				
		2.2	0.872				
		2.3	0.873				
		2.4	0.873				
		2.5	0.873				
		2.6	0.873				
		2.7	0.873				
		2.8	0.873				
		2.9	0.873				
		3	0.873				

5.2.6 Equipment Sizing

The next logical step for model development was equipment sizing using the simulation data and equipment information described earlier. Equipment sizing was carried out in Aspen Icarus Process Evaluator as explained in the following discussion:

5.2.6.1 Aspen Icarus Process Evaluator (IPE)

Aspen IPE is a software system provided by Aspen Technology, Inc. and can be termed as an extension of Aspen plus software used extensively for rigorous sizing calculations and economic analysis. Some of the information about IPE in the following paragraph has been reproduced from the course notes prepared by Dr. Robyn B. Nathanson and his peers at University of Pennsylvania **(Robyn B. Nathanson 2008)**:

IPE determines the capital expenditure, operating costs, and the profitability of proposed designs. Aspen IPE has an automatic, electronic expert system which links to process simulation programs. It is used to: (1) extend the results of process simulation, (2) generate rigorous size and cost estimates for processing equipment, (3) perform preliminary mechanical designs, and (4) estimate purchase and installation costs, indirect costs, the total capital investment, the engineering-procurement-construction planning schedule, and profitability analyses. Aspen IPE usually begins with the results of a simulation from one of the major process simulators (e.g., ASPEN PLUS, HYSYS, CHEMCAD, and PRO/II), it is noted that users can, alternatively, provide equipment specifications and request investment analysis without using the process simulators

In later chapters, IPE use for cost estimation will be described. Aspen Icarus works in tandem with Aspen Plus. As mentioned earlier, IPE utilizes the process simulation results generated from Aspen Plus and performs rigorous sizing calculations based on the Icarus database.

It is normally necessary to adapt the simulation file in two ways. First, to estimate equipment sizes, Aspen IPE usually requires estimates of mixture properties not needed for the material and energy balance, and phase equilibria calculations performed by the process simulators. For this reason, it is necessary to augment the simulation report files with estimates of mixture properties, such as viscosity, thermal conductivity, and surface tension, for the streams in the simulation flow sheet. Second, Aspen IPE requires specifications to estimate equipment sizes that are not determined by some of the approximate simulation models. This is the case, for example, when the DISTL and RSTOIC models are used in ASPEN PLUS. To circumvent this, these are replaced by more rigorous models, such as the RADFRAC and RPLUG models. This replacement can be viewed as the first step in computing equipment sizes and costs.

5.2.6.2 Equipment Sizing Results

Detailed equipment sizing results are provided in Table 4.1 through 4.4. Note that the tables have been categorized based on the type of equipment they describe.

Table 5.12: Equipment sizing results for heat exchangers (Bubble column condenser, Heat 1, Heat 2)

Heat Exchanging Equipment			
Name	**DHE TEMA EXCH BUBLCOL (Cond)**	**DHE TEMA EXCH HEAT1**	**DHE TEMA EXCH HEAT2**
Mapping	BUBLCOL	HEAT1	HEAT2
Heat transfer area [SF]	6.51	0.09	1.32
Front end TEMA symbol	B	B	B
Shell TEMA symbol	E	E	E
Rear end TEMA symbol	M	M	M
Tube design gauge pressure [PSIG]	60.304	110.304	110.304
Tube design temperature [DEG F]	250	377.8	377.8
Tube operating temperature [DEG F]	95	327.8	327.8
Tube outside diameter [INCHES]	1	1	1
Shell design gauge pressure [PSIG]	35.30	68.63	68.63
Shell design temperature [DEG F]	250	267.4	296.2
Shell operating temperature [DEG F]	149.73	217.4	246.2
Tube length extended [FEET]	20	20	20
Tube pitch [INCHES]	1.25	1.25	1.25
Number of tube passes	1	1	1
Number of shell passes	1	1	1

Table 5.13: Equipment sizing results for separation columns (Bubble column tower, Separat 1, Separat 3)

Separation Column (RADFRAC and Flash columns)			
Name	**DTW TRAYED BUBLCOL-tower**	**DTW TRAYED SEPARAT1**	**DTW TRAYED SEPARAT3**
Mapping	BUBLCOL-tower	SEPARAT1	SEPARAT3
Tray type	SIEVE	SIEVE	SIEVE
Vessel diameter [FEET]	1.5	1.5	1.5
Vessel tangent to tangent height [FEET]	56	36	32
Design gauge pressure [PSIG]	15	15	15
Design temperature [DEG F]	265.33	289.39	471.91
Operating temperature [DEG F]	225.40	260.08	421.91
Number of trays	22	12	10
Tray spacing [INCHES]	24	24	24
Molecular weight Overhead prod	43.77	18.61	33.89

Table 5.14: Equipment sizing results for separation columns (Separat 2)

Separator Column (Sep 2)	
Name	**DVT CYLINDER SEPARAT2**
Mapping	SEPARAT2
Liquid volume [GALLONS]	634.56
Vessel diameter [FEET]	3
Vessel tangent to tangent height [FEET]	12
Design gauge pressure [PSIG]	15
Design temperature [DEG F]	310.08
Operating temperature [DEG F]	260.08

Table 5.15: Equipment sizing results for Hydrolysis Reactor

Hydrolysis Reactor (RStoich)	
Name	**DAT REACTOR HYDREACT**
Mapping	HYDREACT
Liquid volume [GALLONS]	7.34
Vessel diameter [FEET]	2
Vessel tangent to tangent height [FEET]	5
Design gauge pressure [PSIG]	15
Design temperature [DEG F]	289.39

Table 5.16: Equipment sizing results for Bubble Column Reboiler

DRB U TUBE	
Name	**DRB U TUBE BUBLCOL-reb**
Mapping	BUBLCOL-reb
Heat transfer area [SF]	3.67
Tube design gauge pressure [PSIG]	110.304
Tube design temperature [DEG F]	377.8
Tube operating temperature [DEG F]	327.8
Tube outside diameter [INCHES]	1
Shell design gauge pressure [PSIG]	68.63
Shell design temperature [DEG F]	265.33
Shell operating temperature [DEG F]	215.33
Tube length extended [FEET]	20
Tube pitch [INCHES]	1.25
Tube pitch symbol	TRIANGULAR
Number of tube passes	2
Duty [MMBTU/H]	0.048
TEMA type	BKU

5.3 Summary

In this chapter, the steps for model development have been described. The lactic acid process described in Chapter 4 is the basis for process development. Aspen Plus is the process simulator that was used to carry out the simulation. Following is the step-wise methodology that was implemented to accomplish model development:

1) Thermodynamic Model Selection
2) Unit Operation Model Selection in Aspen Plus
3) Process Flow Diagram (PFD) Generation
4) Sensitivity Analysis
5) Process Parameter Optimization
6) Equipment Sizing

The first five steps were implemented in Aspen Plus while Equipment Sizing was carried out in Aspen IPE. The results obtained from process simulation in Aspen Plus and Equipment Sizing in Aspen IPE are the basis for further sustainability analysis and has been described in the following chapters.

CHAPTER VI

ECONOMIC ANALYSIS AND OPTIMIZATION

6.1 Project Economics

Although environmental and social aspects have been determined to be equally important while considering the sustainability index of a process, economics was and still is the considered to be the most important aspect. Even if a certain process is deemed to be viable in terms of design, companies will not consider any design as an option unless it is economically viable. In other words, money continues to drive process design and selection in industry **(El-Halwagi 2012)** .

Thus it becomes vital to study process economics which enables a chemical engineer to do the following as stated by **(El-Halwagi 2012)**):

- Evaluate feasibility of new projects
- Improve performance of existing processes
- Make design and operating decisions
- Compare alternatives
- Decide strategic directions for the company
- Establish sound policies for process and product objectives

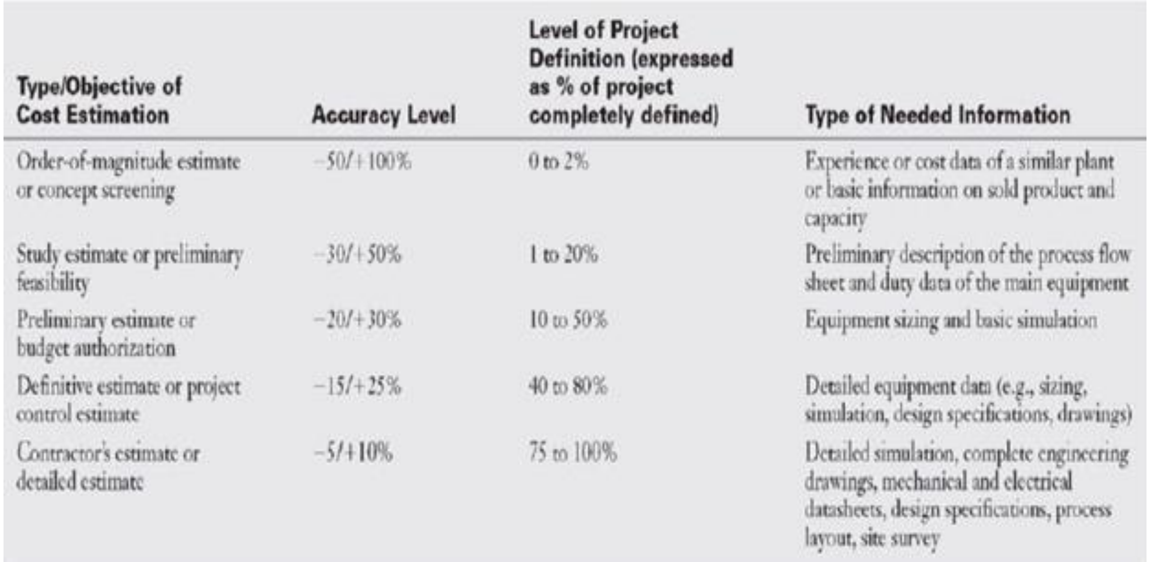
Generally, in any industrial setting, the economic analysis is used for a combination of the above factors in a step-wise manner. At an initial stage, a process engineer has to conduct a rough cost estimate to decide whether pursuing the process further is of any benefit. If the process is already being implemented then it could be improved further using economic optimization. When it comes to decision-making about different process configurations or alternative choice of equipment, cost analysis is the first thing to be considered.

There are two types of costs that need to be evaluated: capital costs and operating costs.

The capital cost is the cost entailed for to purchase process equipment, as well as the installation and also includes the expenses required for plant start-up. The expenses required to run the plant are termed as operating cost

Costing can be categorized based on the level of its accuracy as shown in Table 6.1:

Table 6.1: Costing Categories on basis of accuracy intended (Reproduced from **(El-Halwagi 2012))**



Type/Objective of Cost Estimation	Accuracy Level	Level of Project Definition (expressed as % of project completely defined)	Type of Needed Information
Order-of-magnitude estimate or concept screening	−50/+100%	0 to 2%	Experience or cost data of a similar plant or basic information on sold product and capacity
Study estimate or preliminary feasibility	−30/+50%	1 to 20%	Preliminary description of the process flow sheet and duty data of the main equipment
Preliminary estimate or budget authorization	−20/+30%	10 to 50%	Equipment sizing and basic simulation
Definitive estimate or project control estimate	−15/+25%	40 to 80%	Detailed equipment data (e.g., sizing, simulation, design specifications, drawings)
Contractor's estimate or detailed estimate	−5/+10%	75 to 100%	Detailed simulation, complete engineering drawings, mechanical and electrical datasheets, design specifications, process layout, site survey

The foremost thing to be considered here is to understand the accuracy level of cost estimate required at that particular stage of the project. For example, if the project is in its primitive stage and the initial screening of process alternatives is being done then a rough cost estimate would suffice. Alternatively, if the project is at a stage where a decision on whether to continue with it is to be made, a more detailed cost analysis is required. A rough estimate at this stage could lead to serious consequences.

6.1.1 Capital Cost Estimation

According to El-Halwagi **(El-Halwagi 2012)**, the capital cost or Total Capital Investment (TCI) of a process can be defined as the money needed to purchase and install the plant and all its ancillaries and to provide for the necessary expenses required to start up the process operation. It is further classified into two types of expenditures: *fixed capital investment (FCI)* and *working capital investment (WCI)*

$$TCI = FCI + WCI \qquad (6.1)$$

The FCI is the expenses incurred for the equipment, auxiliaries, acquiring and preparing the land, procuring and installing the control systems etc.

On the other hand, the **working capital investment** (WCI) can be defined as the money required for the operating expenditures up to the time when the product is sold as well as the expenses required to pay for raw materials inventories before production starts.

6.1.1.1 Equipment Cost Estimation

Equipment cost is the major contributor towards the capital investment in a project.

The following methods could be used to estimate the cost of individual pieces of equipment:

1. Manufacturer's quotation
2. Cost-analysis software (example: Aspen ICARUS)
3. Equipment capacity ratio with exponent **(El-Halwagi 2012)**

6.1.2 Operating Cost Estimation

As explained earlier, the operating cost consists of all of the continuous expenses required to run the plant. It includes raw material cost, utility cost, labor and maintenance cost etc. The estimation of each type of cost is explained in the following section.

6.1.2.1 Raw Material Cost

Based on the material balance data, the quantities of raw material is calculated. The unit price for each component can be obtained from specialized costing agencies (like ICIS) or from vendors (Sigma Aldrich etc.) in the form of price quotations.

6.1.2.2 Utility Cost

The utilities could be further divided into two types: material utilities and energy utilities

Material Utilities: These consist of all chemicals that are used in conjunction with reactants and products for various objectives. Solvents, catalysts, adsorbents, surfactants etc. are included in this category. Although generally these materials are required in small quantities and are regenerated in the process, the cost of make-up needs to be considered even for small losses.

Energy Utilities: Fuel, water, steam, cooling/heating air, other coolants (oil etc.) etc. are categorized as energy utilities. The quantities for energy utilities are obtained from the energy balance. The unit cost depends on the location and quantity of the utility and may vary significantly.

6.1.2.3 Labor Cost

Labor costs depend on several factors including location, hourly wages, shift timings, number of shifts etc. The labor costs vary significantly from one country to another. It is primarily controlled by the prevailing government labor policies in that particular country. The U.S Bureau of Labor website (http://www.bls.gov/) provides an insight into government policies in the United States.

6.1.2.4 Maintenance Cost

Maintenance could be further categorized into preventive maintenance and responsive maintenance. Preventive maintenance ensures that day-to-day operations are carried out in an efficient and safe manner. Responsive maintenance deals with maintenance work needed to remediate certain situations that might occur during plant operation. Maintenance costs mainly consists of costs for labor and maintenance equipment and material and therefore may vary distinctly with location and conditions in general.

6.1.2.5 Production Cost

The production cost is that portion of the operating cost that includes expenses needed to run the process as well as the cost of the capital investment needed for the process equipment and ancillary systems.

6.2 Cost Estimation for Lactic Acid Process

For the lactic acid process, a detailed cost analysis was performed using the Aspen Process Economic Analyzer (APEA) **(AspenTech 2012).** The Aspen Plus Integrated Analysis combines the functionalities of Aspen Plus and the Aspen Process Economic Analyzer (APEA). The analyzer uses the process parameters generated by the Aspen simulator for the subsequent cost analysis. Based on the simulation results it maps the unit operation with the model equipment in Aspen Plus and performs costing estimates. Alternatively, it allows the user to carry out a customized mapping of equipment. The estimates are based on the Aspen Plus and Aspen Icarus equipment database. The integrated analyzer also allows the user to change equipment parameters such as Material of Construction (MOC), equipment dimensions etc. as well utility parameters, if the user has them readily available. This tool is particularly useful for process engineers working in industry because it allows them to optimize their design more efficiently in a shorter duration.

The integrated economics workflow enables users to include cost estimation into the process design calculations. This offers a more holistic view and is helpful especially while screening alternatives. The integrated analyzer also allows the user to make a more informed decision based on technical, safety, environmental and economic factors, which is essentially the basis for sustainable process design.

Depending on the level of process data available and/or level of control that the user would like to exercise over the economic analysis, “steps could be detailed or can be skipped in favor of a quick, automatic evaluation based on default-assigned “mapping” and sizing algorithms” as described in the Aspen manual (AspenTech, 2013)

Thus, the utility of this integrated analysis lies in the fact that it gives the freedom to the user to carry out studies ranging from a very crude, rudimentary evaluation to a very accurate, rigorous one.

6.2.1 Cost Estimation Methodology

The steps to perform an economic analysis are as follows:

1) Obtain a converged simulation:

   A converged simulation is required to proceed to the integrated economics step of the workflow.

2) Map:

   The second step in the workflow is to map the unit operations from the simulation to Aspen Process Economic Analyzer. The analyzer has the ability to map the equipment by default, utilizing the best-engineering solution within the available software package. As mentioned earlier, the software allows the user to modify the default mapping based on user knowledge and/or experience. In the lactic acid process the reactive distillation column (RadFrac unit operation in Aspen Plus) has been mapped into the economics software as a collection of equipment models, including a column, pumps and some other complementary equipment items.

There might be some unit operations which cannot be correlated to actual equipment available in the Aspen Plus environment. In these cases the analyzer provides placeholders, or 'C' units. For example, a splitter is actually a T-junction in the piping and would not contribute towards equipment cost. Both the splitters in the lactic acid process have been mapped to 'C' units.

3) Size

The integrated analyzer has the capability to use the simulation run data to perform equipment sizing. Missing data is estimated according to basic principles and common practice. The user can also override estimate sizes in the equipment grid. This step can be ignored in case of a quick but less accurate estimate.

4) Evaluate

The evaluation can be performed only after the mapping and sizing is done. If not, the user is directed to mapping, and the sizing is done automatically using estimations as explained earlier.

5) View Equipment

The Results Summary – Equipment form provides the overall results of the evaluation. The 'Summary' tab lists the estimated total capital cost, operating cost and utility cost.

The estimated cost and sizing information for each equipment in the plant is summarized in the 'Equipment' tab. Details for each unit type (heat exchangers, pumps, columns etc.) are displayed under a separate tab. Equipment material, dimensions, choice of auxiliary equipment can be reviewed and edited through this tab if more accurate data is available.

6) Investment Analysis

   One of the best features of this integrated approach is the investment analysis. It is an economic summary of the project in MS Excel format. If the stream costs have been fed initially, an estimated Return on Investment is displayed and reported. This economic analysis is in line with any economic analysis carried out in the process industry and provides Total Project Capital Cost, Total Operating Cost, Total Raw Materials Cost, Total Products Sales, Total Operating Labor and Maintenance Cost, Total Utilities Cost along with a detailed cash flow report.

The workflow described above was implemented for the lactic acid process. First, a converged simulation was obtained in Aspen Plus v8.2. It should be noted that the individual stream price needs to be entered before the simulation is run. The stream prices were calculated in MS Excel based on the material balance and component costs. Table 6.2 illustrates the stream prices used. It can be noted that price for the product is significantly high and the reason for that is the high purity (99% by wt.) product obtained. Table 6.3 lists the individual component prices based on the available source references. The data has been shown in the form that it was obtained from the source. Appropriate unit changes (mass to volume conversion or vice-versa) have been carried out while calculating stream prices.

