2012

A Modeling, Optimization, and Analysis Framework for Designing Multi-Product Lignocellulosic Biorefineries

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A MODELING, OPTIMIZATION, AND ANALYSIS FRAMEWORK FOR DESIGNING MULTI-PRODUCT LIGNOCELLULOSIC BIOREFINERIES

A Dissertation

Submitted to the Graduate Faculty of the Louisiana State University and Agricultural and Mechanical College in partial fulfillment of the requirements for the degree of Doctor of Philosophy in The Department of Chemical Engineering

by

Paritosh Sharma
B.S. Texas Tech University 2007
August 2012
This dissertation is dedicated
to the memory of my father,

Prem Kumar Sharma
ACKNOWLEDGEMENTS

I want to begin by thanking my research advisor, Professor Jose A. Romagnoli, for his the manner in which he handled my 4 years of doctoral work with him. He gave me ample room to guide my research the way I saw fit while providing me with very pointed remarks and critique throughout my work. Under him, I have grown into a person that I myself did not think I could be.

“Jose I can’t thank you enough for helping me become the person I am today.”

I also want to acknowledge my family, and especially my mother, my grandmother, my uncle (Arun Prakash) and my aunt (Anu Prakash). For the past 10 years that I have been in school (undergraduate and doctorate) they have persevered with me through thick and thin. I could not have asked for a better support system around me, as I was able to dedicate myself to research work without having to worry about any extraneous distractions.

“Mom, Mausi, Mausaji, Nani I couldn’t have gone through these 10 years without you”

Next, I really want to take a moment and thank my fiancé, Hayley Mosher. She has put up with a lot over the past four years we’ve been together. My all-nighters at the chemical engineering department and mood swings because of workload; really I don’t know how she put up with me.

“Hayley, I hope someday I can make up these 4 years up to you”
Finally, I want to thank my research group peers, who have always been there to guide me through the daily gyrations of research work. Many a time, when I came to a stalemate at moving my research forward, my research mates were always there to help through my problems. This research work, in part, has come to fruition through their efforts.

“Guys, this dissertation belongs to you as much as it does to me. Thank you for all your help!”
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ABSTRACT

The objective of this research is to propose a methodology to develop modular decision analysis frameworks to design value chains for enterprises in the renewable fuels and chemicals sector. The decision support framework focuses on providing strategic decision support to startup and new product ventures. The tasks that are embedded in the framework include process and systems design, technology and product selection, forecasting cost and market variables, designing network capacities, and analysis of risks.

The Decision support system (DSS) proposed is based on optimization modeling; systems design are carried out using integer programming with multiple sets of process and network configurations utilized as inputs. Uncertainty is incorporated using real options, which are utilized to design network processing capacity for the conversion of biomass resources. Risk analysis is carried out using Monte Carlo methods.

The DSS framework is exemplified using a lignocellulosic biorefinery case study that is assumed to be located in Louisiana. The biorefinery utilizes energy crops as feedstocks and processes them into cellulosic biofuels and biobased chemicals. Optimization modeling is utilized to select an optimal network, a fractionation technology, a fermentation configuration, and optimal product recovery and purification unit operations.

A decision tree is then used to design incremental capacity under uncertain market parameters. The valuation methodology proposed stresses flexibility in decision making in the face of market uncertainties as is the case with renewable fuels and chemicals. The value of flexibility, termed as “Option Value” is shown to significantly improve the net present value of the proposed biorefinery.
Monte Carlo simulations are utilized to develop risk curves for alternate capacity design plans. Risk curves show a favorable risk reward ratio for the case of incremental capacity design with embedded decision options.

The framework proposed here can be used by enterprises, government entities and decision makers in general to test, validate, and design technological superstructures and network processing capacities, conduct scenario analyses, and quantify the financial impacts and risks of their representative designs. We plan to further add functionality to the DSS framework and make available the tools developed to wide audience through an “open-source” software distribution model.
1. INTRODUCTION AND BACKGROUND

1.1 Energy Production – History and Future Drivers

In the past couple of decades, the world population has increased 25 percent largely driven by growth in emerging market countries, namely, China, India, Brazil and Russia. Additionally, it is predicted that this number, currently at approximately 6 billion, will increase nearly 50 percent to 9 billion by 2050 (figure 1-1).

![Figure 1-1: Projected world population trend](image)

This increase is and will be largely driven by Asian and African nations where an emerging middle class and improved healthcare and civic amenities have increased family disposable income levels and extended life expectancies, respectively. Two major consequent trends that are bound to follow this population and income growth are increasing demand for commodities, such as energy and food, to satiate the needs for this emerging middle class. In terms of energy, electrification of previously rural and desolate areas around the world, emerging highway and road connectivity in individual emerging nations, and higher levels of
disposable income coupled with an aspirational middle class consumer will undoubtedly put significant pressure on the world energy resources to satisfy these demands. Consequently, a sharp rise in energy supply is necessitated in order to maintain a semblance of supply-demand balance in world energy markets and prevent runaway energy price inflation. Over the last century the world has derived most of its energy needs from fossil-based resources primarily composed of crude oil and its derivatives, natural gas and other short-chain liquid hydrocarbons, and thermal coal. By their very nature, fossil fuels are formed underground and the entire process takes millions of years before they are available in usable form, making these resources essentially non-renewable. While they have been a very important driver of the world engine in the past, the depletion of these resources has put in doubt their long-term sustainability in subsidizing the lion share of the world energy needs going into the future. The confluence of the aforementioned observations and factors has brought to the forefront the role that renewable resources of energy can play as a part of a comprehensive solution to growing energy demanded by the world population, currently and in the future.