Table 6.2: Stream price data

Stream	**Price (USD/kg)**
LA-FEED	0.6790
FIN-PROD	40.0000
METHFEED	0.3482
PURE-LA	40.0000
WATER	0.5082
DISTTOP	0.5082
SEP2TOP	0.5082
WASTE	0.3837

Table 6.3: Component price data

Chemical	**Grade/Composition**	**Price (weight/volume basis)**	**Reference Source**
Lactic Acid	88% (Food Grade)	0.72-0.85 USD / lb	http://www.icis.com/chemicals/channel-info-chemicals-a-z/
Sulfuric acid	93% purity	67 USD / ton	http://www.icis.com/chemicals/channel-info-chemicals-a-z/
Methanol	US Gulf, spot dom. Barge	0.94-2.73 USD / Gallon	http://www.icis.com/chemicals/channel-info-chemicals-a-z/
Calcium Lactate	98%	1 - 3 USD / Kilogram	http://www.alibaba.com/product-gs/521469783/L_calcium_lactate.html
Methyl Lactate	Food Grade	2-7 USD / Kilogram	http://www.alibaba.com/showroom/methyl-lactate-price.html
Water	Distilled Water	3.7 USD / Gallon	http://www.enasco.com/product/SB07177%28LM%29M

6.2.2 Cost Estimation Results

As described earlier, the Aspen Process Economic Analyzer extracts the simulation results from the converged simulation. The next logical step was to proceed to the Economic Analysis. Mapping, sizing and evaluation was carried out in the manner described earlier. The equipment specifications like material specification and sizing dimensions were modified wherever data was available. The Investment Analysis feature of the Process Analyzer provided a detailed economic analysis of the process.

While evaluating various process configurations in terms of economics, two configurations came forward as the best possible options. A more detailed analysis was therefore carried out for these two configurations to evaluate their advantages and shortcomings. Configuration 1 has been shown in Figure 1 and configuration 2 is depicted in Figure 2. It can be seen from the two figures that there is only a minor difference in the two configurations. Configuration 2 is devoid of the separator column which purifies the methanol before it is recycled back to the feed and the preheater before the separator column. The separator in configuration 1 separates the methanol from water and other impurities and therefore increases the purity of methyl lactate produced in the bubble column reactor. However, the separator and the heater come at a cost and therefore it is a case of trade-off between quality and economy as is the situation in most industrial settings. Table 6.4 provides the brief results of the economic analysis of the two configurations. Please note that the only difference between the two configurations is the separator column and the preheater as discussed and therefore the variations in the cost can be attributed directly to the inclusion/exclusion of the separator column.

Table 6.5 through Table 6.12 lists the key data obtained from the Investment Analysis for Configuration 2. Additional Investment Analysis data for configuration 2 and extensive Investment Analysis data for configuration 1 has been included in Appendix.

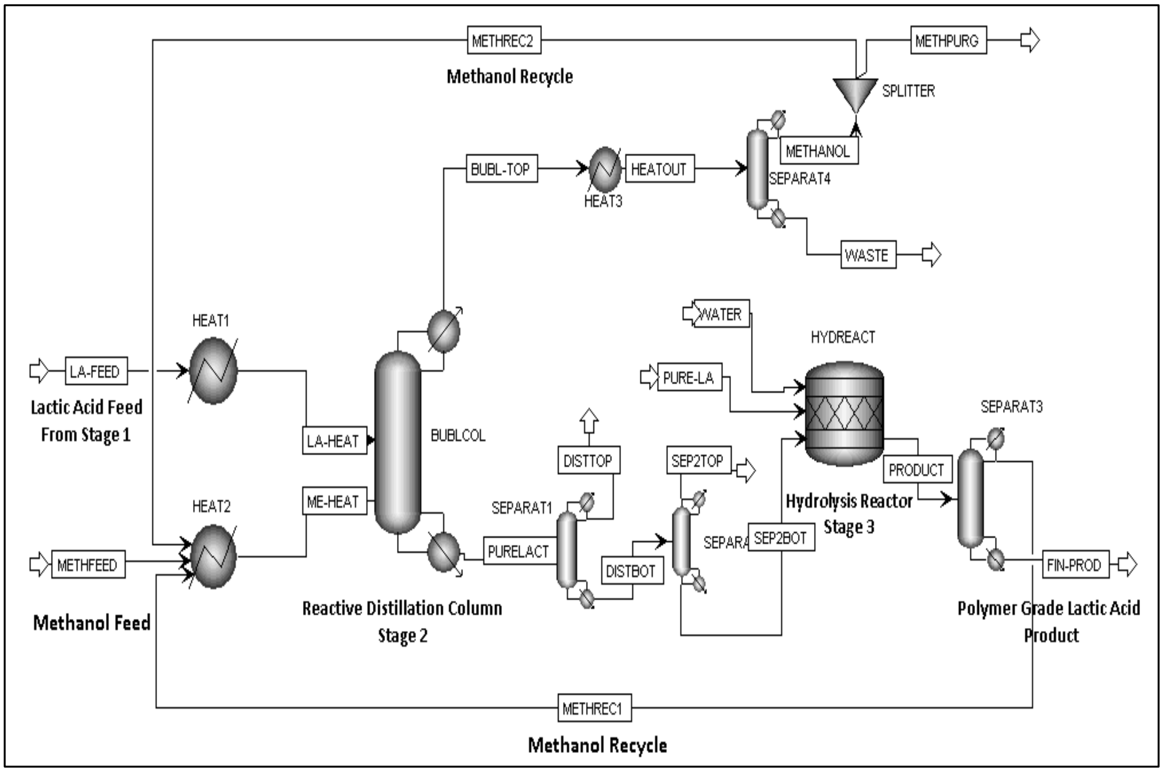


Figure 6.1: Configuration 1 which includes the separator column (Separat4) and preheater (Heat3) for methanol purification before recycle

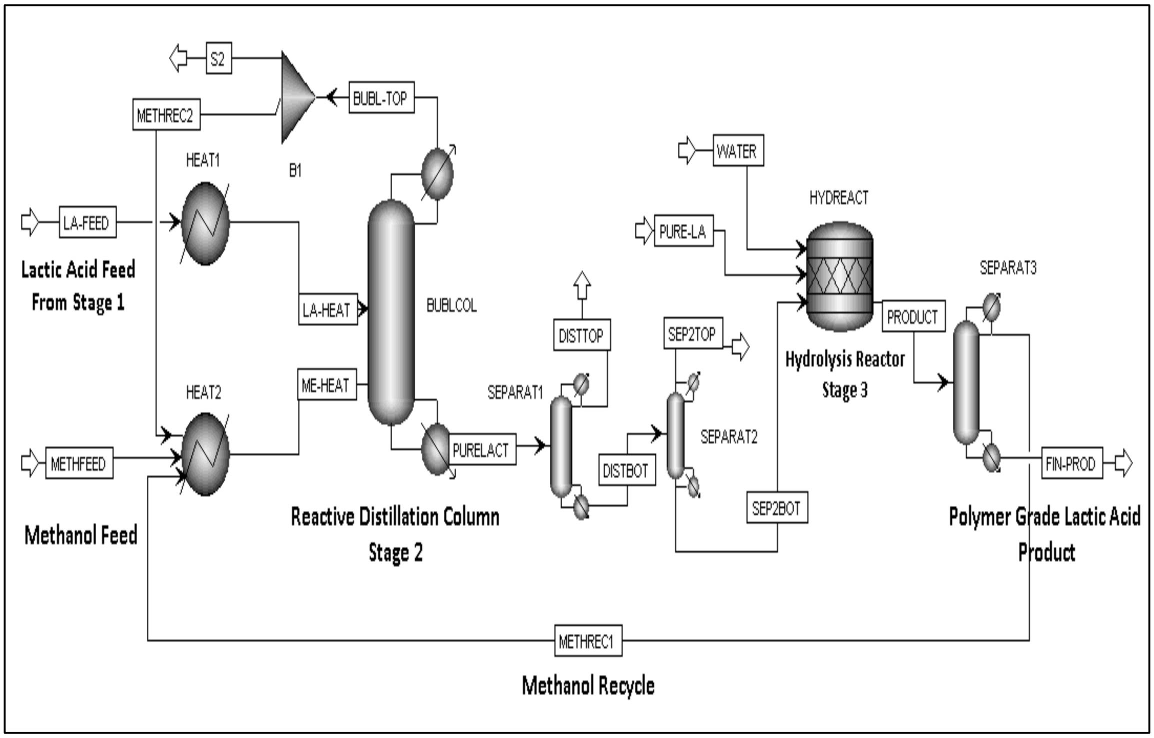


Figure 6.2: Configuration 2 which excludes the methanol separator column and preheater

Table 6.4: This table shows the results of an economic analysis conducted on the two configurations

Configuration	Total Project Capital Cost (USD)	Total Operating Cost (USD per year)	Total Raw Materials Cost (USD per year)	Total Utilities Cost (USD per year)	Total Product Sales (USD per year)	Payback Period (Years)
Configuration 1	5,753,800	1,918,520	246,500	41,659	4,743,180	**6.28**
Configuration 2	4,689,640	1,913,990	246,500	40,422	4,723,020	**4.59**

Table 6.4 clearly indicates the difference in terms of the total capital cost. Configuration 1 costs 57,538,000 USD as initial investment as compared to 46,896,400 USD. The difference can be mainly credited to the cost due to the additional separator column and the preheater in Configuration 1 as explained earlier. Consequently, the

payback period goes down from 6.28 years to 4.59 years due to the decreased total cost. It can also be observed that there is a slight decrease in the total operating cost and total product sales in Configuration 2. This decrease is due to the fact that less methanol per unit mass is recycled back to the bubble column and therefore less methyl lactate is formed leading to lesser production of pure lactic acid.

Table 6.5: Project Economic Summary for Configuration 2

Cost Type	**Value**	**Units**
Total Project Capital Cost	4,689,640	USD
Total Operating Cost	1,913,990	USD/Year
Total Raw Materials Cost	246,500	USD/Year
Total Utilities Cost	40,421.7	USD/Year
Total Product Sales	4,723,020	USD/Year
P.O. Period	4.59	Year

Table 6.6: Project Cash flow Details

ITEM	**Value**	**Units**
TW (Number of Weeks per Period)	52	Weeks/period
T (Number of Periods for Analysis)	20	Period
DTEPC (Duration of EPC Phase)	0.38	Period
DT (Duration of EPC Phase and Startup)	0.77	Period
WORKP (Working Capital Percentage)	5	Percent/period
OPCHG (Operating Charges)	25	Percent/period
PLANTOVH (Plant Overhead)	50	Percent/period
CAPT (Total Project Cost)	4.69E+06	Cost
RAWT (Total Raw Material Cost)	246500	Cost/period
PRODT (Total Product Sales)	4.72E+06	Cost/period
OPMT (Total Operating Labor and Maintenance Cost)	851398	Cost/period
UTILT (Total Utilities Cost)	40421.7	Cost/period
ROR (Desired Rate of Return/Interest Rate)	20	Percent/period
AF (ROR Annuity Factor)	5	
TAXR (Tax Rate)	40	Percent/period
IF (ROR Interest Factor)	1.2	
ECONLIFE (Economic Life of Project)	10	Period
SALVAL (Salvage Value (Percent of Initial Capital Cost))	20	Percent

DEPMETH (Depreciation Method)	Straight Line	
DEPMETHN (Depreciation Method Id)	1	
ESCAP (Project Capital Escalation)	5	Percent/period
ESPROD (Products Escalation)	5	Percent/period
ESRAW (Raw Material Escalation)	3.5	Percent/period
ESLAB (Operating and Maintenance Labor Escalation)	3	Percent/period
ESUT (Utilities Escalation)	3	Percent/period
START (Start Period for Plant Startup)	1	Period
PODE (Desired Payout Period (excluding EPC and Startup Phases))		Period
POD (Desired Payout Period)		Period
DESRET (Desired Return on Project for Sales Forecasting)	10.5	Percent/Period
END (End Period for Economic Life of Project)	10	Period
GA (G and A Expenses)	8	Percent/Period
DTEP (Duration of EP Phase before Start of Construction)	0.15	Period
OP (Total Operating Labor Cost)	832770	Cost/period
MT (Total Maintenance Cost)	18627.8	Cost/period

Table 6.6 gives a detailed listing of the cash flow for the project. From economics point of view, these parameters are of utmost importance. It can be observed from the table that there is high level of detailing in this cost analysis. Factors like equipment depreciation, salvage value etc. have been taken into consideration to make this analysis more accurate.

Table 6.7: Equipment Costing

Component Name	**Component Type**	**Total Direct Cost**	**Equipment Cost**	**Equipment Weight**	**Installed Weight**
		(USD)	**(USD)**	**LBS**	**LBS**
BUBLCOL-bottoms split	C (Placeholder)	0	0	0	0
BUBLCOL-condenser	DHE TEMA EXCH	44,400	7,700	270	2,798
BUBLCOL-condenser accessories	DHT HORIZ DRUM	102,100	15,300	2,700	9,542
BUBLCOL-overhead split	C (Placeholder)	0	0	0	0
BUBLCOL-reboiler	DRB U TUBE	58,700	12,200	320	3,968
BUBLCOL-reflux pump	DCP CENTRIF	27,600	4,400	200	2,218
BUBLCOL-tower	DTW TRAYED	220,900	65,700	17,500	34,602

HEAT1	DHE TEMA EXCH	47,800	7,700	270	4,137
HEAT2	DHE TEMA EXCH	47,800	7,700	270	4,137
HYDREACT	DAT REACTOR	151,400	22,000	1,000	13,561
SEPARAT1	DTW TRAYED	169,700	31,600	4,500	19,101
SEPARAT2	DVT CYLINDER	119,800	15,200	2,600	14,899
SEPARAT3	DTW TRAYED	172,900	28,800	4,000	19,631

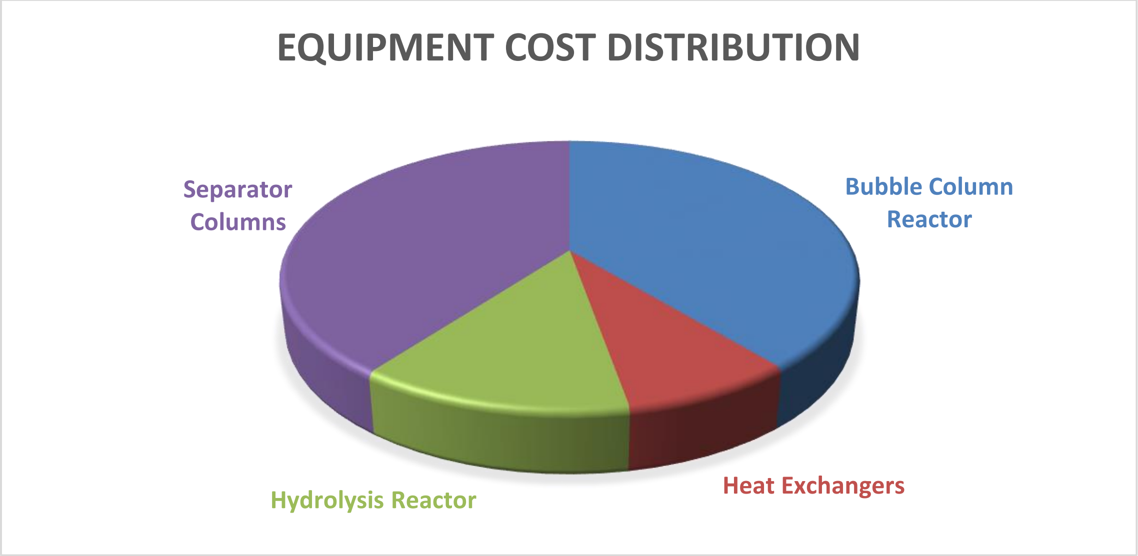


Figure 6.3: Equipment Cost Distribution

Table 6.7 shows a detailed list of equipment costing. The equipment sizing is based on the process simulation data obtained from the converged simulation. It can be observed that although we have been treating the bubble column as a single piece of equipment, it actually consists of several pieces of equipment like the column, condenser, reboiler, reflux pump etc. There is therefore no surprise in the fact that the bubble column incurs the maximum cost. Thus, it can be concluded that the bubble column is not only the most important equipment qualitatively but is also crucial economically.

Table 6.8: Project Capital Summary

PROJECT CAPITAL SUMMARY	**Design, Engg, Procurement**	**Construction Material**	**Construction Man-hours**	**Construction Manpower**	**Construction Indirects**	**Total Cost**
	USD	**USD**	**USD**	**USD**	**USD**	**USD**
Purchased Equipment	-	217,510	-	-	-	217,510
Equipment Setting	-	-	267	8,092	-	8,092
Piping	-	118,686	4,758	141,842	-	260,528
Civil	-	30,464	1,215	29,587	-	60,051
Steel	-	33,870	220	6,131	-	40,001
Instrumentation	-	670,905	4,243	128,804	-	799,708
Electrical	-	430,865	2,332	67,199	-	498,064
Insulation	-	34,321	1,429	32,313	-	66,634
Paint	-	6,451	711	15,829	-	22,280
Other	1,363,300	158,100	-	-	652,000	2,173,400
G and A Overheads	-	51,035	-	12,894	19,560	83,489
Contract Fee	98,158	42,053	-	42,941	65,141	248,293
Contingencies	263,062	322,967	-	87,414	132,606	806,049
Total Project Cost						5,284,100

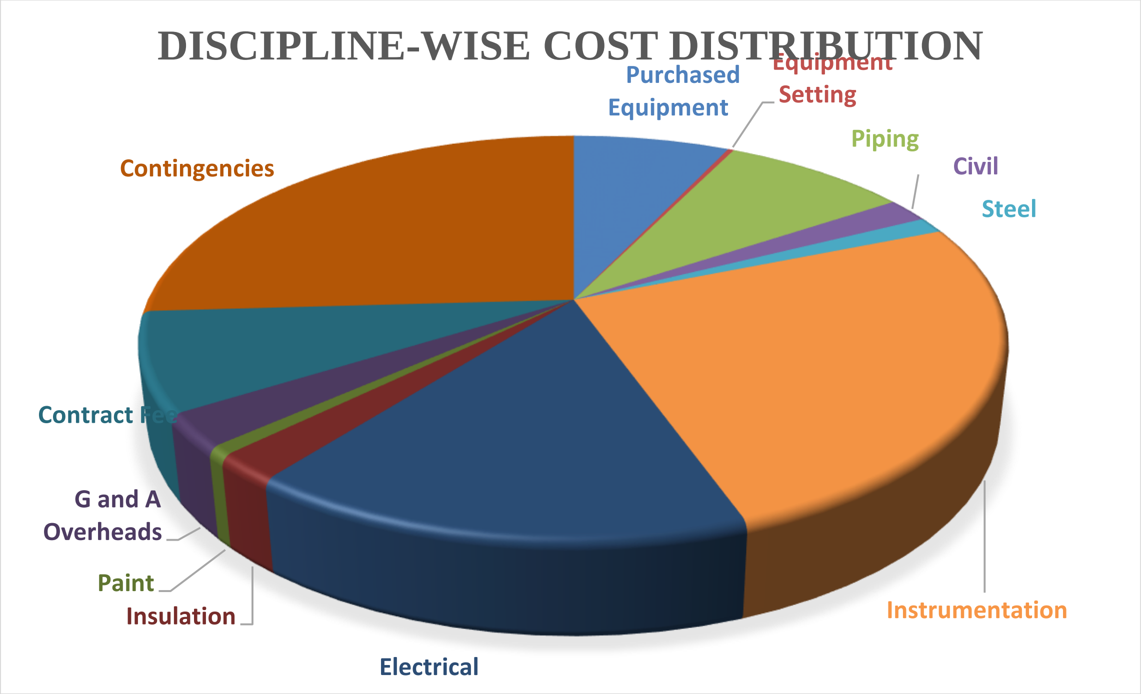
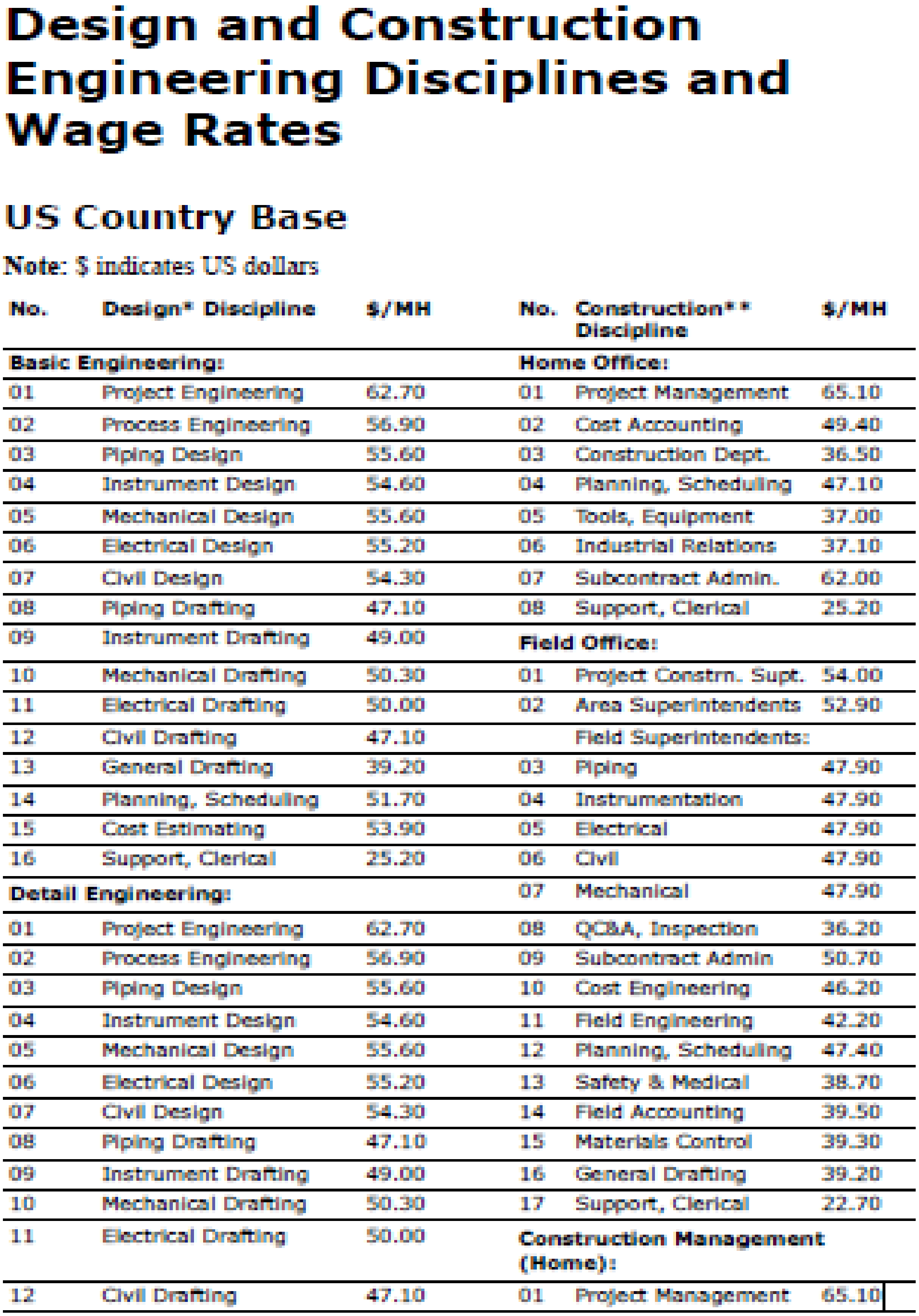


Figure 6.4: Discipline-wise cost distribution

Table 6.8 gives the information about the cost distribution across various engineering disciplines. In a typical process industry setting where these different disciplines work towards design of a plant, it becomes very important to track down the effort of each discipline. This information helps the project manager control the resources more effectively. They can easily identify the areas which need to improve and can mobilize them more efficiently. This analysis also helps each discipline keep a track of their progress in terms of economics. The eventual aim is to make profit and therefore this analysis turns out to be very useful. As discussed earlier, this data should be generated at several stages of the project, starting from the design stage till the installation is completed. Table 6.9 and Table 6.10 enlist the cost basis for this analysis. Aspen Icarus has separate cost databases for different countries. The one used here is from the US database.

Table 6.9: Design and construction engineering disciplines and wage rates reproduced from AspenTech **(AspenTech 2012)**



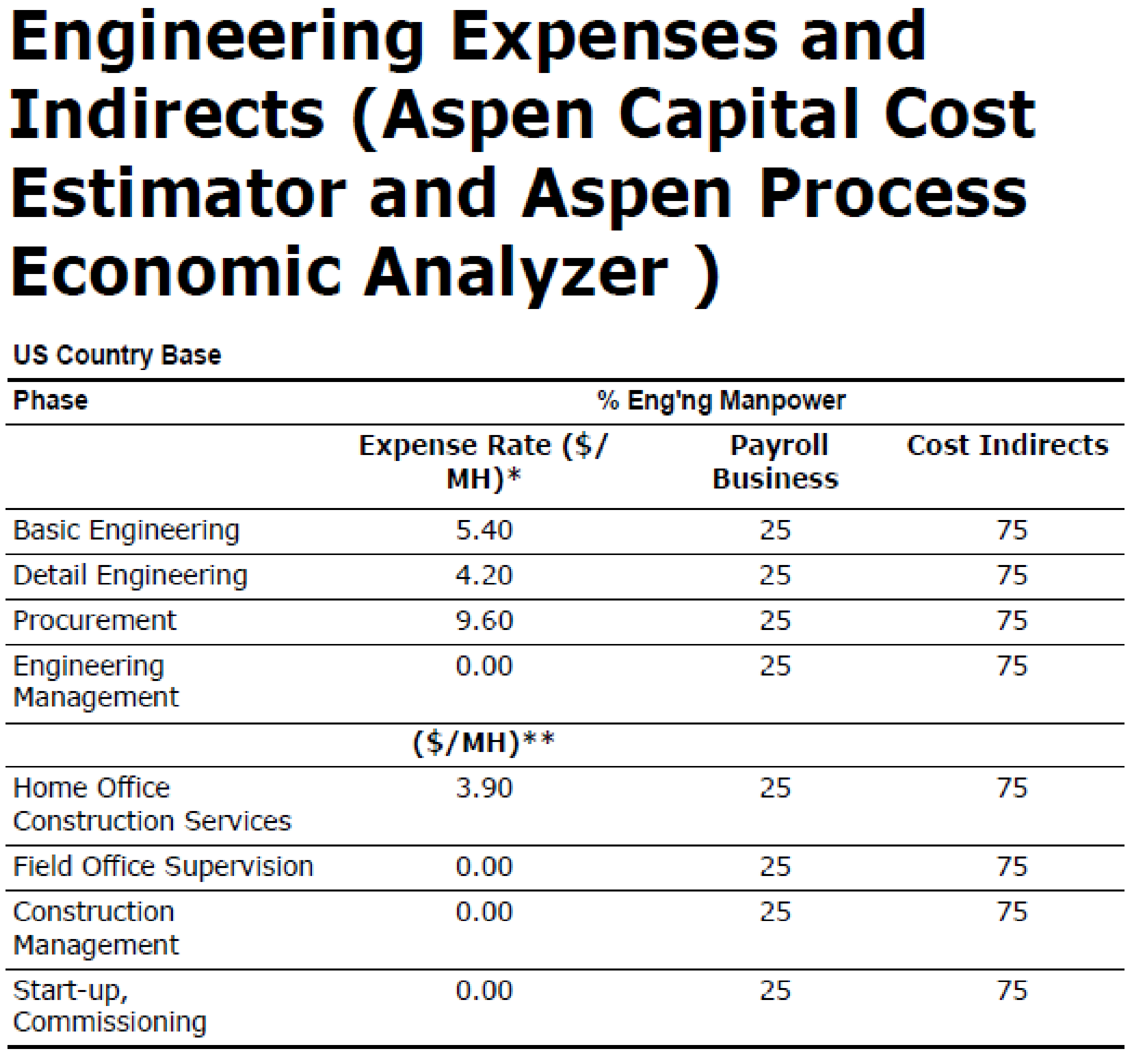
Design and Construction Engineering Disciplines and Wage Rates

US Country Base

Note: $ indicates US dollars

No.	Design* Discipline	$/MH	No.	Construction** Discipline	$/MH
Basic Engineering:			**Home Office:**		
01	Project Engineering	62.70	01	Project Management	65.10
02	Process Engineering	56.90	02	Cost Accounting	49.40
03	Piping Design	55.60	03	Construction Dept.	36.50
04	Instrument Design	54.60	04	Planning, Scheduling	47.10
05	Mechanical Design	55.60	05	Tools, Equipment	37.00
06	Electrical Design	55.20	06	Industrial Relations	37.10
07	Civil Design	54.30	07	Subcontract Admin.	62.00
08	Piping Drafting	47.10	08	Support, Clerical	25.20
09	Instrument Drafting	49.00	**Field Office:**		
10	Mechanical Drafting	50.30	01	Project Constrn. Supt.	54.00
11	Electrical Drafting	50.00	02	Area Superintendents	52.90
12	Civil Drafting	47.10		Field Superintendents:	
13	General Drafting	39.20	03	Piping	47.90
14	Planning, Scheduling	51.70	04	Instrumentation	47.90
15	Cost Estimating	53.90	05	Electrical	47.90
16	Support, Clerical	25.20	06	Civil	47.90
Detail Engineering:			07	Mechanical	47.90
01	Project Engineering	62.70	08	QC&A, Inspection	36.20
02	Process Engineering	56.90	09	Subcontract Admin	50.70
03	Piping Design	55.60	10	Cost Engineering	46.20
04	Instrument Design	54.60	11	Field Engineering	42.20
05	Mechanical Design	55.60	12	Planning, Scheduling	47.40
06	Electrical Design	55.20	13	Safety & Medical	38.70
07	Civil Design	54.30	14	Field Accounting	39.50
08	Piping Drafting	47.10	15	Materials Control	39.30
09	Instrument Drafting	49.00	16	General Drafting	39.20
10	Mechanical Drafting	50.30	17	Support, Clerical	22.70
11	Electrical Drafting	50.00	**Construction Management (Home):**		
12	Civil Drafting	47.10	01	Project Management	65.10

Table 6.10: Engineering expenses and indirects reproduced from AspenTech **(AspenTech 2012)**



Engineering Expenses and Indirects (Aspen Capital Cost Estimator and Aspen Process Economic Analyzer)

US Country Base

Phase	**% Eng'ng Manpower**		
	Expense Rate ($/ MH)*	**Payroll Business**	**Cost Indirects**
Basic Engineering	5.40	25	75
Detail Engineering	4.20	25	75
Procurement	9.60	25	75
Engineering Management	0.00	25	75
	($/MH)**		
Home Office Construction Services	3.90	25	75
Field Office Supervision	0.00	25	75
Construction Management	0.00	25	75
Start-up, Commissioning	0.00	25	75

Table 6.11: Utility Summary

Description	**Fluid**	**Rate**	**Rate Units**	**Cost per Hour**	**Cost Units**
Electricity		53.159	KW	4.119822	USD/H
Cooling Water	Water	0.000198	MMGAL/H	0.02376	USD/H
Steam @100PSI	Steam	0.07479	KLB/H	0.608791	USD/H

Table 6.11 enumerates the cost database of the utilities. Electricity, cooling water and medium pressure steam were used as utilities in the process.

Table 6.12: Maintenance and Labor Cost

OPERATING LABOR AND MAINTENANCE COSTS	**Value**	**Units**
Operating Labor		
Operators per Shift	3	
Unit Cost	20	Cost/Operator/H
Total Operating Labor Cost	525960	Cost/period
Maintenance		
Cost/8000 Hours	18800	
Total Maintenance Cost	20600.1	Cost/period
Supervision		
Supervisors per Shift	1	
Unit Cost	35	Cost/Supervisor/H
Total Supervision Cost	306810	Cost/period

The above table (Table 6.12) shows the cost incurred for the maintenance, labor and supervision. This specific Aspen Icarus database for the operating, labor and maintenance costs is for the US. As can be observed, the labor and maintenance costs are significant.

This economic analysis evidently reveals exactly which part of the process is dominating the total expenses of the project. This analysis forms the basis for the optimization studies conducted and described in the following part of the chapter. In actuality, the optimization studies have been carried out in tandem with economic analysis to avoid excessive effort. Hence, the parameter values obtained from the optimization studies have already been incorporated in the economic results discussed previously.

6.3 Economic Optimization

6.3.1 Optimization Introduction

Optimization is a generic term and has been used frequently in the chemical engineering field. It can be termed as a procedure in which a parameter or a set of parameters is optimized so as to achieve a certain goal, within a given set of constraints. The goal could be anything ranging from minimizing cost to maximizing output and from minimizing energy requirement to maximizing product purity **(Rhinehart 2013).** For a sustainable process it is imperative that the process parameters are optimized to minimize energy consumption and environmental effluents and maximize profit. In most of the cases these will be conflicting interests. For example, for a process where it is desired to try to maximize profit it leads to corresponding increase in environmental effluents and/or energy consumption. Thus there is always a quest to find the right parameters which will attempt to satisfy the conditions as best as possible.

An optimization problem will consist of an objective function. The objective function can be defined as the procedure to measure goodness (or badness) associated with the thing that needs to be maximized or minimized **(Rhinehart 2013).** The optimization problem will be based on certain decision variables which are the choices that are available or values that can be changed in order to optimize the objective function. The decision variables and the objective function will be related by model equations which describe the system in question. While solving the optimization problem there will be some constraints that need to be satisfied to make the solution a feasible one. The constraints can be further divided into soft constraints and hard constraints.

Hard constraints are the conditions that cannot be violated under any circumstances. For example, the CO_2 emission of a chemical process has to be restricted within a given limit set by the EPA. This condition if violated may lead to the plant being shut down and therefore shouldn’t be compromised. Soft constraints, on the other hand, can be violated up to a certain limit. A classic example of soft constraint is the speed limit while driving. The driver can exceed the speed limit by 3-5 mph without getting any penalty. However, beyond a certain speed he will be penalized. This grey area beyond the limit and before the penalty sets in is variable in every case.

In case of competing objective functions, as described earlier, we need to introduce Equal Concern factors (EC) **(Rhinehart 2013)**. Equal Concern factors (EC) or weighing factors are used to combine all the objective functions in to a single objective function which needs to be minimized or maximized. The EC factors are different for different processes and can be modified based on the requirement. For example, in a chemical process, if the user decides that minimizing environmental effluents is of highest priority then he would assign higher weightage to that term in the combined equation. The general equation would be of the following form:

$$Max\,J = \frac{\text{Process Cost}}{\text{EC1}} - \frac{\text{Environmental effluent}}{\text{EC2}} - \frac{\text{Energy consumption}}{\text{EC3}} \quad (6.2)$$

Note the negative sign that is used for the environmental effluent and energy consumption. The reason for this is that the objective function is set to maximize the expression and our intent is to minimize those two factors. Although the above expression tries to integrate the three objective functions into one, selecting the Equal Concern factors is tricky. Firstly, it is advisable to convert all the objective functions in terms of a single variable type like cost or mass flow rate. The reason being that it is much more difficult to compare different types of quantities; like comparing the proverbial apples to oranges.

6.3.2 Economic Optimization Philosophies

Economic optimization was carried out using three distinct philosophies as described in this section.

6.3.2.1 Optimum Process Configuration

The cost estimation for the lactic acid process was carried for two different process configurations (Configuration 1 and Configuration 2). Table 6.3 illustrates the abridged results for the two combinations. It should be noted that although only the data for the two configurations is shown, several other configurations were considered as well. The configuration without the separator column and heater in the methanol recycle (Configuration 2) is significantly more cost-effective but the methyl lactate purity is compromised. It is essentially a trade-off between product purity and cost as discussed previously. Therefore, the end user can select a configuration to suit their needs based on budget. If purity of methyl lactate is not of particular concern then it is advisable to go for Configuration 2. However, if methyl lactate purity is of utmost concern then the user needs to opt for Configuration 1.

Parameter optimization was carried out on a heuristic basis with the help of green design principles which are explained in detail in the Chapter 7.

From the equipment cost analysis data it is clear that the bubble column reactor contributes the most towards the total equipment cost. Therefore, it makes sense to optimize the parameters of the bubble column reactor in order to minimize its cost.

The optimization of the bubble column reactor could be carried out in several different ways, based on various factors. The philosophy used by Luyben **(Luyben 2006)** was adopted to optimize the bubble column reactor.