1.1.1 Renewable Energy Production

Renewable energy in its broad sense is energy that is derived from natural resources such as sunlight, wind, water, and geothermal heat; these resources have shorter cycles of replenishment and are provided by nature on a “near-continuous” basis. Renewable energy, as a final product, comes in 2 essential forms; (1) electricity that is transported geographically using fixed transportation mediums such as utility grids and wires, and (2) transportation fuels, such as biodiesel, ethanol and butanol, whose mediums (vehicles) are mobile in nature. It is essential to make this distinction between electricity and transportation fuels as a lot of times in the myriad of political arguments what is lost is this subtle yet
defining difference. As a general rule of thumb, renewable electricity sources do currently- and will in the future, replace thermal coal, while renewable transportation fuels are- and will replace crude oil and its derivatives. Of course, electric cars is one caveat where the distinction between static and mobile mediums is bridged, electricity still has to be generated at a fixed source and transported through fixed intermediate mediums in order to reach its final source, the vehicle. Once we have categorized the type of renewable energy, we can start to focus on the renewable resources that are currently utilized to produce these energies. Solar, wind, water, and hydrothermal sources in their native forms are used mostly to produce electricity. Renewable energy as a percentage of total energy supplied in the United States has been stuck at around 7-12 percent, although with recent initiatives and policies there seems to be a breakout in the trend with a larger percentage of our total energy supply coming for renewable (figure 1-2). In order to democratize the use of renewable energy specifically as transportation fuels, a seamless transformation where the renewable resources are converted from their native forms to a more usable and convertible form, is necessary. Fortunately nature provides such a transformative process through the use of photosynthesis, where carbon inputs are chemically altered into organic compounds using energy from sunlight. These compounds, primarily in the form of sugars and lipids, are used to form the structure and backbone of almost all plants and trees we see around us. The question then becomes, what processes and technologies are needed to harvest this natural energy and convert them into usable forms for use as portable, transportation fuels in an economically viable and environmental and socially responsible manner.
1.1.2 Sustainability and Energy Production

Sustainability in its broad sense is defined as the ability to endure something towards an objective. In the context of energy production, sustainability is referred to as the ability to transition from a global energy system based on consuming depletable fossil fuels to one based on non-depletable fuels (Brown et al.). A sustainable enterprise is often defined as an enterprise that does not have a negative socio-environmental impact on the society (Petrini and Pozzebon, 2009). Socio-environmental sustainability is intimately tied-in with the business sustainability of an enterprise; this proposed research aims at merging these broad aspects to yield an analytical system that can aid renewable energy enterprises in achieving their sustainability goals in the most efficient and cost-effective manner. Incorporating business sustainability implies further refining the definition of a sustainable enterprise; an enterprise that not only has the ability to positively impact the environment and the
community, but can also maintain such an impact through continued value creation and profitability.

In recent history of political cycles the world has seen the debate featuring energy (renewable versus non-renewable) go through multiple phases and faces; from climate change, their causes and solution to mitigating catastrophic consequences, to maintaining sovereign energy security by self-producing more energy for national use and reducing the dependence on foreign-imported energy, a lot of times from politically unstable regions of the world. In either case, renewable energy makes a strong case to hold a salient position in a well-diversified energy portfolio for any sovereign nation and warrants all the debate and discussion that it has received over the past 20-30 years. Development of a sustainable renewable energy portfolio has been recognized as a top priority by governments and enterprises around the United States to wean the country off our dependence on fossil resources and, within this broad category, reduce our dependence on foreign oil (figure 1-3).

![Figure 1-3: The historical ratio of oil imports versus total energy demand in the United States; Source: EIA.gov](image-url)
While higher economic capacities for solar and wind energy are highly desirable over the long run for electricity production, they are primarily replacing coal and natural gas, and consequently have little impact on the gross crude oil imports of the United States. A significant portion of our foreign oil imports are utilized in the production of transportation fuels, such as fuel oils (gasoline and diesel), and petrochemicals that are processed through value-added operations to produce high-value chemicals and polymers. Over the past five years demographic trends, geopolitical tensions, and loose central bank monetary policies have all put upward pressure on the market prices for crude oil (figure 1-4). With a significant portion of our oil purchases coming from foreign, often politically unstable regions, higher crude prices don’t only pose a significant risk to consumerism in the United States, but also pose a national security threat as we export more of our money to undesirable political regimes (figure 1-4).

**Figure 1-4:** Exported dollar value as a percentage of US GDP (superimposed on crude oil prices); *Source: EIA.gov*
More efficient energy production and utilization is one way to reduce the demand side of the supply-demand equation; but to improve the supply side for energy, more domestic oil drilling, and domestic resource diversification are the most plausible options. To truly embrace the resolve to concomitantly reduce gross fossil usage and dependence on imported energy, we as a country need to embrace a complete energy strategy; over the short-to-medium term time horizon we need to increase domestic resource production (fossil) and improve utilization efficiencies, while longer-term we need to execute a plan that will sustainably build in an efficient infrastructure to develop, produce, and distribute renewable energy and biobased chemicals.

1.1.3 Biobased Energy Generation

The concept of a biobased facility had been prevalent in the United States and the world in general, for hundreds of years. Paper and sugar mills are quintessential examples of bio-facilities where renewable raw materials such as wood pulp and sugarcane are converted to value-added products. The use of composting facilities and waste digesters in farms and rural areas around the world has been a source of sustainable generation of electric power from renewable resources for decades. In recent times, the emphasis on biobased production using renewable resources has significantly broadened its footprint to incorporate production of fuels, power and chemicals derived from a wider variety of renewable resources. Renewable power, a mainstay of the world’s electrification endeavors with hydropower being one of the world’s first commercially-viable renewable power source, has expanded in recent times to incorporate solar and wind-based generation. Some renewable transportation fuels that are already in the commercial production phase include first generation ethanol (corn ethanol) and biodiesel (from vegetable oils and animal fats). Yet the growth itself in
renewable energy supply is dwarfed in front of the growth produced in the fossil energy generation sectors (coal, natural gas and liquids, crude oil). While coal, natural gas and natural gas liquids, are used primarily for electricity generation, crude oil’s primary purpose is to supply energy for surface transportation. Additionally, crude oil is also a primary source for jet fuel derivation which is used for aviation purposes. Figure 1-5 shows the gross energy supply from renewable and non-renewable resources over the past 6 decades.

![Image of Figure 1-5: The gross energy supplied from different energy resources in the United States; Source: EIA.gov](image)

We notice from figure 1-5 a steepening of the growth rates in gross renewable energy outputs over the past decade, driven by policy initiatives, consumer behavior, and a sense of corporate environmental responsibility. Despite this uptick, recent ventures into renewable energy have been fraught with corporate failures. A driving reason for these unsuccessful
ventures, in part is governed by the lack of proper strategic planning in designing renewable energy plants and supply networks. Often exuberant forecasts of market evolution and insufficient levers in plant and supply chain design for risk mitigation have lead to companies failing to maintain solvency when lab- and bench-scale innovations are commercialized for the production of renewable products. An essential part of the planning process is garnering sufficient decision support to guide long-term strategic actions in the face of process and policy uncertainty, and market and competitive risks. The following dissertation is meant to introduce the development of a framework that can be used for the modeling, optimization, analyses, and design of renewable product systems and value chains. The framework’s functions are to provide strategic and tactical guidance, through the use of mathematically-driven decision modeling, for emergent renewable product system developers, startup enterprises, and government-sponsored entities and endeavors. My project is the first in hopefully a series of projects under the Process Systems Engineering banner at Louisiana State University, that will incrementally develop a fully functional and “renewable system-agnostic” decision support software framework, which can be distributed to enterprises in a multitude of biobased product industry in the years to come.