It was decided to find the optimum number of trays since it would be a major contributor to cost. Here are a few considerations to find the optimum number of trays:

6.3.2.2 Heuristic Optimization

a) Using Fenske equation the total trays can be set to twice the minimum number of trays.

$$N_{min} + 1 = \frac{\log[\left(\frac{x_D}{1-x_D}\right)\left(\frac{1-x_B}{x_B}\right)]}{\log(\alpha_{average})} \qquad (6.3)$$

$x_D: mole\ fraction\ of\ more\ volatile\ component\ in\ distillate$

$x_B: mole\ fraction\ of\ more\ volatile\ component\ in\ bottoms$

$\alpha_{average}\ : Relative\ volatility\ of\ components$

For the lactic acid process we have $x_D = 0.99$ and $x_B = 0.02$ (from process stream data)

$\alpha_{average}\ = 2.61\ (for\ methanol - water\ system\ from\ literature)$

$N_{min} = 7.84 \Rightarrow 8\ (No. of\ trays\ should\ be\ an\ integer)$

Using the heuristics the total number of trays totals to 8 × 2 = 16. Please note that this was also the same number of trays obtained from the shortcut distillation which was the starting point for the bubble column reactor for the Aspen simulation.

b) Another way to use heuristic optimization is to set the reflux ratio to 1.2 times the minimum reflux ratio.

$$RR_{min} = \sum_{i=1}^{N} \frac{\alpha_i x_{Di}}{\alpha_i - \theta} - 1 \qquad (6.4)$$

Calculating we get $RR_{min} = 2.9$

Therefore, Reflux Ratio = 2.9 × 1.2 = 3.48

6.3.2.3 Optimization using the Optimizer Block in Aspen Plus

Aspen Plus has the capability to perform single objective optimization through its optimization block. Optimization in Aspen is used to optimize a user-defined objective function by changing decision variable values **(AspenTech 2000).** The decision variables in Aspen could range from mass flow for any stream to process conditions like pressure, temperature and can even include equipment parameters. Aspen Plus uses FORTRAN to perform the optimization calculations. Therefore, the objective function needs to be in the form of a valid FORTRAN expression. The user can define equality as well as inequality constraints for the objective function. The tolerance needs to be specified, both for the objective function as well as the constraints.

Aspen Plus utilizes the following two types of algorithms for solving the optimization problems **(AspenTech 2000)**:

Table 6.13: Table describing types of algorithms used in Aspen Plus

Path Method	**Information**
Feasible	Requires that tear streams and equality constraints (design specifications), if any, be converged at each iteration of the optimization
Infeasible	Can converge tear streams, equality constraints, and inequality constraints simultaneously with the optimization problem

Aspen Plus has two algorithm options to select from:

- The COMPLEX Method
- The SQP Method

COMPLEX Method

As the name suggests, the COMPLEX method utilizes the well-known Complex algorithm **(AspenTech 2000)**. It is a basically a black box pattern search which can handle inequality constraints and bounds on decision variables. It generally requires several iterations to converge but the computational effort is less as it doesn't require calculation of derivatives.

Sequential Quadratic Programming (SQP) Method

This method is based on the quasi-Newton nonlinear programming algorithm **(AspenTech 2000)**. The advantage with SQP is that it can converge tear streams, equality constraints and inequality constraints simultaneously. Also, it requires fewer iterations to attain convergence. However, it requires numerical derivative and consequently additional computational effort. SQP is the default convergence procedure in Aspen and was also used in this work.

Following are the steps for defining an optimization problem in Aspen Plus. This procedure is reproduced from AspenTech **(AspenTech 2000)**

1. Creating the optimization problem.
2. Identifying the sampled flow sheet variables used in the objective function.
3. Specifying the objective function for a sampled variable, or some function of sampled variables, and identify the constraints associated with the problem.
4. Identifying the simulation input variables to be adjusted to maximize or minimize the objective function, and specify the limits within which they can be adjusted.
5. Entering optional FORTRAN statements.
6. Defining the constraints for the optimization problem.

The above procedure was implemented for the lactic acid process. In this work only economic optimization has been performed. The environmental and energy factors are dealt with separately in following chapters on Environmental Impacts and Sustainability Evaluator.

As discussed earlier, economic optimization based on profit maximization (cost minimization) for the bubble column reactor was carried out. The major pieces of equipment in a distillation column are: the vessel (length L and diameter D, the reboiler, and the condenser. Smaller piece of equipment like pumps, valves, pipe fittings were ignored as they wouldn’t affect the optimum solution significantly and would only lead to excessive effort.

Subsequently, an expression was developed which relates the bubble column parameters to its operating cost and profit. Operating cost in this case is based upon feed flow, distillate flow, bottoms flow, and reboiler duty. Profit is defined as the income from products minus cost of feed minus energy cost minus capital cost for the defined period (payback period).

$$Profit = Income - (Capital\ Cost + Operating\ Cost) \tag{6.5}$$

Using parameter values from process simulation data we get the following equation:

$$Profit = D \times 0.365\ +\ B \times 2.21 - F \times\ 0.541 -\ QR \times 5.3 - Capital\ Cost \tag{6.6}$$

Where,

D: Distillate Flow rate (kg/s)

B: Bottoms Flow rate (kg/s)

F: Feed Flow rate (kg/s)

QR: Reboiler Duty (kJ/s)

For capital cost the plant life has been assumed as 5 years and the cost has been pro-rated.

Equations for capital cost are as follows:

$$Capital\ Cost = Shell\ Cost + Heat\ Exchanger\ Cost \tag{6.7}$$

$$Capital\ Cost = (17640 \times d^{1.066} \times l^{0.802}) + (7296 \times reboiler\ area^{0.65} \times condenser\ area^{0.65}) \tag{6.8}$$

Where,

$$l = \frac{No.of\ trays\ (N) \times 2 \times 1.2}{3.281} \tag{6.9}$$

Equations and parameters are obtained from Luyben **(Luyben 2006)**

Solving we get the following equation for prorated capital cost

$$Capital\ Cost = 0.289 \times N^{0.802} + 0.343 \tag{6.10}$$

$$Profit = D \times 0.365\ +\ B \times 2.21 - F \times\ 0.541 -\ QR \times 5.3 - (0.289 \times N^{0.802} + 0.343)$$

(6.11)

The following constraints were used:

1. F=B+D (Material balance)
2. 8 <= N <= 40 (Minimum no. of trays calculated by Fenske Equation)
3. B,D,N > 0 (Flow Rates and No. of Trays cannot be negative)

The above equation was setup in Aspen Plus as a FORTRAN statement using the steps described in the previous discussion. The optimization details are shown in Table 6.14.

Table 6.14: Optimization Parameters used in Aspen Plus Optimizer

Algorithm:	Sequential Quadratic Programming
Tolerance:	0.001
Maximum number of flow sheet iterations:	100

The following results were obtained (Table 6.15) as the optimum values.

Table 6.15: Optimum operating conditions obtained from the Aspen Plus optimizer

Parameter	Units	Optimum Value
No. of stages	-	16.4
Distillate	kg/hr	66.7
Bottoms	kg/hr	12.1
Reboiler Duty	J/s	9866.5

The number of stages can be assumed to be 17 since it has to be a whole number. The above-mentioned parameters have been used as the optimum operating conditions to maximize profit. Please note that although economic optimization has been mentioned at the end of the chapter, it has been carried out in tandem with the economic analysis. Therefore, the optimum conditions obtained have already been utilized in Configuration 2 and the economic results are based on the same.

6.4 Summary

Economic aspect being the distinguishing factor in determining sustainability of a process, needs to be carefully analyzed. In this work, a comprehensive economic analysis has been carried out for the lactic acid process. The analysis was carried out in Aspen Process Economic Analyzer (APEA) utilizing the results from a converged Aspen Plus simulation. It generated a detailed economic analysis report which could be utilized in the process industry.

Different process configurations were tested to determine the most economic option. This exercise yielded two configurations (Configuration 1 and Configuration 2) which competed for product purity and cost. Configuration 2 was found to be the more economic option.

Simultaneously, the Bubble Column Reactor was optimized to determine the process parameters which maximized the profit. Optimization was performed using the Aspen Plus Optimizer Block. The optimum parameters were determined and utilized for further analysis.

CHAPTER VII

ENVIRONMENTAL SUSTAINABILITY AND LCA

7.1 Introduction

Environmental sustainability primarily deals with atmospheric emissions and their impacts on nature and society. The impacts vary on global, local and regional scales **(Allen and Shonnard 2001)**. Global warming and a climate change worldwide is attributed to Greenhouse gas emissions such as CFC refrigerants (chlorofluorocarbons), CO2, methane. On a regional scale, NOx emissions from combustion process in combination with hydrocarbon release amounts to degradation in air quality extending to several kilometers. Other atmospheric concerns include atmospheric acidification, eutrophication, ozone depletion etc. Figure 7.1 gives a brief listing of the various environmental impacts and their causes.

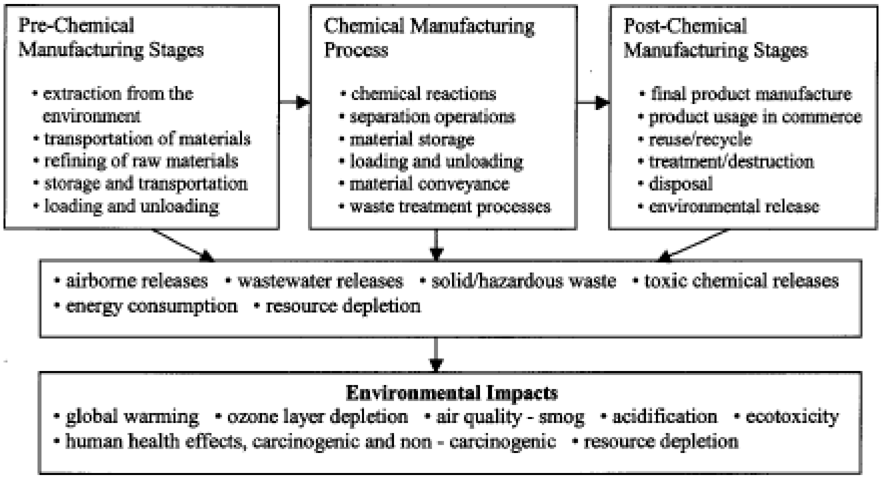
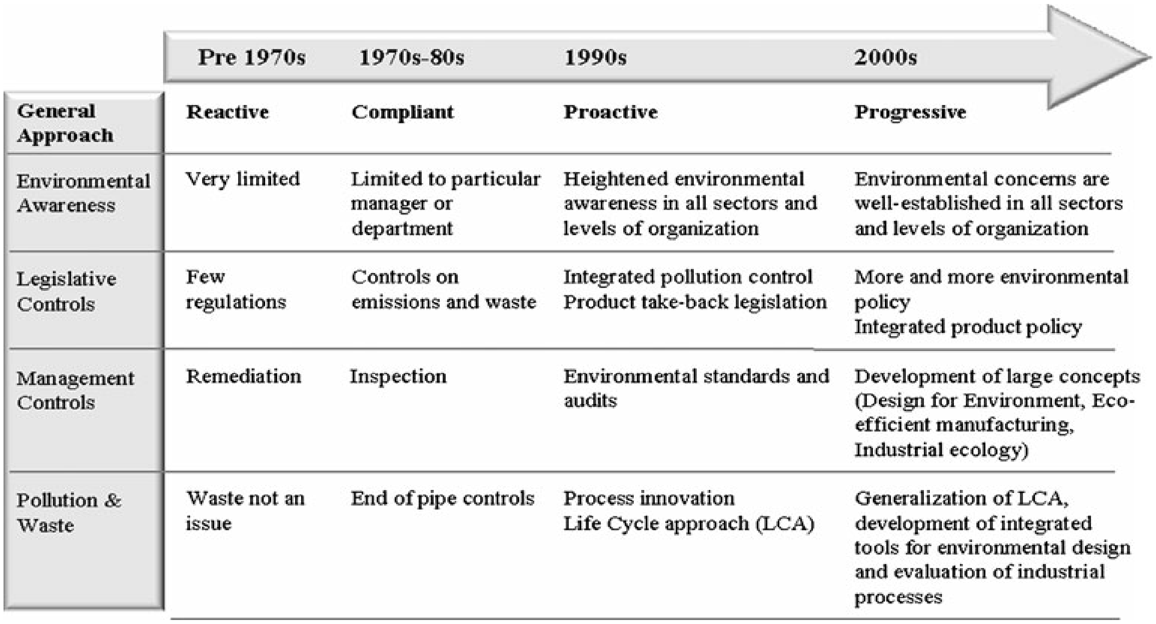


Figure 7.1: Environmental impacts and their causes reproduced from **Chen, et al.(Chen, Wen et al. 2002)**

In recent years, environmental awareness among researchers has peaked, mainly because of the drastic potential consequences. Azapagic describes how environmental assessment has progressed over the past fifty years (Figure 7.2). As can be seen, the approach has gone from being reactive in the pre 70s to being progressive in the 21st century.



	Pre 1970s	1970s-80s	1990s	2000s
General Approach	**Reactive**	**Compliant**	**Proactive**	**Progressive**
Environmental Awareness	Very limited	Limited to particular manager or department	Heightened environmental awareness in all sectors and levels of organization	Environmental concerns are well-established in all sectors and levels of organization
Legislative Controls	Few regulations	Controls on emissions and waste	Integrated pollution control Product take-back legislation	More and more environmental policy Integrated product policy
Management Controls	Remediation	Inspection	Environmental standards and audits	Development of large concepts (Design for Environment, Eco-efficient manufacturing, Industrial ecology)
Pollution & Waste	Waste not an issue	End of pipe controls	Process innovation Life Cycle approach (LCA)	Generalization of LCA, development of integrated tools for environmental design and evaluation of industrial processes

Figure 7.2: Changes in Environmental Approach reproduced from Azapagic (Azapagic 1999)

Polymer plastics have always been under scrutiny for their adverse effect on the environment. From a restriction on PVC (Polyvinyl Chloride) use in the European Union and the USA to a generic ban on plastic bags world-wide, plastic products have always run into controversy **(Tolinski 2012)**. This and several other reasons have led to increased interest in research on plastic pollution (Figure 7.3):

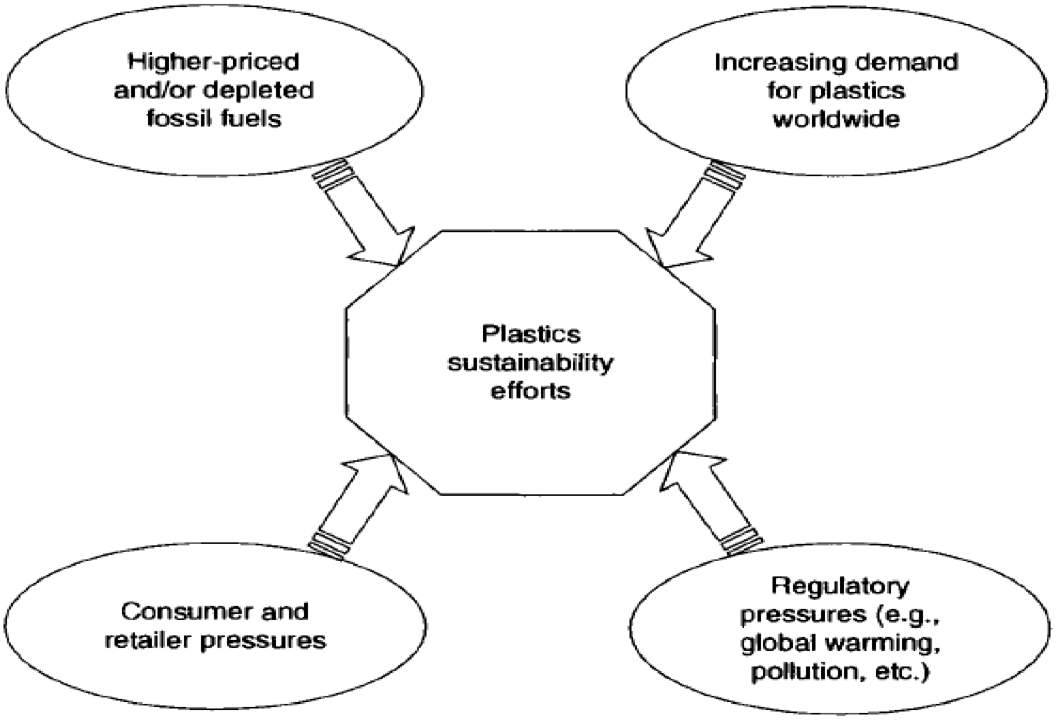


Figure 7.3: Large-scale social and natural forces are pressuring efforts toward making plastics and plastic products more sustainable and environmentally friendly reproduced from Tolinski **(Tolinski 2012)**

7.2 Environmental Analysis

As mentioned before, any process that is eventually going to produce plastic needs to be thoroughly analyzed. In this work the process has been analyzed using two methods:

1) Green Design Principles

2) Life Cycle Assessment (LCA) study

The green design principles are guidelines for a process designers to be able to design an environmental friendly process. Life Cycle Assessment (LCA) on the other hand is a study of the environmental emissions and impacts. It is a tool for measurement of these emissions and impacts. Together they provide a more holistic view about the environmental impacts of the process.

7.2.1 Green Design Principles and Application

The following discussion is based on the 12 principles of green engineering by Anastas **(Anastas 2003)** and their relevance regarding polymer plastics studied by Tolinski **(Tolinski 2012).** In their work on sustainability and green engineering, Anastas and. Zimmerman have developed a framework which could be used by process designers to conceive of processes that are benign to humans and the environment. The 12 principles developed by them can be considered as interdependent components of a sophisticated system. Just as each parameter in a process cannot be optimized at a given time due to competing objectives and conflicting constraints, these principles may end up leading to contradictory solutions and it is up to the user to prioritize which principle is the most important. The principles are explained one by one along with their application in this work in the next section. Some of the principles are not relevant to this work but have been mentioned as they could be relevant for other processes. Most of the process improvements have been explained qualitatively as they have been quantified elsewhere in this work.

Principle 1: Inherent rather than circumstantial

Although the undesirable effects of inherently hazardous substances could be minimized, it will generally come at the cost of excess use of time, material and energy resources. Therefore, for a process designer it is often beneficial to select inherently benign material and energy inputs wherever possible. In the lactic acid process, the raw materials as well as end product are non-toxic. As seen from Table 7.1, the only minor toxicity is due to methanol which can be recycled appropriately so as to not be released via the waste streams.

Table 7.1: Acute toxicity category of main chemicals in the lactic process

Chemical	Acute Toxicity Category (As per GHS)
Methanol	Category 3
Methyl Lactate	-
Lactic Acid	Category 5

Note: Category 1 is the most severe toxicity category and Category 5 is the least severe.

Principle 2: Prevention instead of treatment

A process cannot be a “zero-waste” process as it would violate basic thermodynamic laws. However, the concept of waste is human. Therefore, a material that might be considered as waste for a particular process may actually be useful in another process. Process designers should try to integrate processes if possible. Generating excessive “waste” not only undermines the value of the material but also wastes the energy content of the material which increases the cost as well as the carbon footprint. Also, additional system equipment is required for waste treatment, which leads to further wastage of resources. Although, the “waste” created in the lactic acid process isn’t utilized for another process, the amount is so small that it leads to insignificant amount of material, energy and capital resources being lost.

Principle 3: Design for separation

Separation and purification processes consume the most energy and material in the chemical process industry. An astute design of separator columns and proficient design of process configurations could lead to significant energy and cost savings. Configuration 2, of the lactic acid process, is a good illustration of this fact. Optimum process parameters and appropriate use of equipment ensures minimal energy requirements and capital costs.

Principle 4: Maximize mass, energy, space and time efficiency

Using more time, space, energy and material than required causes the process to become “inefficient.” Using the appropriate safety factors for all aspects becomes very important as erring on one side may lead to safety issues while erring on the other increases the cost. Finding the right balance between the two comes from thorough fundamental knowledge of the process and experience.

Principle 5: Output-pulled versus input-pushed

The equilibrium law, more commonly known as Le Chatelier’s principle, is used to explain the effect of a change in conditions on a chemical reaction. It states that if a chemical system at equilibrium is subject to change in the physical conditions like temperature, volume, pressure or concentration then there is a shift in equilibrium to counteract the change and the equilibrium is shifted. Many times a reaction is forced to completion based on Le Chatelier’s principle by adding more energy or materials to the system. This system can be described as an input-pushed system. However, there is a better way to drive a reaction to completion and that is by continuously removing the product without adding excess energy or material. This is an output-pulled system and is much more efficient in terms of resource usage. In the lactic acid process, water was continuously removed in order to facilitate the esterification reaction in the Bubble Column Reactor

Principle 6: Conserve complexity

The amount of sophistication that goes into a product is usually a direct function of material, energy and time resources. Thus it is not advisable to recycle the material and it should rather correspond to reuse. Also, end-of –life recycle or disposal decisions should be based on the amount of resources required on all fronts.

Principle 7: Durability rather than immortality

Products are normally designed for a certain amount of time depending on their application. If a product lasts well beyond their use, it creates environmental concern due to the difficulty of disposal. Therefore, it is advisable to design products which will last only as long as required and not make it immortal. Targeting durability and avoiding immortality, as a design principle, could greatly reduce the environmental burden.

Principle 8: Meet need, minimize excess

It is important to determine at the design stage what is the capability of a process i.e. how efficient and flexible the process can be. There is a tendency to design for worst case scenarios or for unrealistic conditions which then leads to added material and energy costs for overdesign. This tendency could be reduced if accurate process information is available and if the designer knows the nuances of the process.

Principle 9: Minimize material diversity

Products and processes generally have diverse components. Even an individual plastic consists of additives, plasticizers, dyes etc. This becomes a problem when end-of-life decisions are to be made, determining the ease of recycle and reuse. Final disposal becomes easier and cheaper if material diversity is reduced in the design upfront.

Principle 10: Integrate local material and energy flows

Material and energy integration is one of the most important considerations for a process designer while performing process intensification. The design should minimize the overall material and energy usage. Therefore, heat from an exothermic reaction could be utilized to heat up another process stream. The added cost and fuel use for the heat exchanger however should be taken into consideration while assessing this option. Material streams should be purified and recycled wherever possible thereby reducing material. In the lactic acid process two methanol recycles streams have been used thus minimizing methanol input to the process. The energy intensification was also considered. However, adding a heat exchanger for this would actually be costlier.

Principle 11: Design for commercial “afterlife”

In the current world, commercial end of life for most of the plastic products occurs due to being technologically or stylistically obsolete rather than its functional failure. Thus components that retain their functionality could be recycled/reused.

Principle 12: Renewable rather than depleting

Use of renewable resources rather than using diminishing resources both for material and energy is probably one of the most important step towards designing a sustainable process. According to Anastas **(Anastas 2003),** *every unit of finite substance used in a consumptive manner incrementally moves the supply of that substance toward depletion.* Thus, using renewable sources for material and energy has become one of the prime objectives of a process designer while deciding the process philosophy. The calcium lactate that is a raw material in the lactic acid process comes as a fermentation product from a biodegradable source. Anastas and Warner came up with 12 principles of green chemistry **(Anastas 1998)**. These principles compliment the 12 principles of green engineering described earlier and have been considered while designing the process:

1) Prevention
2) Atom Economy
3) Less Hazardous Chemical Syntheses
4) Designing Safer Chemicals
5) Safer Solvents and Auxiliaries
6) Design for Energy Efficiency
7) Use of Renewable Feedstocks
8) Reduce Derivatives
9) Catalysis
10) Design for Degradation
11) Real-time analysis for Pollution Prevention
12) Inherently Safer Chemistry for Accident Prevention

7.2.2 Life Cycle Assessment Studies

There has always been a search for a framework that could compare products/processes on the basis of their effectiveness, primarily in terms of economic and environmental aspects. There is no single framework so far that has been able to effectively capture all the parameters and yet be simplistic enough for general use. One of the reasons behind this is the vast variety of processes that we deal with and the diverse nature of purpose of the LCA studies.

LCA or Life Cycle Assessment is one of the recent alternatives which can be a solution. It is especially useful when environmental impact is the major aspect in focus. LCA coupled with sound economic analysis generally provides a reasonable basis for comparison.

In this work LCA studies have been performed with a focus on the following intention:

- To evaluate the Base Case and the two process configurations (Configuration 1 and Configuration 2) for the lactic acid process based on their environmental impact.

7.2.2.1 Background

Part of the this section has been reproduced from yet unpublished work done by me and Ife Olukoya **(Ife Olukoya 2014).**

Life Cycle Assessment can be defined as a technique used to assess the environmental impacts of a process or a product which can be attributed to the life cycle of the product or process **(Rebitzer, Ekvall et al. 2004)** . The impact categories generally used are ozone layer depletion, global warming, aquatic acidification, eutrophication, stress on human health and ecosystems, depletion of natural resources like land and water. Tolinski **(Tolinski 2012)** defines LCA as “a methodology or technique for identifying, measuring, and evaluating all the energy and material flows that result from making, using, and disposing of a target product or material.” LCA came to attention in the 1970s when it transitioned from a mere energy analysis to a more inclusive environmental burden analysis **(Guinée, Heijungs et al. 2010)**. LCA developed further in the 1980s and 1990s with the inclusion of environmental costing, making it a more pragmatic option for overall environmental analysis. However, it wasn’t until the 21st century, when the social feature was incorporated, that it got a comprehensive outlook and industries started using it for decision making. Subsequently, environmental policies and standards have now started to become life-cycle based. In USA, the Environmental Protection Agency (EPA) started to promote LCA and various LCA networks have now been established **(Guinée, Heijungs et al. 2010)** .

Tolinski (Tolinski 2012) discusses the following possible motivating factors for conducting a LCA on a product or process in an industrial setting:

1) The ecosystem is being adversely affected by human activities leading to polluting the environment and this damage could be controlled if the LCA reveals any specific source of pollution.
2) Earth’s resources, especially non-renewable fuels and water have been declining at an alarming rate due to overuse and the same could be used more efficiently.
3) A process is being operating at less than optimal conditions leading to higher environmental costs coupled with a less flattering public image

7.2.2.2 Methodology

As mentioned earlier this study focusses on a comparative study of two process configurations to produce polymer grade lactic acid. As both process configurations produce the same end product, we have concentrated our efforts on the gate to gate stage of the process. LCA results for the cradle to gate and the gate to grave stages for both the configurations will be identical and therefore wouldn't affect the decision making. Impact 2002+ is the LCA methodology that has been used for this study.

Jolliet, et al (Jolliet, Margni et al. 2003) describes the Impact 2002+ methodology as follows: "*The new IMPACT 2002+ life cycle impact assessment methodology proposes a feasible implementation of a combined midpoint/ damage approach, linking all types of life cycle inventory results (elementary flows and other interventions) via 14 midpoint categories to four damage categories.*"

There are four basic steps adopted in any LCA study:

1) Goal Definition and Scoping
2) Inventory Analysis
3) Impact Assessment
4) Improvement Assessment

7.2.2.2.1 Goal and Scope Definition

The goal of an LCA study states its intended purpose, the intended application, the reason for the study, the audience and how the results will be used. The scope includes the products under investigation, its function, allocation procedures, impact categories, impact assessment methodologies, assumptions, functional unit and system boundary

(ISO 2006, ISO 2006). Since an LCA is in iterative process, as more data is collected, the goal and scope can be revised during the LCA process but setting a goal and scope at the beginning of the analysis is crucial. The functional unit for any LCA must be explicitly stated and should be related to the function of the final product. It is what all inputs and outputs are related to and when a comparative LCA is performed, both systems should have the same functional unit **(Baumann and Tillman 2004)**.

The selection of a system boundary is one of the most important aspects of an LCA; different system boundaries for the same process can result in different outcomes and conclusions. The system boundary includes unit processes that will be part of the analysis and as the LCA is conducted, the system boundary may need to be refined. As the system boundary is being developed, different parts of the life cycle need to be taken into consideration: raw material acquisition, transportation and distribution, usage and maintenance of products, waste disposal, reuse and recycling of products, manufacturing of equipment, and inputs and outputs into the main process **(ISO 2006)**.

The goal of this LCA is to quantify the environmental impacts in the global warming impact, non-renewable energy use, and respiratory inorganics impact categories of the production of polymer grade lactic acid at a 50,000 kg/year capacity facility with a ten year lifespan. The three categories have been selected since only these categories have significant impacts. A comparison between the two process configurations previously derived, Configuration1 and Configuration 2 is conducted. The analysis was performed in SimaPro 8.0.0 using the Impact 2002+ impact assessment method. This LCA is a cradle-to-gate LCA; it takes into consideration all impacts from the production of raw material to the development of the final product. All unit processes present in the simulation have been included in the system boundary and so are impacts from raw material production and transportation to the facility. Impacts from construction of the facility are not included in the analysis, it is assumed to be negligible when spread out over the lifespan of the process.

7.2.2.2.2 Inventory Analysis

The inventory analysis step of an LCA involves collection of input and output data for the unit processes that are included within the system boundary. Just like the goal and scope definition, as the LCA is performed, more is known about the process or if there are changes to the system boundary, there might be new data requirements or changes to the goal and scope based to the collected data. Data required include: energy and raw material inputs, products, co-products, waste, emissions, and other environmental factors **(ISO 2006)**.The data collection also includes relating each input and output to the functional unit and reference flow, validation, and allocation of impacts when co-products are present.

7.2.2.2.3 Life Cycle Impact Assessment (LCIA)

This step involves taken data collected from the inventory analysis and quantifying the environmental impacts for the chosen impact categories. Doing this allows the LCA practitioner to understand the environmental impacts. Impact categories for Impact 2002+ include: carcinogens, non-carcinogens, respiratory inorganics, ionizing radiation, ozone layer depletion, respiratory organics, aquatic eco toxicity, terrestrial eco toxicity, terrestrial acidification/nitrification, land occupation, aquatic acidification, aquatic eutrophication, global warming, non-renewable energy use, and mineral extraction **(Jolliet, Margni et al. 2003)**.

7.2.2.2.4 Interpretation

Using results from the inventory analysis, and impact assessment the LCA practitioner draws conclusions that are consistent with what is laid out in the goal and scope definition in the interpretation step. Also called improvement assessment, this step requires critical evaluation of the LCA **(Klöpffer 1997)**. Conclusions and recommendations are made based on the findings. Just like the previous steps, this is in iterative process and ISO 14040 states that “The interpretation should reflect the fact that the LCIA results are based on a relative approach, that they indicate potential environmental effects, and that they do no predict actual impacts on category endpoints” **(ISO 2006)**. A visual representation of how the four categories on a LCA related and some direct application of LCAs can be seen in Figure 7.4.

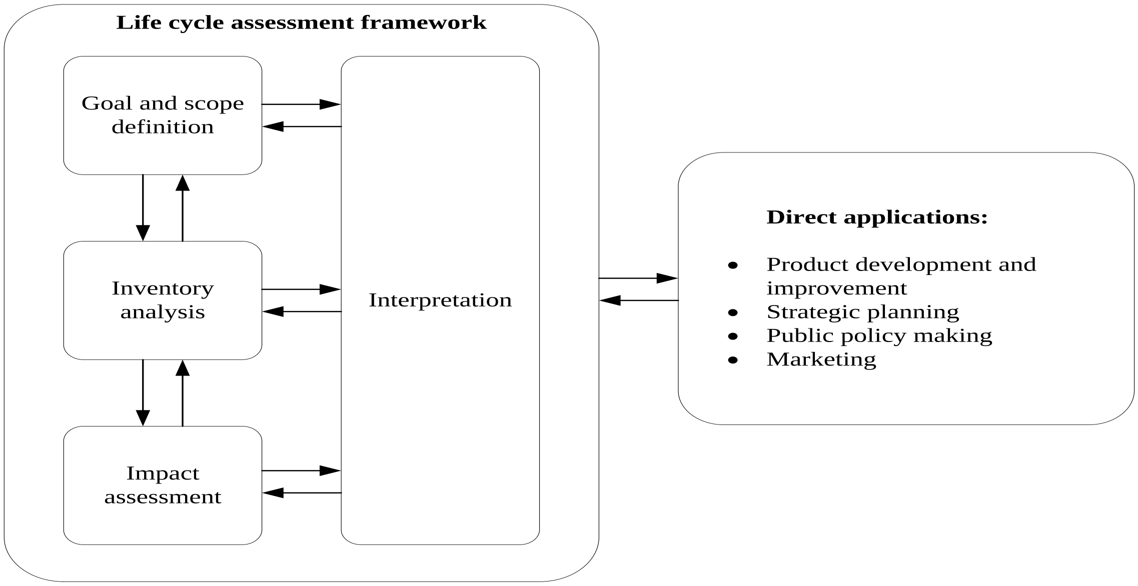


Figure 7.4: Life cycle assessment framework, adapted from ISO 14040

7.2.2.3 Results and Discussion

LCA results generated in SimaPro and are shown in Table 7., and it can be seen that Configuration 1 with Separator 4 has lower environmental impacts for each impact category than Configuration 2 without Separator 4. The results are presented in per kg of polymer grade lactic acid produced in the facility.

Table 7.2: Life cycle impact assessment results, per kg of polymer grade lactic acid produced

Impact category	Configuration 1	Configuration 2	Unit
Respiratory inorganics	4.2×10^{-2}	6.6×10^{-2}	kg of particulate matter
Global warming	116.3	181.8	kg CO_2 equivalent
Non-renewable energy	2132.6	3318.1	MJ

7.2.2.3.1 Respiratory Inorganics

This impact category deals with human health impacts from inorganic particulate matter release into the air. The reference unit is particulate matter than is 2.5 microns or less, this can include dust, sulfur and nitrogen oxides

Table 7.3: Unit process contribution to respiratory inorganics impact category, per kg of polymer grade lactic acid produced, units of kg of particulate matter

Unit process	Configuration 1	Configuration 2
Methanol	2.5×10^{-4}	2.5×10^{-4}

Process water	2.1x10^{-7}	2.1x10^{-7}
Lactic acid	9.1x10^{-6}	9.1x10^{-6}
Heater 1	2.2x10^{-4}	2.2x10^{-4}
Heater 2	2.3x10^{-3}	2.3x10^{-3}
Heater 3	2.8x10^{-4}	–
Bubble column	2.3x10^{-2}	5.3x10^{-2}
Separator 1	1.2x10^{-3}	4.9x10^{-3}
Separator 3	5.2x10^{-3}	5.1x10^{-3}
Separator 4	1.0x10^{-2}	–
Waste water treatment	6.7x10^{-5}	3.0x10^{-5}

Table **7.3**7.3 breaks down each unit process contribution to the impacts for the respiratory inorganics category. When both configurations are compared the Bubble Column Reactor and Separator 1 both see an increase in impacts in Configuration 2 where Separator 4 and Heater 3 are removed. Waste water treatment is the only unit process that sees a decrease in Configuration 2. **Error! Reference source not found.** shows the relative contribution of each unit process in both the Configuration 1 and Configuration 2. In both configurations, the Bubble Column Reactor accounts for a majority of impacts. In the

Configuration 1 it accounts for 53% and in Configuration 2 it accounts for 81% of the impacts.

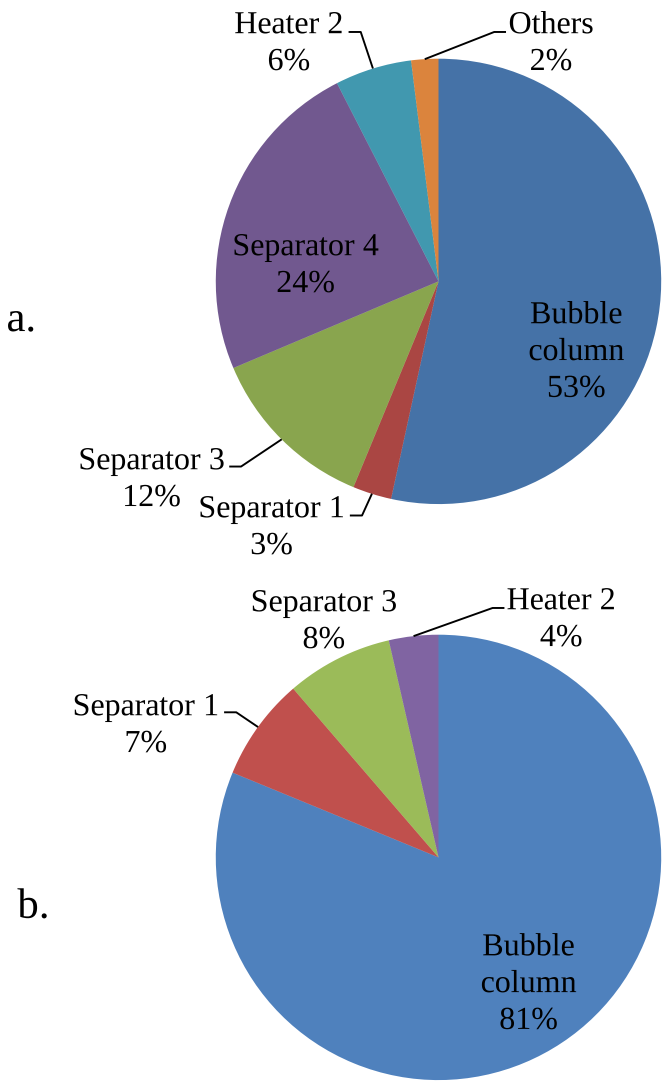


Figure 7.5: Breakdown of impact for respiratory inorganics impact category, a. Configuration 1, b. Configuration 2

7.2.2.3.2 Global Warming

The global warming impact category in the Impact 2002+ impact assessment method takes into account the potential global warming impacts of greenhouse gases (GHG) like methane (CH_4), carbon dioxide (CO_2), nitrous oxide (N_2O), hydrofluorocarbons and perfluorocarbons. The reference unit for this impact category is kg of CO_2 emitted during the life cycle of the process. Other greenhouse gases that are emitted have their global warming potential (GWP) used to convert their impacts to an equivalent CO_2 basis.