1.2 Literature Review

1.2.1 Decision Support Frameworks across Industries

Decision modeling frameworks are ubiquitously classified as decision support systems in a variety of industry verticals including the food and services industries, retail and grocery services, healthcare, and the process and manufacturing industries. In its most basic form, a decision support system is used to help value chain actors make mission-critical decisions that have an economic, social, or environmental impact on the stakeholders of the
value chain. Additionally, the nature of the decisions can be (1) strategic in nature leaning towards longer term decisions that will have an extended impact on stakeholders, (2) tactical which help stakeholders develop tactics to execute the strategies that are developing through strategic planning, or (3) operational in nature where the daily or weekly management of value chain functioning is emphasized. Table 1 shows a list of industries and corresponding decision support functions for a representative support framework.

<table>
<thead>
<tr>
<th>Industry</th>
<th>Decision Support Functions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pharmaceutical</td>
<td>R&amp;D product pipeline design; Manufacturing process design; Clinical trial study design</td>
</tr>
<tr>
<td>Retail</td>
<td>Supplier selection; supply chain management; store design; Product price optimization</td>
</tr>
<tr>
<td>Auto</td>
<td>Vehicle demand forecasting; parts’ supplier selection; production planning;</td>
</tr>
<tr>
<td>Agriculture</td>
<td>Crop yield predictions; operations management; risk analysis and cost/price hedging</td>
</tr>
</tbody>
</table>

1.2.2 Decision Support for Renewable Product Value Chains

Within the renewable products industry, decision support systems are relatively new, somewhat driven by the nascence of the industry itself. Owing to the complex nature of supply chains, conversion processes, and product markets, the use of decision support to aid in decision-making seems appropriate and in many cases it does lead more sound actions being taken by stakeholders based on a more complete picture of what is actually happening around them. Most decision support systems use complex mathematical formulations to model the interactions and interplay of actual physical phenomena that may go unaccounted for in case of ad-hoc decision making; consequently they are considered a valuable tool for any decision maker to compliment the “due diligence process” that they would go through before finalizing and executing critical decisions that would impact stakeholders over the
short, medium, and long terms. Table 2 shows a list of renewable product industries and corresponding support functions for a prototypical decision support framework.

**Table 1-2: Decision support functions specifically in renewable energy production systems**

<table>
<thead>
<tr>
<th>Renewable Energy Sub-industry</th>
<th>Decision Support Functions</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Solar</strong></td>
<td>Solar resource assessment; Power market analysis (supply, demand, price), load forecasting</td>
</tr>
<tr>
<td><strong>Wind</strong></td>
<td>Wind resource assessment, load and power forecasting, discrete parts’ inventory management</td>
</tr>
<tr>
<td><strong>Biomass (Electricity)</strong></td>
<td>Regional feedstock inventory analysis (GIS), feedstock logistics management, emissions management</td>
</tr>
<tr>
<td><strong>Hydropower</strong></td>
<td>Water resource assessment and planning, Hydropower forecasting, environmental management</td>
</tr>
</tbody>
</table>

1.2.3 Strategic Decision Support (SDS)

From the perspective of new renewable product value chains, we have to be cognizant of the fact that most of these endeavors are still in their design and pre-feasibility study phase, wherein, the processes that execute the purpose of the value chain are still non-existent. For example, 2nd and 3rd generation biofuels including cellulosic ethanol and butanol, and algae oil are still in the research, development and demonstration (RD&D) phase in their commercialization cycle, where feedstock supplies, processing technology yields, and product markets are still being studied and developed. When developing a decision support framework for such enterprises, the initial functions of the framework should therefore focus on aiding stakeholders in the intelligent design of the supply and production chains that will impact all actors and participants over strategic time horizons (10-30 years). Some key features that should be included for the design of a strategic decision support system are listed below:
Table 1-3: Strategic decision problems and proposed solutions for renewable product systems

<table>
<thead>
<tr>
<th>Strategic Decision Support Function</th>
<th>Model-based Decision Support Solution</th>
</tr>
</thead>
<tbody>
<tr>
<td>Technology selection and analysis</td>
<td>Integer-based systems optimization model governed by first-principles models</td>
</tr>
<tr>
<td>Market analysis</td>
<td>Long-term causal models for forecasting supply, demand, and prices in markets</td>
</tr>
<tr>
<td>Supply chain design</td>
<td>Spatial Optimization model for network design</td>
</tr>
<tr>
<td>Capital structure design</td>
<td>Monte Carlo model for simulation of projected cash flows</td>
</tr>
</tbody>
</table>