Table 7.4: Unit process contribution to global warming impact category, per kg of polymer grade lactic acid produced, units of kg of equivalent CO_2

	Configuration 1	Configuration 2
Methanol	0.9	0.9
Process water	$2.6\text{x}10^{-4}$	$2.6\text{x}10^{-4}$
Lactic acid	$1.0\text{x}10^{-2}$	$1.0\text{x}10^{-2}$
Heater 1	0.6	0.6
Heater 2	6.5	6.5
Heater 3	0.8	–
Bubble column	62.0	146.4
Separator 1	3.3	13.5
Separator 3	14.4	13.9
Separator 4	27.7	–
Waste water treatment	0.2	0.1

The unit process contribution for the global warming impact category in Table 7.4 shows a similar trend that is seen in the respiratory inorganics unit process contribution in Table **7.3**7.3 where Configuration 2 results in an increase in impacts from the Bubble Column Reactor and Separator 1. There is a decrease in equivalent CO_2 for Separator 3 and the waste water treatment. Figure **7.6**7.6 shows each unit process contribution as a percentage of impacts, once again, the Bubble Column take up the majority of impact for this category for both Configuration 1 and Configuration 2.

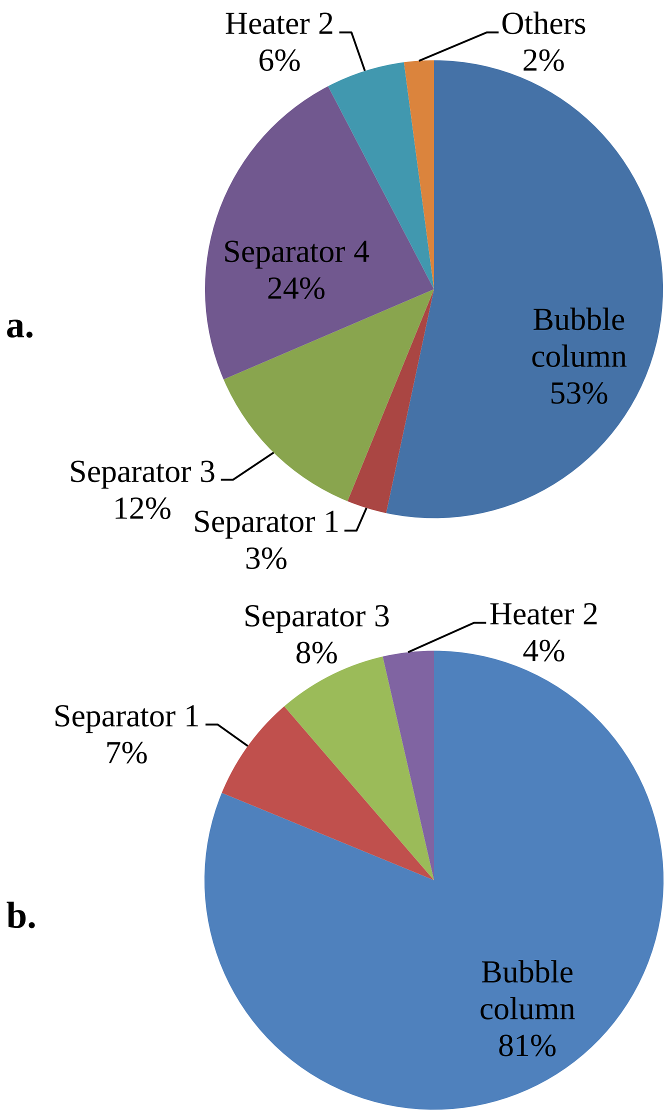


Figure 7.6: Breakdown of impact for global warming impact category, a. Configuration 1, b. Configuration 2

7.2.2.3.3 Non-renewable Energy Use

The non-renewable energy use category accounts for energy use from sources that can be depleted. These include crude oil, natural gas, coal, and uranium usage from the raw material acquisition stage to the final production of the polymer grade lactic acid. The reference unit for this impact category is MJ of energy from crude oil. Table 7.5 shows unit process contribution for this category and it exhibits trends that have already been observed in Table 7.3 and Table . Increase in contribution from the Bubble Column Reactor and Separator 1, and a decrease in contribution from Separator 2 and waste water treatment. In Figure **7.7**7.7 the percentage contributions are shown and the Bubble Column Reactor again is the largest contributor for both the Configuration 1 and Configuration 2 with an 80% contribution in Configuration 1 and a 53% contribution in Configuration 2.

Table 7.5: Unit process contribution to non-renewable energy use impact category, per kg of polymer grade lactic acid produced, units of MJ

	Configuration 1	Configuration 2
Methanol	49.2	49.2
Process water	$5.8\text{x}10^{-3}$	$5.8\text{x}10^{-3}$
Lactic acid	0.2	0.2
Heater 1	10.9	10.9
Heater 2	116.9	116.9
Heater 3	13.9	–
Bubble column	1121.3	2645.5
Separator 1	59.2	243.3
Separator 3	260.3	251.8
Separator 4	500.0	–
Waste water treatment	0.6	0.3

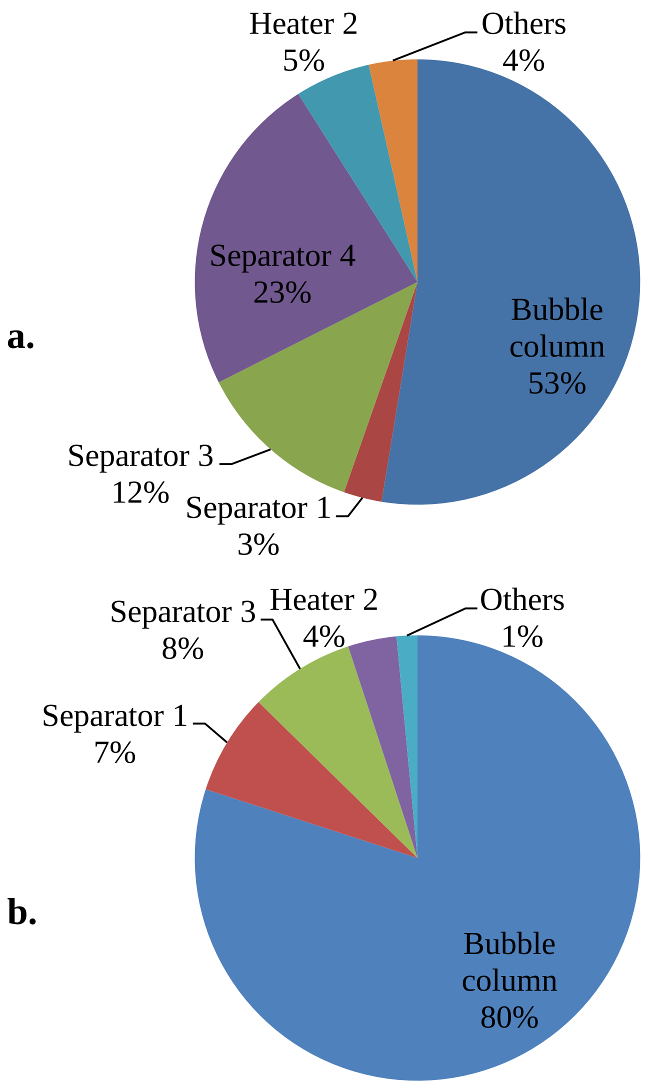


Figure 7.7: Breakdown of impact for non-renewable energy use impact category, a. Configuration 1, b. Configuration 2

7.2.2.4 Conclusion

The LCIA results have been able to highlight the stages of the process that have the largest contributions to the environmental impacts and the unit processes can be singled out for improvement. The bubble column is the largest contributor in each impact category that is investigated in this LCA. For Configuration 2, when the separator column in the recycle is removed, the bubble column unit process contribution for all three impact categories more than doubles. Another conclusion that can be drawn from the LCA is that the economic optimization of the process produces a configuration that is better from an economic standpoint but worse from an environmental standpoint.

Figure 7.8 gives a comparative summary of the two configurations for their environmental impact contribution towards each of the three categories. It can be noticed that Configuration 2 has ~40% higher impact in every category than Configuration 1. This result is attributable to the fact that since the methanol recycled back to the Bubble Column Reactor is of lesser purity, it leads to a higher steam requirement. This increased steam requirement is the direct cause of the increased environmental impact. It can be noted that the steam requirement for the Bubble Column Reactor in Configuration 2 (3848.61 kg/day) is much higher than the combined steam requirement of the Bubble Column Reactor and Separator in Configuration 1 (2358.62 kg/day). Therefore, although Configuration 2 has higher profitability, it also has higher environmental impacts owing to higher steam requirement.

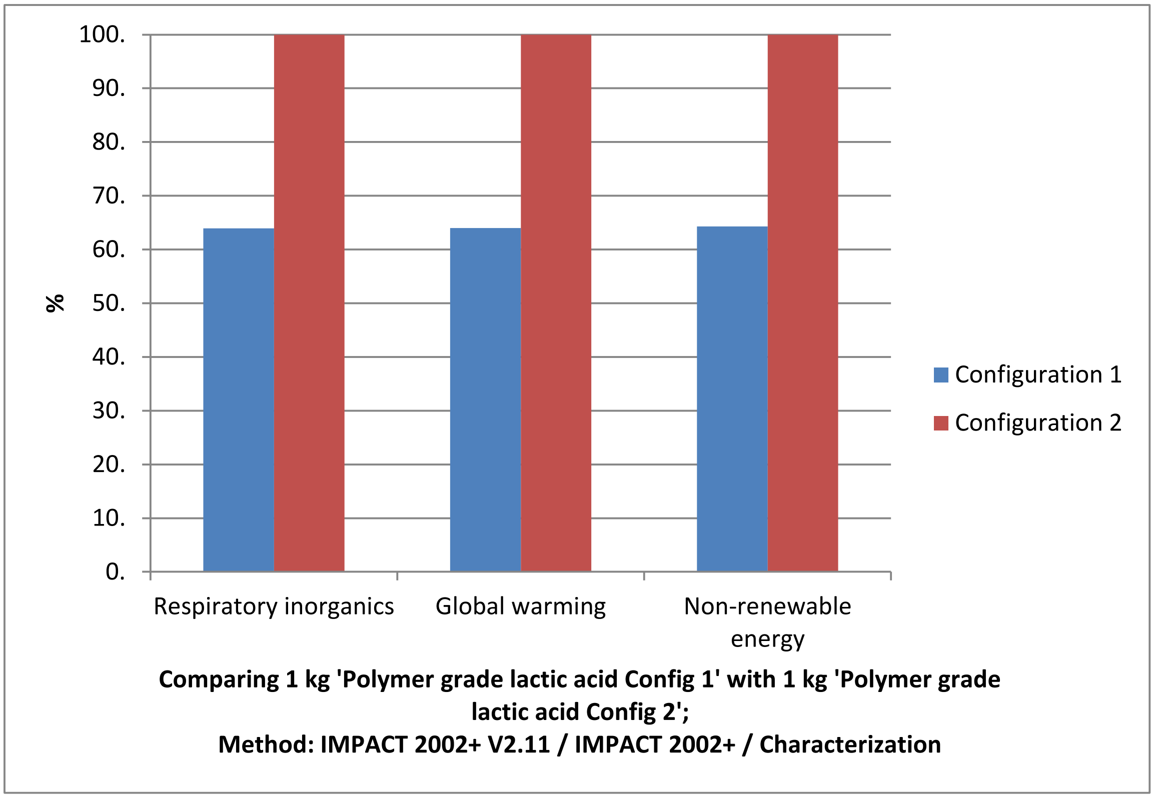


Figure 7.8: Comparison of Configuration 1 and Configuration 2 for each Impact Category

The environmental aspect being a crucial part of sustainability has been thoroughly studied in this work. Green Design principles have been used while designing the process in order to minimize toxic emissions. Life Cycle Assessment (LCA) study has been carried out on the two process alternatives (Configuration 1 and Configuration 2) in order to assess their impact on the environment. The LCA analysis has been carried out using SimaPro software **(Consultants 2010)** and the Impact2000+ methodology has been adopted. Three impact categories, global warming impact, non-renewable energy use and respiratory inorganics were found to have significant impact on the environment and were therefore studied in depth. The study provided results which were contradictory to initial expectation. However, an in-depth analysis reveals the reasoning as explained earlier in the chapter. Thus, Configuration 1 was found to be more eco-friendly than Configuration 2, although the latter is more lucrative.

CHAPTER VIII

SUSTAINABILITY EVALUATOR

8.1 Introduction

There has always been an effort to develop a tool which integrates all three aspects of a sustainable process – economic, environmental and social. One such attempt has been made by Shadiya and High in their development of the SUSTAINABILITY EVALUATOR **(Shadiya and High 2013).** The SUSTAINABILITY EVALUATOR is an MS Excel based software program that utilizes simulation parameters to evaluate sustainability of a chemical process **(Shadiya 2010)**. The SUSTAINABILITY EVALUATOR is unique because it not only manages to incorporate all three facets of sustainability but also produces a single score based on weighing factors assigned by the user. The single score gives the user a quick and easy-to-read number in order to assess the sustainability index of the process. It also provides details about the contribution of each aspect towards overall impact thereby making it easy to zero-in on the area which requires improvement. The evaluator is mainly used to 1) Evaluate the sustainability of a process in order to ascertain its industrial feasibility. 2) Compare sustainability of products or process alternatives to choose the best option.

In this work the SUSTAINABILITY EVALUATOR has been utilized to evaluate and compare configuration 1 and configuration 2 on a more holistic basis. The evaluator has also been utilized to show the process improvements when compared to the base case.

8.2 Metric Development

As mentioned earlier the SUSTAINABILITY EVALUATOR integrates the economic feasibility, environmental impacts and social factors. Following is a brief description of the factors that have been considered while formulating the evaluator. Some of the description about the sustainability evaluator metrics has been reproduced from **Shadiya (Shadiya 2010).** Also, all of the reference data for the metrics calculations has been acquired from **Shadiya (Shadiya 2010)**

8.2.1 Economic Impact

Economic Impact needs to be evaluated prudently because if the process is not going to make reasonable profit, it is deemed infeasible. In fact, one of the first things that a process engineer/project manager looks at while evaluating a process is whether there is any realistic chance of economically sustaining the process. The sustainability evaluator incorporates the following economic analysis factors. The factor descriptions have been obtained from **Shadiya (Shadiya 2010)**

a) Product Revenue: This is a measure of the revenue that is generated from the manufactured product and by-products. The higher the product revenue, the more profitable the process will be.
b) Raw Material Costs: This is defined as costs of the raw materials used in manufacturing the product.

c) Waste Treatment Costs: This is defined as the expenses associated with treating wastes generated in a process.

d) Operating costs: This is defined as the costs of energy used in manufacturing a particular product.

e) Material Value Added: This is defined as the difference between the product revenue and the raw material costs.

f) Annualized Capital Costs: This is the conversion of the capital costs to an annual value by multiplying by a capital recovery factor. The capital recovery factor is evaluated using the following equation

$$CRF = \frac{i(1+i)^n}{(1+i)^n - 1} \tag{8.1}$$

Where,

CRF = Capital Recovery Factor

n = Number of Years

i = Interest Rate

g) Profit: This is defined as shown in the following equation

$$\text{Profit} = \text{Product Revenue} + \text{By product Revenue} - (\text{Raw Material Cost} + \text{Waste Treatment Cost} + \text{Operating Cost} + \text{Annualized Capital Cost}) \tag{8.2}$$

8.2.2 Environmental Burden

The following nine impact categories listed below are suggested: global warming, stratospheric ozone depletion, photochemical smog, aquatic oxygen demand, atmospheric acidification, aquatic acidification, eco-toxicity to aquatic life, eutrophication and resource usage. A detailed description of the impact factors could be found in **Shadiya (Shadiya 2010)**

Resources usage

Resource utilization is an important indicator while assessing the sustainability of a process.

This metric evaluate resource usage of a chemical process, while addressing energy and water usage as well as reaction efficiency. The sub-metrics under this category include, E-factor, mass productivity, reaction mass efficiency, energy intensity and water consumption. Equations 8.3 through 8.8 are used for calculation.

$$E - Factor = \frac{Total\ Waste}{Mass\ of\ Product\ (kg)} \qquad (8.3)$$

$$Reaction\ Mass\ Efficiency = \frac{Mass\ of\ Product\ (kg)}{Mass\ of\ Reactant\ (kg)} \qquad (8.4)$$

$$Mass\ Productivity = \frac{1}{Mass\ Intensity} \times 100 \qquad (8.5)$$

$$Mass\ Intensity = \frac{Total\ Mass\ used\ in\ Process\ Step}{Mass\ of\ Product\ (kg)} \qquad (8.6)$$

$$Energy\ Intensity = \frac{Energy\ Consumed}{Mass\ of\ Product\ (kg)} \qquad (8.7)$$

$$Water\ Intensity = \frac{Water\ Consumed}{Mass\ of\ Product\ (kg)} \qquad (8.8)$$

8.2.3 Social Concerns

Social awareness has traditionally been the most neglected aspect out of the three – environmental, economic and social. In recent years however, there has been an increased focus on social sustainability from researchers. The realization that social impact factors have an indirect impact on environmental and economic factors has prompted this change. The problem faced by researchers however is that of quantifying the impact. The SUSTAINABILITY EVALUATOR is one such attempt at quantifying social impact **(Shadiya 2010).** The factors have been categorized into two categories as follows:

- Process Safety Risks
- Health Risks

Process Safety Risk

The following process safety metrics have been incorporated in the SUSTAINABILITY EVALUATOR: heat of main and side reaction index, flammability index, explosivity index, corrosive index, toxic exposure index, temperature index, pressure index, equipment process safety index and process safety structure index.

Health Risk

The following health metrics have been incorporated in the SUSTAINABILITY EVALUATOR: carcinogenic health risk, developmental health risk, reproductive health risk, cardiovascular health risk, endocrine system health risk, liver damage health risk, immune system damage health risk, kidney damage health risk, skeletal system damage health risk, neurological damage health risk and respiratory system health risk.

8.2.4 Impact Calculations

Overall Sustainability Impact (Sustainability Index)

As discussed in the introduction of the SUSTAINABILITY EVALUATOR, the exclusivity of THE SUSTAINABILITY EVALUATOR lies in the fact that it gives one single score by combining the impacts due to the three categories. Thus the three concerning factors are weighted and combined into a single objective known as the overall sustainability impact (SUI) and is described by the following equation:

$$SUI = 0.2 * EI + 0.4 * ENVI + 0.4 * SCI \tag{8.9}$$

EI: Economic Impact
ENVI: Environmental Impact
SCI: Social Impact

The weight factors used in the above equation are essentially Equal Concern (EC) factors as described in the Economic Analysis and Optimization chapter. The weighing factors enable us to obtain a single solution instead of obtaining multiple Pareto-Optimal solutions **(Shadiya 2010).** The weighing factors were chosen based on overall risks. The economic impact was assigned a weight of 0.2 and the social and environmental factors were assigned a weight of 0.4 to each. Therefore, although economics is the driving force for decision-makers, environmental and social factors have been given higher weightage due to the fact that the risks associated are costlier. It can be observed that the weighting factors add up to 1 and therefore the overall sustainability impact will range from 0 to 1. Higher the impact value lesser the sustainability index. Therefore, a value closer to 0 indicates that the process is more sustainable as compared to process with a value close to 1.