The inception of decision support tools and framework is a relatively new concept in the field of renewable energy and chemicals. Additionally, complete frameworks that can support a multitude of strategic and tactical tasks that a renewable products franchise is faced with are still scarce. Ramachandra et al (2005) presented a model based decision support tool that helped solar power companies estimate the probable amount of solar energy regionally. TOWNSCOPE II is an information management system developed by Teller and Azar (2001) that provides tools for solar energy evaluation in 3 dimensions. Rylatt et al (2000) developed a GIS-based decision support system for solar energy planning in urban environments. Munoz et al (2011) developed a model-based decision making tool to evaluate project investments in wind power generation taking into account uncertainty in wind regimes and in electricity market prices. They utilize Real options analysis as a means to develop strategic investment plans for project investment that hedge against market prices risks. Ouammi et al (2011) published a model based environmental decision support system that stressed optimal technology selection and site location for wind power generation. Arbaoui and Asbik (2010) presented a decision support tool for site-specific design of wind turbine system using constraint-based programming and detailed cost modeling. Olteanu (2011) developed a support system to study the impact of oilseed markets, crude markets, and policy directions on biodiesel value chains. The DSS was proposed as a constrained
systems optimization model that optimizes the major value chain activities and supports management decisions in strategic and tactical planning. In recent times, several analytical models have been suggested to study the effect of biomass species, technology choices, and plant capacities on the production and profitability of cellulosic ethanol (Kerstetter and Lyon; Huang et al, 2010; Brechbill and Tyner, 2008). NREL has developed several analytical models (Aden, 2007; Phillips et al, 2008; Kazi et al, 2010) that analyze different process configurations for the production of cellulosic ethanol. Huang et al (2010) provided a comparative analysis on the effect of feedstock choice and plant size on the economics of ethanol production. Laser et al (2009) quantified the impact of different technology scenarios on the production of cellulosic ethanol and power from switchgrass. The traditional Net Present Value (NPV) was used by Haas et al. (2005) to estimate production costs for biodiesel production. An increased emphasis on efficient supply chain management and NPV optimization has yielded substantial literature concerning supply chain modeling and strategic value optimization (Naraharisetti et al., 2008; Puigjaner et al., 2007; Lainez et al., 2009; Lu, 2003; Varma et al. 2006). Application of these techniques specifically to a biorefinery is an area which has recently started to receive considerable attention. To this end, Chambost et al. (2008) provided a qualitative summary describing a methodology to integrate the idea of a forest biorefinery into existing pulp and paper mills in Canada. Sammons et al. (2007) developed a framework for optimal product allocation for a flexible biorefinery. Their methodology provides a framework for process design and product slate selection based on optimization. Marvin et al (2011) developed an economic optimization model for a cellulosic ethanol value chain in the Midwest. Tursun et al. (2008) developed a multi-year transshipment and facility location model to determine the optimal size and time
to build each plant, the amount of raw material processed by individual plants, and the
distribution of bioenergy crops and ethanol across Illinois. Economic analyses have been
carried out for biorefineries on a project-by-project basis. Slade et al. (2009) analyzed the
effect of supply chain design on commercial feasibility of cellulosic ethanol. Dunnett et al.
(2008) provided an assessment methodology to measure the feasibility of decentralized
lignocellulosic ethanol processing in Europe. Tembo et al. (2003) presented an MILP
investment appraisal model for ethanol process facility location in Oklahoma. Eksioglu et al.
(2009) developed a methodology to analyze and manage a biomass-to-biorefinery supply
chain. As a part of government endeavors, Lynd et al. (2002) presented a comprehensive
strategic analysis of current biorefining capabilities, while suggesting co-product integration
as a means to achieving higher profitability. Wellisch et al. (2010) reported a general
overview of how different facets of sustainability intersect for biorefining systems. The
authors suggested a product-driven instead of process-driven approach to build sustainability
into biorefining systems. Along these lines, Mansoornejad et al. (2010) suggested and
exemplified a strategy for hierarchical product, process, and network design for biorefining
systems. Huang et al. (2010) developed a multi-stage supply chain optimization model for
biofuel supply chain. The decision variables included facility locations and capacity design.

1.2.4 Design of Strategic Decision Support Systems

The basic idea for a decision support framework is based on figure 1-6. This figure
shows how a standard, enterprise-wide decision analysis framework fits into a process
enterprise’s operating and management hierarchy. Specifically for a process enterprise,
decision support tools can encompass process simulation software, resource planning software, and supply chain management tools.

**Figure 1-6: Standard decision making process work flow through an enterprise's structure**

Following the figure above, starting from the ideation phase, engineers and/or management will discuss and identify major bottlenecks and issues in the process enterprise’s supply and demand chains; following the identification, solutions and ideas will be identified to tackle these issues. A major component of any decision support system is a forecasting module that estimates the future parameters that will impact the design and operation of the enterprise; these parameters can include feedstock/raw material supplies, input costs, process yields, product supplies, demand, and prices, and expenditures necessary to achieve the long- and short-term goals of the enterprise. The forecasting module can utilize a multitude of techniques, qualitative and quantitative, to generate forecasts for parameters that the stakeholders deem necessary to know accurately. Some forecasting techniques include time
series based methods, regression analyses, and causal models; each technique has its own place within the forecasting umbrella. Time series forecasts and regression analyses utilize historical data to predict future outputs and are more suitable for short to medium-term forecasting (based on time scale, 0-1 years) and for parameters that have sufficient historical data available. The applicability of time series forecasting and regression analyses diminishes when dealing with new products and technologies for which historical data is scarce. Causal models are suitable for long term forecasting and are usually based on experts’ understanding of the future evolution of macro-conditions; usually trends spotted using time series and regression analyses hold true over shorter time lengths, but over longer time horizons these trends seem to breakdown. For strategic decision support causal models are deemed the most apt, as they eliminate short term trends from the modeling endeavor and focus on the evolution of the macro-environment and how this impacts the parameters that are being forecasted. Additionally, for new products and technologies, it is important to “play-around” with the forecasting model parameters and judge qualitatively if the forecasted variables make sense; this step leads to an iterative development of the forecasting models where due diligence is necessary to develop remotely accurate forecasts. It has been shown that forecasts generated over longer time horizons usually tend to be inaccurate as the forecasted variables evolve in real-time; consequently the forecasting parameters and models need dynamic readjustment as new information becomes available in order to maintain a semblance of accuracy in the forecasted values. Additional methods for long range forecasts can involve judgment based methods, where industry experts can be surveyed to gauge their views of the future. These data can be combined with regression methods and causal models in order to forecast important enterprise parameters. Once again, this is an iterative process
and dynamically updating these models is deemed as important as the initial model
development itself.

Once the requisite parameter forecasts are generated over desired time scales
(strategic, tactical, or operational), these parameters are input into the decision analysis
framework where decision tools are used to model and generate actions that the enterprise
can then execute; the decision tools’ are meant to be a guiding force towards making the final
decision that is executed in real time and not an “end-all be all”. This implies that the
framework results are complimentary to human knowledge and should be used as a “support”
tool by stakeholders and not as a defining line set in stone. There are many reasons for taking
this “soft” approach as opposed to a hard-line stance, the primary one being that seldom are
real world phenomena and constraints represented accurately and completely in a decision
analysis framework. Although a decision modeler should spend significant effort in
representing, as closely as possible, what is actually happening in real life, the framework
can get over-complicated, cumbersome, and often incorrect to use if too much detail is built
into the framework. Nevertheless, having decision tools to aid in real-time decision making is
instrumental in studying the impacts of a variety of input actions on the long- and medium
term goals of an enterprise, without actually executing the actions. Additionally, for new
products and technologies, it is rare to have a complete understanding of the supply and
demand chains in the absence of actually design and operational history; in such scenarios a
decision analysis framework is absolutely essential to study the impact of multiple future
scenario realizations and the respective uncertainties in expected results from enterprise
actions. Often it is also noticed, especially for new products and technologies, that “hidden”
and unexpected correlations between various design, operational, and market parameters can

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be uncovered by simply representing the prospective supply and production chains as a complete system where upstream inputs, actions and outputs have an inescapable impact on the functioning of downstream nodes in the value chain. In the next section we will provide examples of value chain issues pertaining to hypothetical enterprises in different industries and demonstrate how a decision analysis framework can be utilized to resolve these issues.

1.2.5 Hypothetical Examples of SDS Systems

In this section, examples are provided of hypothetical enterprises in different industries, faced with realistic design and operational issues, and how decision framework can be used to guide their actions.

I. **Industry: Accessory Retail**

**Problem:** An accessory retailer has designed a new line of teenage accessories which they believe can be a game changer in the accessory retail market for teens between the ages of 13-18. The retailer has an approximate idea of their current input costs that it would take to commercially manufacture and distribute their product lines across the country. The retailer wants to develop a strategy to manufacture, market, and distribute this product line to consumers, which they believe will continue to buy the current development and future incremental changes over the next 5 years.

**Issues that need resolution:**

- Securing raw material supplies and managing input costs over the 5 year planning horizon;
Developing price points for accessories that balances expected profits against product demand (price elastic demand);

Developing a manufacturing strategy to manufacture the product lines by balancing manufacturing costs against product quality;

Developing a marketing and distribution strategy to maximize reach to consumer markets with the least possible costs;

Developing a strategy to add incremental design changes to the initial product line over the 5 year horizon in order to maintain profitable sales levels and even drive higher sales in the future.

Tackling these issues with the aid of a decision framework: As can be seen from the problem, a simple action to manufacture and sell a new consumer product is plagued by problems that scale multiple time periods, impact different aspects of the retail enterprise, and additionally, are inherently correlated as a decision to resolve one issue can impact a multitude of other issues spatially in the value chain and temporally over the planning and execution horizon. To tackle such a problem holistically, a decision framework, in conjunction with expert judgments, can- and should be utilized. The following are some possible tools that can be utilized to help decision makers in their decision making process.

1. First and foremost all planned iterations to the initial product line that the retailer plans to introduce over the 5 year horizon need to be enlisted, with raw material and labor requirements stated.
2. A forecasting model to predict future raw material requirements, market costs for securing adequate supplies, possible suppliers to supply these raw materials, and predicted macro-conditions that may impact these costs, can be developed.

3. Once the possible costs are determined and forecasted, the retailer can select appropriate locations for manufacturing facilities that balance the raw material purchase and transportation costs, with manufacturing (labor, taxes, and energy) and product distribution costs.

4. Once the spatial structure of the supply and demand chains are fixed, the retailer needs to develop an efficient marketing strategy to market these products to the consumers. Here human intervention is necessary as marketing models are based on expert judgments about consumer needs and aspirations, and what aspects of the prospective product line will appeal most to consumers.

5. Additionally, pricing models that develop price points for final products are necessitated; while prices should be high enough to account for input costs and appropriate profit margins, too high a price point can lead to demand destruction. Such a scenario, where product demands are extremely sensitive to retail price points require forecasting models that incorporate demand elasticity to prices and optimize the price points under input cost and consumer demand constraints.

6. Finally, upon execution of the first design iteration, consumer sentiment should be gauged and the aforementioned strategy should be tweaked if necessary in order to re-calibrate the enterprise expectations with the consumer response to
the new product line. In this way, a dynamic strategy that optimizes enterprise bottom-line through each step of the product life cycle can be executed.

II. **Industry:** Polymer Manufacturer

**Problem Statement:** A polymer manufacturer believes that it has discovered a new polymer that addresses a significant market need. The polymer production process is designed in-house and can utilize two different catalysts with similar functions but marginally different costs, properties, and final product yields. Additionally, the polymerization process utilizes as feedstock, outputs from a petroleum refinery that is currently utilized to produce another polymer with a stable market.

**Issues that need resolution:**

- Whether production of the polymer should be executed on a commercial scale;
- If executed, what catalyst should be utilized?
- How should the enterprise secure the feedstock – should some of the current feedstock be diverted or should new feedstock supplies be secured?
- What scale should the process be design for commercially (capacity)?
- What markets should be served?

**Tackling these issues with the aid of a decision framework:** For the aforementioned problem there are several issues that need to be addressed before a commercial scale production process is brought online. The following solutions implemented within a decision analysis framework can help guide decision makers in the right direction.
1. The first comment necessary to make here is about the length of the planning horizon over which the enterprise should execute a prospective strategy; in this case, a commercial facility will involve construction and startup time, and then a learning curve over which customer adoption rates will increase. This problem fits into the strategic planning case as longer time horizons are required for technology development and demonstration followed by market acceptance.

2. The first task at hand is to develop a process simulation that can simulate the lab-scale process using commercial simulation software or in-house process models.

3. For pre-feasibility studies, a market analysis can be conducted to gauge who are the potential customers. This can be conducted using surveys or through one-on-one meetings with potential customers.

4. Following the generation of the customer list, the quantitative market potential for the product should be determined in order to assess what possible production capacities may be installed. This again should be done through an engagement process with potential customers.

5. If the product is a commodity polymer, that is, it can be sold into multiple industry verticals and utilized different ways, a forecasting model (regression-based causal forecasting) can be utilized to assess the future market potential of the product. Independent parameters that are used to derive the potential demand over a strategic time horizon can include macro-economic variables such as GDP predictions, employment and income levels, and interest and inflation rates.

6. If the polymer is replacing an older product (produced by the same enterprise or rivals), product competition/cannibalization also needs to be accounted for.
Additionally, for non-patented technologies or in the case of rival technologies, product supplies (from competition) should also increase as the market expands. This in-turn will impact the price dynamics for the new product.

7. Once a preliminary forecasting model is conjured to forecast potential polymer production costs, supplies, demands, and prices, the enterprise needs to design an implementation strategy to decide when to and how much capacity should be installed, and what are the feedstock, resource, and capital requirements to execute the plan.

8. To gauge the financial performance of the simulated process, a traditional discounted cash flow (DCF) analysis can be utilized. Additionally, scenario analyses (what ifs) should be utilized in order to determine alternative strategies for commercial scale-up and production.