Overall Economic Impact (EI)

The overall economic impact factor was calculated as a ratio of profit to investment (PRI)

$$PRI = \frac{Profit}{Expenses} \times 100 \qquad (8.10)$$

The reason behind selecting the metric is that generally this ratio is an important criterion while making investment decisions. An impact score in the range of 0-1 was assigned based on the criteria shown in Table 8.1.

Table 8.1: Economic impact score based on PRI

PRI	Economic Impact
0	1
5%	0.75
15%	0.5
20%	0.25
>25%	0

A PRI in excess of 25% is assigned an impact score of 0 and a PRI of 0 (non-profitable process) is assigned an impact score of 1. It is obvious that a lower impact score is desirable.

Overall Environmental Impact (ENVI)

The environmental impact was calculated using both the resource usage index (RUI) and environmental burden metrics (EVI) as shown in the following equation:

$$ENVI = 0.25 * RUI + 0.75 * EVI \qquad (8.11)$$

The weights of 0.25 and 0.75 were made based on the fact that resource usage measures a single category of environmental concern whereas environmental burden accounts for eight other ecological categories. The overall environmental impact (ENVI) was normalized to yield a value between 0-1 as explained in **(Shadiya 2010).** As is the case with EI, a lower value of ENVI indicates lesser environmental burden and therefore is preferred.

Overall Social Impact (SCI)

The overall social impact was developed using an equal weighing factor of 0.5 for both Safety Impact (SAI) and Health Impact (HEI) as depicted in the following equation.

$$SCI = 0.5 * SAI \; + \; 0.5 * HEI \qquad (8.12)$$

This indicates that both the categories are equally important for accurate assessment of the social impact. A score range of 0-1 was developed by normalization of the impacts and is listed in Table 8.2. An impact value of 0 indicates that the process has the lowest possible risk whereas a score of 1 points to a high safety risk process.

Table 8.2: Safety impact score based on process safety value index

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

8.3 SUSTAINABILITY EVALUATOR Results

The SUSTAINABILITY EVALUATOR was thus used to examine the impacts in each category as well as the overall sustainability index.

Figure 8.1 through Figure 8.3 provide a comparative chart for the three cases (Base Case, Configuration 1 and Configuration 2 for economic, environmental and social impacts respectively. Configuration 1 is the one with the extra separator column and heater in the recycle stream and Configuration 2 is devoid of both.

8.3.1 Economic Impacts

Figure 8.1 provides a comparative chart for the three cases based on their economic impact. Complete SUSTAINABILITY EVALUATOR results are provided in the Appendix. It can be observed from the Figure 8.1 that the base case is much less lucrative than Configuration1 and Configuration 2 in terms of Revenue and Profit. The two configurations also score better in the Material Value Added category. When we compare Configuration 1 with Configuration 2 it can be observed that the latter is more profitable. This observation is as expected because of the extra separation column and preheater in Configuration 1 contributes to the added capital cost. Configuration 2 also yields higher profit because of the slight increase in mass flow rate of the product. In conclusion, it can be said that in terms of economic factors, Configuration 2 is the best among the three.

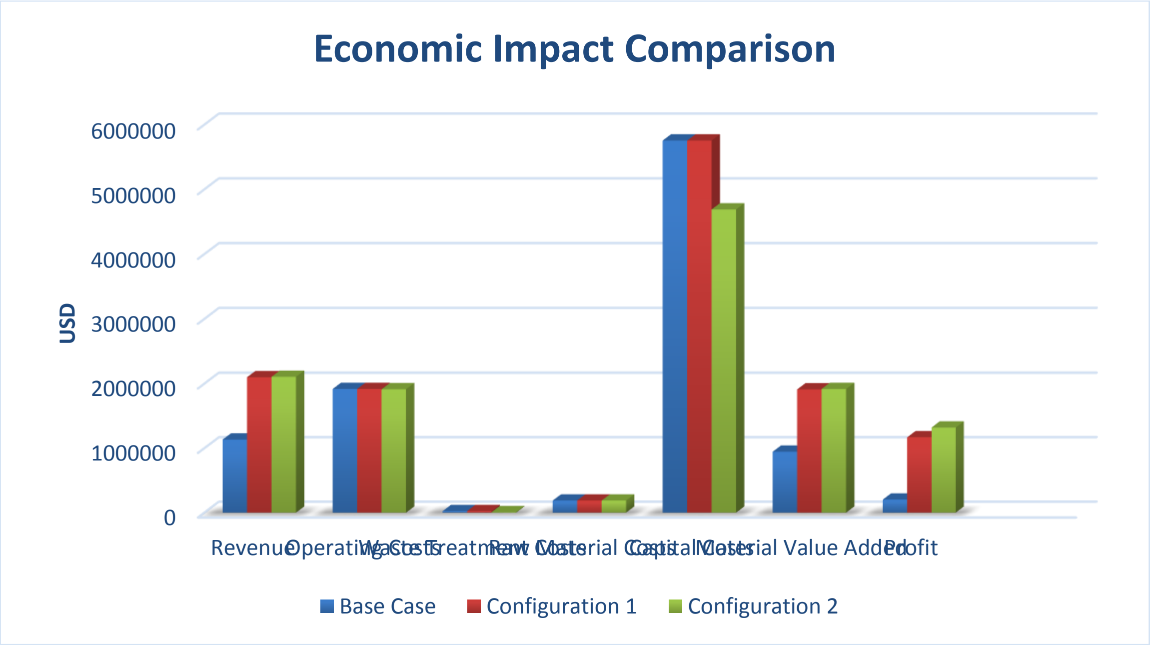


Figure 8.1: Comparison chart of the three cases for economic impact

8.3.2 Environmental Impacts

Figure 8.2 shows the environmental impact of the three cases for various categories as described previously. It is evident that the global warming is the dominating factor in terms of environmental impact categories. The reason for this is that both methyl lactate and methanol contribute towards global warming. Global warming is primarily caused by CO_2 and therefore the impact of other effluents is calculated by potency factors. Methyl lactate and methanol have enough potency so as to cause significant global warming compared to lactic acid. The other significant impact category is the aquatic oxygen demand. It can be termed as the measure for increase in oxygen needed by aerobic microorganisms due to water-pollutants **(Shadiya 2010).** This metric is based on converting all substances that increase the aquatic oxygen demand to oxygen equivalent. Methanol is the major contributor to this category.

In terms of comparison of the three cases, it is evident that configuration 2 has the least environmental impact and therefore is the best choice.

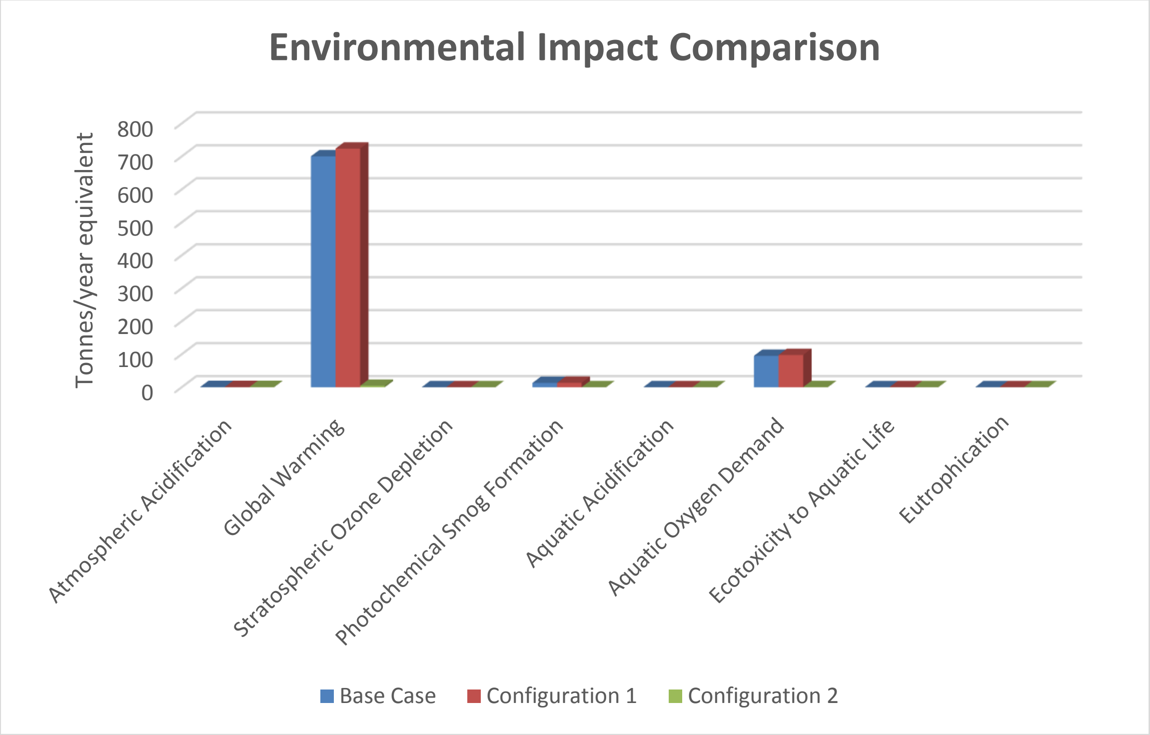


Figure 8.2: Comparison chart of the three cases for environmental impact

Table 8.3: Resource Usage Evaluation for the three cases

Environmental Impact	Units	Base Case	Configuration 1	Configuration 2
E-Factor	kg/kg	2.5	2.3	0.7
Reaction Mass Efficiency	%	30	33	33
Mass Productivity	%	27	30	30
Mass Intensity	kg/kg	2.3	2	2
Energy Intensity	kW/kg	0.0021	0.00109	0.00077
Water Intensity	kg/kg	3.8	3.4	3.4

8.3.3 Social Impacts

Figure 8.3 summarises the health risks attached with the three cases based on the factors discussed at the start of the chapter.

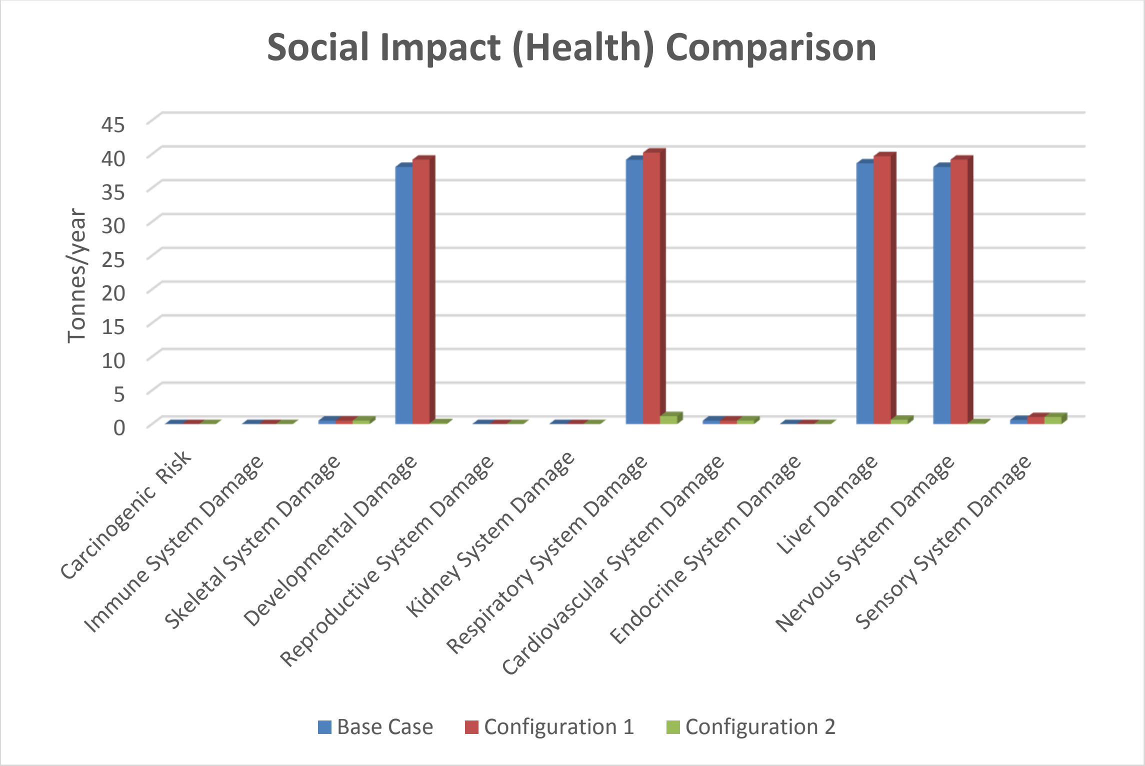


Figure 8.3: Comparison chart of the three cases for social impact

The chart shows that the there is equal contribution from development damage, respiratory system damage, liver damage and nervous system damage towards health concerns. This impact stems from the methanol in the waste stream.

Development damage index deals with the risks posed to a pregnant woman due to exposure to toxic chemicals. Chemicals known to be development toxicants were assigned a score of 1 and those suspected were assigned a score of 0.6.

The respiratory system damage index measures the risks associated primarily with the nasal passages and the lungs when are exposed to toxicants. A score of 0.6 was assigned to suspected toxicants.

The nervous system damage index takes into consideration the risks posed by toxicants to the central nervous system and each toxicant is again assigned a score of 0.6

The liver damage index takes into account the risks posed to the liver and gastrointestinal tract.

To calculate the total impact for each category, the individual score was multiplied by the amount of the toxicant in the waste stream.

8.3.4 Overall Impact

Table 8.4 summarizes the impact scores for each process case.

Table 8.4: Comparison of three cases in terms of overall sustainability index

Aspect(→) Case (↓)	Economical	Environmental	Social	Total
Base Case	0.25	0.10	0.25	0.19
Configuration 1	0.00	0.10	0.25	0.14
Configuration 2	0.00	0.07	0.25	0.13

It can be observed that the overall impact for all three processes is low. A lower impact value is an indicator of an inherently sustainable process and therefore all three process alternatives (Base Case, Configuration 1 and Configuration 2) could be termed as sustainable **(Shadiya 2010)**. This is expected s since there has been minimal use of toxic chemicals in the process which leads to lower environmental and social impacts. The process is also very economical since polymer grade lactic acid is priced high.

As far as comparison between process alternatives goes, Configuration 2 has the lowest impact in all three categories and consequently its overall impact index is also the lowest. This result is also as per initial expectations since Configuration 2 minimizes equipment use and maximizes material usage efficiency. However, as discussed in Chapter 7, Configuration 2 actually has higher environmental impact according to LCA analysis. This contradiction can be attributed to the fact that unlike LCA, the sustainability evaluator does not include indirect sources for environmental impact calculation. Therefore, the environmental impact due to fossil fuel use is not considered for impact assessment in the sustainability evaluator. It can be thus concluded that the environmental impact calculation part of the sustainability evaluator needs to be used with caution. In cases where the impact due to fossil fuels is known to be comparatively lower, the sustainability evaluator will be a highly efficient tool for impact assessment. However, if the fuel usage dominates the environmental impacts, it is advisable to use a comprehensive analysis tool like LCA.

CHAPTER IX

CONCLUSIONS AND RECOMMENDATIONS

9.1 Conclusions

This work deals with sustainable development of a process to produce polymer grade lactic acid which is used for Poly Lactic Acid (PLA) manufacture. The following step-wise methodology was adopted for the analysis (Figure 9.1)

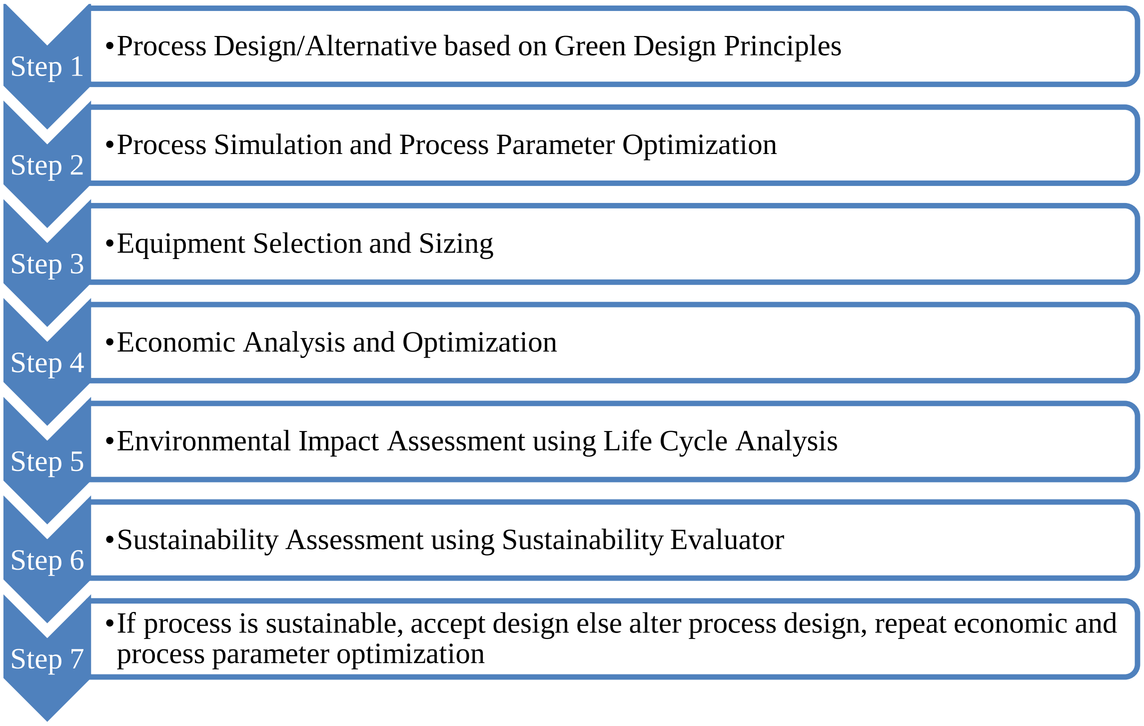


Figure 9.1: Sustainable process design methodology

The methodology depicted above can be used as a general framework for sustainable process design. Table 9.1 summarizes the details about the details of each step along with tools utilized.

Table 9.1: Summary of step-wise design procedure along with the tool used in each step

Steps	Action	Tools
1.	General process design based on process description, literature and material and energy balance conforming to green design principles.	Process Simulator (Aspen Plus)
2.	Process simulation and process parameter optimization utilizing sensitivity analysis results	Process Simulator (Aspen Plus)
3.	Equipment Selection based on process information and sizing calculations based on process simulation results.	Process Simulator (Aspen Plus) and Equipment Sizing tool (Aspen Icarus Process Evaluator)
4.	Economic analysis and optimization based on process simulation data	Process Simulator (Aspen Plus) and Economic Analyzer (Aspen Process Economic Analyzer)
5.	Environmental impact assessment using Life cycle Assessment (LCA) studies based on process simulation data	SimaPro
6.	Sustainability Assessment for process alternatives	Sustainability Evaluator

Therefore, in this work, not only a sustainable process is developed but also a general sustainable process design framework has been established.