9. Once the lab-process is validated and a strategy is developed to implement the process on a commercial scale, most process enterprises will necessitate the use of a demonstration scale plant to test if the simulated process mirrors what actually happens. It should be kept in mind that the process models previously developed may require tuning following the operation of the demonstration plant in order to reconcile differences in simulated and observed data.

We can see from the aforementioned examples that even simple decisions with low complexity (at least on the surface) entail a significant amount of due diligence before any actions are implemented. Especially for strategic investment decisions such as plant and supply chain design, irreversible capital outlays are required upfront, with the future cash flows that are, in large part, highly uncertain. For renewable product value chains, this issue
is magnified owing in large part to the nascence of the industry as a whole. Processes to supply and convert resources to final products and then distribute them across end markets are still at the beginning of their developmental cycle and end markets are still underdeveloped at best. Add to that competition from rival product value chains that are highly established and efficient in their operations, such as crude oil, natural gas, and coal, and what we get is an industry in renewable energy and chemicals that is plagued by significant uncertainty and risk about what will unfold in the near and distant future. This is the driving force behind the conception of the proposed decision support system. With such uncertainty manifesting into capital risks, the DSS developed here has to be rooted under a strong theoretical basis, but exemplify capabilities to incorporate several practical considerations while providing strategic decision support. Given that there are such intricacies in strategic planning and a whole host of options to choose from, even for the simplest decision, I chose to utilize a model-based optimization approach as the basis for the development of the DSS. The next section will provide a bit more color on the optimization framework that is developed here and discuss in detail different aspect of the framework that make it amenable for strategic decision analysis and support.

1.3 Dissertation Motivation: A Case for Optimization Modeling for Decision Support

Despite a flurry of work in the field of renewable energy decision support, an integrated strategy that carefully models, optimizes, and examines multiple aspects of strategic decisions such as spatial network design, technology selection, process design, feedstock and raw material selection, and product portfolio design for renewable product value chains has yet to be investigated within a single framework. Within strategic planning, most models proposed are analytical models that assume a predetermined process, feedstock,
product portfolio, and value chain design; but with a host of configurations that have been identified and proposed in different research communities, an integrated approach that determines, in a fast and efficient manner, what configurations are the most promising is still missing. With innovation at its cutting edge in the renewable products’ sector, it is necessary to have decision models that can help stakeholders evaluate, qualitatively and quantitatively, what feedstock(s), technologies, and product provide the most favorable mix of near-term profitability while generating long-term value for its stakeholders. Some issues that have been under-appreciated to date in renewable product literature include:

1. Strategic optimization models that optimize value of a renewable product venture to all stakeholders including the enterprise, capital providers, suppliers, customers, and the environment;

2. Optimization and integration of business cash flows with process design, execution, and operations;

3. Optimization of capital allocation and financing decisions under uncertain input costs and supplies, technological evolution, and product markets.

The work proposed in this dissertation will incorporate the aforementioned characteristics (or lack thereof) into a complete, model-based decision support system. While the decision system will be formulated with multiple renewable supply chains in mind, the efficacy and applicability of the system will be tested by studying a representative supply and production chain, which converts biomass resources to biofuels and biochemicals, in detail. The arrangement of materials in the rest of the dissertation is done in form sections and chapters. The content of each section and chapter is mentioned briefly below.
1.4 Contributions of this Dissertation

The goal of this research is to develop a decision support platform that can be ubiquitously used by renewable product franchises in order to make more intelligent and mathematically-substantiated decisions and study the impact of their decisions on stakeholders. Through this research we wanted to apply the concepts of enterprise optimization to sustainable planning and development of renewable energy ventures. Given a slew of failures in recent times in renewable product endeavors, we wanted to develop a framework where risks that are inherent in any new product venture can be mitigate through careful planning and evaluation. Additionally, renewable energy and sustainability have received such tremendous attention in recent times that a confluence of research literature has been formed with a multitude of suggested products, feedstocks, and technologies. In such a situation it has become hard to separate the winners from the losers; as a part of our development we wanted to provide researchers and practitioners with a holistic platform based on which the economic, technical, and environmental merits of their innovation can be evaluated and possibly implemented. Finally, renewable energy sits in a very unenviable position; they (renewable energy technologies) are competing with well-established fossil resources in the energy markets. The fossil resource industry is a behemoth industrially, with decades, if not centuries, of experience in running a very lean and efficient supply and demand chain. In such a situation, capital markets can be a very unappetizing proposition for renewables as they compete with a proven industry for consumer acceptance. Although the environmental aspect is a definite positive in favor of renewables, we believe, that in the end sustainable development of the industry will only occur when market forces accept the technology as a viable replacement (or partner) to fossil energy. In that case, it becomes
imperative to evaluate renewable technologies in the presence of competitive markets and study the impact of market risk factors on the development and build out of renewable resource utilization capacity. Through this dissertation, we will analyze a novel structure of decision making and analysis, wherein the process and environmental characteristics are quantified not only based on their technical merits but also represented economically. We stress the monetization of all process- and environmental-related aspects of value chain design for renewable products, under the conception that truly sustainable industries will be built not only on their environmental merit but also in their ability to compete profitably with fossil resources.

1.5 Organization of Dissertation

This dissertation is organized into 5 sections followed by a concluding section and possible extensions to the research work. We also list the contributions, in terms of journal papers and conference presentations that have been made by the authors to general research literature regarding the design of renewable energy systems.

Chapter 2 introduces the concept of optimization-based decision support with applications to renewable product value chains. We try to legitimize the use of the proposed methodology to design complex renewable resource utilization systems. We also suggest a fundamental (first principles based) modeling framework that is developed as a means to carefully study the technical, economic and environmental impacts of renewable product value chains. A model building strategy is suggested in order to optimize material and energy flows across the value chain; the methodology focuses on incorporating real world design, environmental, and financial constraints with the material and energy flow equations and suggests a hybrid economic-environmental objective that can be optimized in order to satisfy
the sustainability-driven goals of a renewable product enterprise. Finally we propose the use of management science as means to bridge the gap between the technical relevance of a technology and its economic sustainability; here we use advanced financial techniques in conjunction with the systems models developed to represent the bioprocesses. Decision options are suggested as a means to mitigate market risks while designing value chains that are promising in their potential, but are characterized by a high degree of uncertainty with regards to their financial impact on stakeholders.

Chapter 3 focuses on exemplifying the suggest modeling framework with the use of a hypothetical biomass-to-bioproducts value chain. We assume an enterprise that is looking to establish a value chain in Louisiana that processes biomass resources to produce biofuels and value-added biobased chemicals. The suggested methodology from Chapter 2 is applied to this hypothetical case study with a detailed quantitative description of the prospective system. We pose a problem regarding network and technology superstructure design that the enterprise is faced with, and utilize a structured approach to mathematically optimize the design of the value chain under real world resource and financial constraints. As a significant value-add to the research, we develop deep environmental, energy, technical, and business analytics for the optimal design in order to lend more color to the design case.

Chapter 4 is dedicated to studying the impact of uncertainty on the optimal design yielded in chapter 3. We suggest a novel options-based integer programming framework in order to optimize the strategic build out of value chain capacity under market uncertainties. We suggest a hypothetical model of a real economy and incorporate the impact of macro-economic and competitive forces on the strategic decisions of the bio-enterprise. The integer model runs yield alternative design plans under different market scenario realizations that can
be used by the bio-enterprise in order to realize their goals of value creation. While options have been applied previously to study strategic aspects of different industry verticals, its applications to a biomass-to-bioproducts enterprise, and more specifically, the use of integer programming to represent real world decision is a novel contribution of this research.

Chapter 5 focuses on simulating the optimal design plans obtained in the previous chapters under market and process uncertainties. We utilize Monte Carlo methods to study the risk characteristics of the optimal designs that are obtained previously. Finally, we generate Value at-Risk metrics for each design plan to quantify the financial risks that may present themselves during the implementation of each design plan from chapter 4. While an optimized enterprise value and design strategy is obtained through options optimization in chapter 4, the trade off with financial risks, especially for marginally higher value creation, will become apparent through this exercise. We suggest that the final decision to implement one of the design strategies obtained through the framework implementation will come down to the risk appetite of an enterprise, that is, what level of financial risks are the stakeholders in the bio-enterprise willing to undertake in order to attain their strategic objectives.

Chapter 6 summarizes the research work that is presented in this dissertation. We summarize the modeling framework that is developed and discuss its implications by using the case study as a cornerstone. Additionally, future research work and possible extensions to the framework are suggested.
2. AN OPTIMIZATION-BASED STRATEGIC DECISION SUPPORT ARCHITECTURE FOR EMERGENT RENEWABLE VALUE CHAINS

2.1 Introduction

The previous chapter showed that the simplest of strategic decisions made by an enterprise involve a lot of due diligence and pre-implementation studies to gauge the impact of the decision across multiple components of a company’s value chain. This is especially true for new product value chains, such as a majority of renewable products, that do not have developed markets and a robust technological basis that is commercially proven to be successful. A slew of academic and industrial research, driven by policy initiatives, have created a large inventory of technologies, process and supply chain configurations, and final products that possess, in some way shape or form, attractive characteristics to supply our energy and chemical needs in the future. With such a confluence of configurations and technologies, it can get extremely difficult for a startup enterprise to select a robust design and operating strategy to implement in real time in order to produce renewable energy and/or biobased chemicals. Current markets for renewable fuels are additionally distorted by policy subsidies and support creating a large amount of uncertainty about how the industry will unfold in the future once government support is removed.

This dissertation provides a novel methodology to deal with a large number of aforementioned issues that plague renewable energy endeavors. We use model-based optimization as a basis to design the DSS as such techniques are inherently able to model underlying processes that govern real world phenomena and represent real-world constraints that govern the decisions made to operate these processes. With a large library of technologies available for the conversion of renewable resources to a variety of value-added
products, such an optimization framework can help stakeholders decipher what is the optimal portfolio of products to produce sustainably over the long-term and what is the optimal technological and network superstructure to convert feedstocks to final products. Granularity in the model can advance the incorporation of real world constraints, such as resource availabilities, capital requirements, market demands, and investor expectations, into the decision problems; these constraints help shape the decisions that are output from the model(s). The next section discusses the formulation of the framework and the individual components of the DSS.

2.2 A Model-based SDS System for Renewable Product Value Chains

2.2.1 Framework Design

Using framework features mentioned previously, we will suggest in this section, the design of a holistic decision analysis framework that can be utilized by a variety of renewable product enterprises to support feedstock, technology and selection decisions and design network processing capacities given uncertainty in product markets. The decision framework suggested here is developed with renewable products in mind, but its application is plausible in multiple industry verticals with minor changes to the content of the framework.
2.2.1.1 Quantitative Discussion of Design

Figure 2-1 shows a systems representation of the SDS System (SDSS); given that the purpose of the SDSS is to provide strategic decision support for new renewable product design decisions, the first step in the decision process is to conceptually formulate product, process, and network configurations that are believed to hold promise into the future. This by no means is a trivial task and requires at the very least, a reasonable amount of qualitative and quantitative market research. Issues such as technological potential, market potential, and supply constraints (for feedstocks and raw materials) should be evaluated in this pre-feasibility study phase; we term this as Life Cycle Inventory Analysis, where data (business, environmental, and socio-economic) about each technological configuration’s life cycle is collected and inventoried. Once a consensus is reached amongst principal stakeholders regarding the prospective configurations that can be executed, optimization modeling is utilized to actually select the optimal technological processes and configurations along with corresponding products, feedstocks, and network structure that can be used to satisfy stakeholder objectives. We use optimization instead of simulation models due their efficacy.
in evaluating multiple technological and product configurations simultaneously as opposed to individual assessment of each configuration (as with simulation models). Indeed once the optimal configuration is obtained, more detailed engineering analyses can and should be conducted (using simulations) to validate the results of optimization.