Following were the step-wise outcomes of this work:

9.1.1 Process Simulation Outcomes

A process flow diagram for the production of polymer grade lactic acid was developed using Aspen Plus. The process was successfully simulated and converged results were obtained. An extensive sensitivity analysis was conducted on each of the key pieces of equipment to obtain high purity methyl lactate and subsequently pure lactic acid. The process conditions were subsequently optimized based on these results. The desired purity of polymer grade lactic acid (99 wt. %, dry basis) was obtained. Also, the purity of methyl lactate was above the desired percentage of 98.5 wt. %.

9.1.2 Economic Analysis and Optimization Outcomes

An economic analysis was carried out based on the converged simulation results for Configuration 1 and Configuration 2. The comparative results are depicted in Table 6.4. It can be observed that Configuration 2 is more profitable as expected. The payback period reduces from 6.28 years for Configuration 1 to 4.59 years for Configuration 2 which is a distinct improvement. The same has been illustrated in Table 6.4.

Table 6.4: This table shows the results of an economic analysis conducted on the two configurations

Configuration	Total Project Capital Cost (USD)	Total Operating Cost (USD per year)	Total Raw Materials Cost (USD per year)	Total Utilities Cost (USD per year)	Total Product Sales (USD per year)	Payback Period (Years)
Configuration 1	5,753,800	1,918,520	246,500	41,659	4,743,180	**6.28**
Configuration 2	4,689,640	1,913,990	246,500	40,422	4,723,020	**4.59**

From the cost analysis it was observed that the Bubble Column Reactor was the biggest contributor to the total cost. Therefore, Economic Optimization was carried out for the bubble column reactor. Optimization was carried out via the Aspen Plus Optimizer Block. The optimizer was used to determine the optimum process conditions for the Bubble Column Reactor. Optimum values for distillate, bottom, reboiler duty and no. of stages were determined and are listed in Table 6.14.

Table 6.14: Optimum operating conditions obtained from the Aspen Plus Optimizer

Parameter	Units	Optimum Value
No. of stages	-	16.4
Distillate	kg/hr	66.7
Bottoms	kg/hr	12.1
Reboiler Duty	J/s	9866.5

9.1.3 Life Cycle Assessment (LCA) Study Outcomes

Life Cycle Assessment (LCA) studies were carried out based on the converged simulation results of Configuration 1 and Configuration 2. The LCA studies reveal that Configuration 2 has approximately 40% higher environmental impact than Configuration 1. This result is unexpected because the overall waste in Configuration 2 is lower than that in Configuration 1 and we therefore would have assumed the impacts to be the other way round. These results could be attributed to the fact that although Configuration 2 gives out lesser waste, it requires higher amount of steam for heating which indirectly leads to higher fuel use. Although the utility cost is not affected greatly because the cooling water cost compensates for the additional steam cost, the environmental impact is varies noticeably. Table 9.2 lists the steam requirement in kg/day for both configurations.

Table 9.2: Total steam requirement comparison

Configuration	Steam Requirement	Units
Configuration 1	2823.48	kg/day
Configuration 2	4313.47	kg/day

A more detailed analysis reveals that the additional steam requirement is because of the fact that as Configuration 2 doesn’t separate out the methanol before recycling, there is added steam requirement for the bubble column reactor to achieve the same. The additional steam used comes from fossil fuel sources and therefore has higher environmental impact.

9.1.4 SUSTAINABILITY EVALUATOR Analysis Outcomes

The final step of process development was the evaluation of the three cases using the SUSTAINABILITY EVALUATOR. The SUSTAINABILITY EVALUATOR provided a detail impact assessment for the three process cases in terms of all three sustainability aspects – economical, environmental and social. The overall sustainability index results are displayed in Table 8.3. As can be observed from the results, Configuration 2 has the least impact in all three sustainability aspects and consequently has the lowest overall impact. The result is on expected lines since in Configuration 2 we are achieving the desired results using the minimum equipment and maximizing the material efficiency. However, it should be noted that although Configuration 2 has lowest environmental impact according to the sustainability evaluator, it has approximately 40% higher impact according to the LCA study. As pointed out in section 9.1.3, the higher impact is due to the higher steam requirements. The SUSTAINABILITY EVALUATOR only accounts for the emissions from the waste streams and does not include the emissions from the fossil fuel used for generating the steam. This is one of the advantages of an LCA study. It gives a more holistic analysis thereby enabling us to make better decisions.

9.1.5 Overall Outcome

From the above analysis it can be concluded that although, prima fascia, Configuration 2 appears to be the more sustainable option in all three sustainability categories, it actually has higher overall environmental impact as explained in section 9.1.4. Having said that, Configuration 2 still fares significantly better in terms of economy and social impact and therefore the decision to choose between the two options is up to the end-user. If the environmental impact is not an important factor in decision making, the end-user should prefer Configuration 2. However, if the environmental impacts are deemed to be significantly affecting the environment and/or if the company policies recommend choosing “greener” process designs then Configuration 1 is preferred. Additionally, government regulatory policies and laws encourage processes with minimum environmental emissions by providing monetary incentives.

9.2 Recommendations

The step-wise methodology adopted in this work could be used for sustainable process design for different types of processes. The framework could also be utilized for testing the feasibility of a process, comparing different process alternatives or optimizing process parameters. The tools used in this work are versatile and adaptable and therefore could suit many different kinds of process/products.

9.3 Future Work

Although this work addresses all the issues associated with developing a sustainable process, especially the incorporation of all three aspects of sustainability into process design, there is still scope for improvement. Following are the suggested approaches

1) Develop a more robust optimizer by linking Aspen Plus optimizer and leapfrogging optimizer **(Rhinehart, Su et al. 2012)**.
2) Improve the sustainability evaluator by including new chemicals and impact categories in order to make it more versatile.
3) Improve social impact quantification
4) Incorporate environmental regulatory laws and policies in the design process.

Develop a framework which integrates process simulator, multi-objective optimization, life cycle assessment (LCA) and the sustainability evaluator

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APPENDICES

This sections provides additional data/results obtained during the study. It primarily includes the detailed sustainability analysis results for both configurations and comprehensive economic analysis for Configuration 1.

Sustainability Evaluator Results – Base Case

OUTPUTS for Environmental Burden Evaluation		
Atmospheric Acidification	0.57	Ton/y Sulfur Dioxide Equivalent
Global Warming	710.07	Ton/y Sulfur Carbon Dioxide Equivalent
Stratospheric Ozone Depletion	0	Ton/y Trichlorofluoromethane Equivalent
Photochemical Smog Formation	13.16	Ton/y Ethylene Equivalent
Aquatic Acidification	0.035	Ton/y H+ Ions Equivalent
Aquatic Oxygen Demand	96.21	Ton/y Oxygen Equivalent
Ecotoxicity to Aquatic Life	0	Ton/y Copper Equivalent
Eutrophication	0	Ton/y Phosphate Equivalent

OUTPUTS for Resource Usage Evaluation		
Effective Mass Yield	0.3	
E-Factor	2.51	Kg/Kg
Atom Economy	1.367	
Mass Intensity	3.71	Kg/Kg
Mass Productivity	0.27	
Reaction Mass Efficiency	0.3	
Material Intensity	2.34	Kg/Kg
Energy Intensity/ Fossil Fuel Usage	0.04	KW/Kg
Water Intensity	3.83	Kg/Kg

OUTPUTS for Process Safety Evaluation		
	Results	Maximum Value
Heat of main reaction index	2	0.25
Heat of side reaction index	0	0
Flammability index	6	0.75
Explosiveness index	4	0.5
Toxic Exposure Index	24	0.8
Corrosiveness index	0	0
Temperature index	6	0.75
Pressure index	0	0
Equipment safety index	4	0.5
Safety Level of Process Structure index	4	0.4
Total Inherent Safety index	50	

OUTPUTS for Economic Evaluation		
Revenue	1133403.84	
Operating Costs	41659.3	
Waste Treatment Costs	24629.62	
Raw Material Costs	188020.27	
Capital Costs	5753800	
Annualized Capital Cost	676071.5	
Material Value Added	945383.57	
Profit	203023.15	

OUTPUTS for Health Evaluation		
Carcinogenic Risk	0	Tons/yr
Immune System Damage	0	Tons/yr
Skeletal System Damage	0.5256	Tons/yr
Developmental Damage	38.11	Tons/yr
Reproductive System Damage	0	Tons/yr
Kidney System Damage	0	Tons/yr
Respiratory System Damage	39.16	Tons/yr
Cardiovascular System Damage	0.52	Tons/yr
Endocrine System Damage	0	Tons/yr
Liver Damage	38.64	Tons/yr
Nervous System Damage	38.11	Tons/yr
Sensory System Damage	0.62	Tons/yr

OUTPUTS for OVERALL SUSTAINABILITY IMPACT		
Economic Impact	0.25	
Environmental Impact	0.1	
Social Impact	0.25	
Sustainability Index	0.19	

Sustainability Evaluator Results – Configuration 1

OUTPUTS for Environmental Burden Evaluation		
Atmospheric Acidification	0.57	Ton/y Sulfur Dioxide Equivalent
Global Warming	733.3	Ton/y Sulfur Carbon Dioxide Equivalent
Stratospheric Ozone Depletion	0	Ton/y Trichlorofluoromethane Equivalent
Photochemical Smog Formation	13.52	Ton/y Ethylene Equivalent
Aquatic Acidification	0.03	Ton/y H+ Ions Equivalent
Aquatic Oxygen Demand	98.87	Ton/y Oxygen Equivalent
Ecotoxicity to Aquatic Life	0	Ton/y Copper Equivalent
Eutrophication	0	Ton/y Phosphate Equivalent

OUTPUTS for Resource Usage Evaluation		
Effective Mass Yield	0.33	
E-Factor	2.34	Kg/Kg
Atom Economy	1.37	
Mass Intensity	3.34	Kg/Kg
Mass Productivity	0.3	
Reaction Mass Efficiency	0.33	
Material Intensity	2	Kg/Kg
Energy Intensity/ Fossil Fuel Usage	0.001	KW/Kg
Water Intensity	3.45	Kg/Kg

OUTPUTS for Process Safety Evaluation		
	Results	Maximum Value
Heat of main reaction index	4	0.5
Heat of side reaction index	0	0
Flammability index	6	0.75
Explosiveness index	4	0.5
Toxic Exposure Index	24	0.8
Corrosiveness index	0	0
Temperature index	6	0.75
Pressure index	0	0
Equipment safety index	4	0.5
Safety Level of Process index	4	0.4
Total Inherent Safety index	52	

OUTPUTS for Economic Evaluation		
Revenue	2099947.2	
Operating Costs	41659.3	
Waste Treatment Costs	24629.62	
Raw Material Costs	188020.27	
Capital Costs	5753800	
Annualized Capital Cost	676071.5	
Material Value Added	1911926.93	
Profit	1169566.51	

OUTPUTS for Health Evaluation		
Carcinogenic Risk	0	Tons/yr
Immune System Damage	0	Tons/yr
Skeletal System Damage	0.52	Tons/yr
Developmental Damage	39.17	Tons/yr
Reproductive System Damage	0	Tons/yr
Kidney System Damage	0	Tons/yr
Respiratory System Damage	40.22	Tons/yr
Cardiovascular System Damage	0.52	Tons/yr
Endocrine System Damage	0	Tons/yr
Liver Damage	39.7	Tons/yr
Nervous System Damage	39.17	Tons/yr
Sensory System Damage	1.05	Tons/yr

OUTPUTS for OVERALL SUSTAINABILITY IMPACT		
Economic Impact	0	
Environmental Impact	0.1	
Social Impact	0.25	
Sustainability Index	0.14	

Sustainability Evaluator Results – Configuration 2

OUTPUTS for Environmental Burden Evaluation		
Atmospheric Acidification	0.57	Ton/y Sulfur Dioxide Equivalent
Global Warming	13.97	Ton/y Sulfur Carbon Dioxide Equivalent
Stratospheric Ozone Depletion	0	Ton/y Trichlorofluoromethane Equivalent
Photochemical Smog Formation	0.18	Ton/y Ethylene Equivalent
Aquatic Acidification	0.03	Ton/y H+ Ions Equivalent
Aquatic Oxygen Demand	1.25	Ton/y Oxygen Equivalent
Ecotoxicity to Aquatic Life	0	Ton/y Copper Equivalent
Eutrophication	0	Ton/y Phosphate Equivalent

OUTPUTS for Resource Usage Evaluation		
Effective Mass Yield	0.33	
E-Factor	0.67	Kg/Kg
Atom Economy	1.36	
Mass Intensity	3.33	Kg/Kg
Mass Productivity	0.3	
Reaction Mass Efficiency	0.33	
Material Intensity	1.99	Kg/Kg
Energy Intensity/ Fossil Fuel Usage	0	KW/Kg
Water Intensity	3.43	Kg/Kg

OUTPUTS for Process Safety Evaluation		
	Results	Maximum Value
Heat of main reaction index	4	0.5
Heat of side reaction index	0	0
Flammability index	6	0.75
Explosiveness index	4	0.5
Toxic Exposure Index	24	0.8
Corrosiveness index	0	0
Temperature index	6	0.75
Pressure index	0	0
Equipment safety index	4	0.5
Safety Level of Process Structure index	4	0.4
Total Inherent Safety index	52	

OUTPUTS for Economic Evaluation		
Revenue	2106254.4	
Operating Costs	40421.7	

Waste Treatment Costs	7053.55	
Raw Material Costs	188020.27	
Capital Costs	4689640	
Annualized Capital Cost	551032.7	
Material Value Added	1918234.13	
Profit	1319726.17	

OUTPUTS for Health Evaluation		
Carcinogenic Risk	0	Tons/yr
Immune System Damage	0	Tons/yr
Skeletal System Damage	0.52	Tons/yr
Developmental Damage	0.13	Tons/yr
Reproductive System Damage	0	Tons/yr
Kidney System Damage	0	Tons/yr
Respiratory System Damage	1.18	Tons/yr
Cardiovascular System Damage	0.52	Tons/yr
Endocrine System Damage	0	Tons/yr
Liver Damage	0.65	Tons/yr
Nervous System Damage	0.13	Tons/yr
Sensory System Damage	1.05	Tons/yr

OUTPUTS for OVERALL SUSTAINABILITY IMPACT		
Economic Impact	0	
Environmental Impact	0.068	
Social Impact	0.25	
Sustainability Index	0.127	

Configuration 1 Investment Analysis Data

Project Cash flow Details

ITEM	**UNITS**	
TW (Number of Weeks per Period)	Weeks/period	52
T (Number of Periods for Analysis)	Period	20
DTEPC (Duration of EPC Phase)	Period	0.692308
DT (Duration of EPC Phase and Startup)	Period	1.07692
WORKP (Working Capital Percentage)	Percent/period	5
OPCHG (Operating Charges)	Percent/period	25
PLANTOVH (Plant Overhead)	Percent/period	50
CAPT (Total Project Cost)	Cost	5.75E+06
RAWT (Total Raw Material Cost)	Cost/period	246500
PRODT (Total Product Sales)	Cost/period	4.74E+06
OPMT (Total Operating Labor and Maintenance Cost)	Cost/period	853370
UTILT (Total Utilities Cost)	Cost/period	41659.3
ROR (Desired Rate of Return/Interest Rate)	Percent/period	20
AF (ROR Annuity Factor)		5
TAXR (Tax Rate)	Percent/period	40
IF (ROR Interest Factor)		1.2
ECONLIFE (Economic Life of Project)	Period	10
SALVAL (Salvage Value (Percent of Initial Capital Cost))	Percent	20
DEPMETH (Depreciation Method)		Straight Line
DEPMETHN (Depreciation Method Id)		1
ESCAP (Project Capital Escalation)	Percent/period	5
ESPROD (Products Escalation)	Percent/period	5
ESRAW (Raw Material Escalation)	Percent/period	3.5
ESLAB (Operating and Maintenance Labor Escalation)	Percent/period	3
ESUT (Utilities Escalation)	Percent/period	3
START (Start Period for Plant Startup)	Period	1
PODE (Desired Payout Period (excluding EPC and Startup Phases))	Period	
POD (Desired Payout Period)	Period	
DESRET (Desired Return on Project for Sales Forecasting)	Percent/Period	10.5
END (End Period for Economic Life of Project)	Period	10
GA (G and A Expenses)	Percent/Period	8
DTEP (Duration of EP Phase before Start of Construction)	Period	0.442308
OP (Total Operating Labor Cost)	Cost/period	832770
MT (Total Maintenance Cost)	Cost/period	20600.1

Equipment Cost Details

Component Name	**Component Type**	**Total Direct Cost**	**Equipment Cost**	**Equipment Weight**	**Installed Weight**
		(USD)	(USD)	LBS	LBS
BUBLCOL-cond	DHE TEMA EXCH	45100	7700	270	3177
BUBLCOL-cond acc	DHT HORIZ DRUM	107000	15300	2700	11651
BUBLCOL-reb	DRB U TUBE	58900	12200	320	4048
BUBLCOL-reflux pump	DCP CENTRIF	27600	4400	200	2218
BUBLCOL-tower	DTW TRAYED	209300	58500	14500	30609
HEAT1	DHE TEMA EXCH	47800	7700	270	4137
HEAT2	DHE TEMA EXCH	47800	7700	270	4137
HEAT3	DHE TEMA EXCH	47800	7700	270	4137
HYDREACT	DAT REACTOR	152800	22000	1000	14337
SEPARAT1	DTW TRAYED	170000	31600	4500	19252
SEPARAT2	DVT CYLINDER	120600	15200	2600	15297
SEPARAT3	DTW TRAYED	172900	28800	4000	19631
SEPARAT4	DTW TRAYED	164800	31200	4500	17245

Project Capital Summary

PROJECT CAPITAL SUMMARY	Total Cost	Design, Eng, Procurement	Construction Material	Construction Manhours	Construction Manpower	Construction Indirects
Purchased Equipment	234110	-	234110	-	-	-
Equipment Setting	8433	-	-	279	8433	-
Piping	293025	-	131246	5426	161779	-
Civil	69901	-	36136	1381	33765	-
Steel	49106	-	41590	269	7516	-
Instrumentation	880242	-	725999	5078	154243	-
Electrical	500082	-	431993	2363	68089	-
Insulation	86874	-	44260	1884	42614	-
Paint	22079	-	6154	714	15925	-
Other	2430200	1532000	169300	-	-	728900
Subcontracts	0	-	-	-	-	-
G and A Overheads	91262	0	54624	-	14771	21867
Contract Fee	271133	107240	43135	-	48685	72074
Escalation	0	0	0	-	0	0
Contingencies	888561	295063	345338	-	100048	148111
Total Project Cost	5753800					

VITA

Susmit Sunil Bapat

Candidate for the Degree of

Master of Science

Thesis: SUSTAINABLE PROCESS DEVELOPMENT FOR POLYMER PRECURSOR BASED ON ECONOMIC ANALYSIS AND LIFE CYCLE ASSESSMENT STUDIES

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