Once an optimal structure has been set, the next step in the strategic planning process is to design capacities for conversion processes in the value chain and evaluate supply and distribution network configurations that will convert the feedstock resources to final products and distribute the products to end markets. Traditionally one utilizes static discounted cash flow (DCF) analysis to estimate the value of a new project and decide whether to implement it or not (go or no-go decision). In DCF analysis, a capacity estimate is used as an input and financial metrics such as net present value (NPV), internal rate of return (IRR), and payback period (PBP) are utilized to estimate the profitability of the project. We posit that this is a rather archaic method for project analysis; with dynamic markets that are constantly evolving, to assume that capacity is established on some scale today with no prospects for expansion in the future, is painting a very incomplete and rather opaque picture of what the actual project’s potential can be. Even if it is assumed that future capacity expansions are possible, a static DCF model in no way values the importance of having this option at management’s disposal. The value of such dynamic capacity expansions in the future can often be the difference between a positive and a negative NPV project. Additionally, most DCF analyses are conducted with static structures for future product costs and markets, sometimes portraying an incorrect representation of what actually will conspire as the “future becomes the present” (as time evolves). Market forecasts that are utilized in most DCF analyses assume that complete information is available of future realizations in project
parameters, such as market demands, product prices, and input costs. While this assumption may simplify the decision problem, it in no way represents what may actually happen. Take for example the crude oil markets; during 2008 we saw a tremendous price spike in the oil markets due to various market- and geopolitical-based factors. For oil exploration companies, and companies that used oil-derived products as inputs, this had varying degrees of impacts on their stakeholders. Exploration companies that utilized static forecasts in projecting oil prices (based on a deterministic value) may not have had the structure in place to take full advantage of such a price rise. On the other hand, companies that had built in flexibility in their oil asset base were able to take advantage of this meteoric price rise (followed by an equally rapid price decline) by producing more oil during the appreciation period and contracting operations during the decline period. This is what we term as “flexibility” in the operating structure; for oil companies this may be represented as additional spare capacity that can be brought online during high oil price scenarios and duly made offline if oil prices are low. The value of this “flexible capacity” was probably not apparent when oil prices were normal, but significant potential (of spare capacity) was realized when oil prices spiked. The decision support system formulated in this dissertation stresses on building this kind of “optionality” in the operating structure for a renewable products enterprise. Given that significant market uncertainties exist in renewable energy and chemical markets, the flexibility to change future investment and operating decisions “on the fly”, holds significant value today. This dissertation will suggest a methodology to value managerial flexibility in making strategic decisions (termed here as “decision options”). Finally, when the optimal structure and capacity design plan has been decided, it is important to study the impact of the optimal design on the stakeholders of the operating supply chain; in this dissertation, this is
termed as impact assessment. Impact assessment can span a variety of stakeholders including the enterprise itself, the shareholders and capital providers, the environment and surrounding ecology, and the communities that will be impacted by the operation of a representative supply and production chain. Some techniques that are utilized for impact assessment include: (1) scenario analysis, where different hypothetical scenarios of process and supply chain parameters are projected and the impact of these scenarios on enterprise performance indicators are then quantified; (2) Monte Carlo simulations, where not only are the parameters projected into the future, but the probabilities of scenario realization are associated with each projection. In this way, a “probability-weighted” impact analysis report can be generated that not only describes the impact of different scenarios on enterprise performance, but also quantifies the probability of each scenario (and the corresponding impact) happening. This dissertation focuses on the utilization of environmental impact analysis of the optimal technology structure and also quantifies the financial risk to project value using Monte Carlo methods. The following figure (figure 2-2) expounds on the DSS that was proposed in figure 2-1 by describing the key components of each block in the figure.
Now that a DSS structure has been proposed, the next step is to populate the individual components of the DSS (termed as modules), with content. The content in this case is represented by optimization models, parameter forecasts, and impact analyses of a representative design structure. The next section provides a methodology to develop optimization model(s) to describe the design and operation of a renewable product supply and demand chain.
2.3 Generic Modeling Methodology

In order to accurately represent a renewable product system, a model-based optimization framework is formulated here. The model content is represented by mass and energy balances to describe physical flows of materials across system nodes and financial flows that result from the systems design and material movements. The financial flows can further be broken up into flow of cash generated at each system node and debt and equity flows in order to exercise design decisions. This section focuses on a methodology to integrate physical flow of materials and energy with financial flows of monetary resources that result from these physical flows. We will start by representing a renewable product system generically using consecutive input/output nodes, sort of like a supply and demand chain. Each node is represented by mass and energy balances resulting from material flows across each node and the financial flows that result from material movement.

![Figure 2-3: A generic nodal structure of a supply and demand chain](image)

2.3.1 Material Flows

Material balances are conducted for each commodity at each node of the aforementioned generic supply and demand chain. Material flows can include primary feedstock(s), ancillary raw materials including water, intermediate conversion products, and final products. Furthermore, yield balances to represent the transformation of upstream raw materials to downstream products are modeled.

\[
    Acc_{jnt} = In_{jnt} - Out_{jnt} + Gen_{jnt} - Cons_{jnt}
\]

(2.3.1)
Equation 1 is a familiar material balance equation where $\text{Acc}_{\text{int}}$ stands for the accumulation term, $\text{In}_{\text{int}}$ and $\text{Out}_{\text{int}}$ are material inflows and outflows through a given system node, and $\text{Gen}_{\text{int}}$ and $\text{Cons}_{\text{int}}$ are generation and consumption terms for material $j$ at node $n$, respectively. For each node $n$ the accumulation terms imply the changes in inventory levels of materials while inflows and outflows imply movement of materials from upstream to downstream nodes. Transformation equations describing the generation and/or consumption terms in equation 1 are provided below. Equation 2 describes the generation of material $j$ transforming incoming material $j'$, while equation 3 describes the consumption of material $j$ which is transformed to material $j'$. The generated material implies intermediate or final products produced while the consumed materials imply feedstock or intermediate materials. Here, $\rho_{jj'}$ is the coefficient of transformation representing the amount of material $j'$ obtained per unit of material $j$.

$$\text{Gen}_{\text{int}} = \sum_{i'} \rho_{jj'} \cdot \text{In}_{jj'_{\text{nt}}} \tag{2.3.2}$$

$$\text{Cons}_{\text{int}} = \sum_{i'} \rho_{jj'} \cdot \text{In}_{\text{int}} \tag{2.3.3}$$

2.3.2 Energy Flows

While the material balance equation (equation 1) can easily be substituted for an energy balance equation, from a systems perspective, it is more efficient to re-formulate equation 1 in terms of energy load requirements for nodal outputs. A general energy load calculation for each product is shown in equation 4 while equation 5 models the amount of energy that is needs to be generated using a combustion fuel.

$$E_{\text{int}}^{\text{req}} = E_{\text{int}}^{\text{cons}} - E_{\text{int}}^{\text{prod}} \tag{2.3.4}$$

$$E_{\text{int}}^{\text{req}} = \frac{E_{\text{int}}^{\text{req}}}{\text{LHV}_{\text{fuel}}} \tag{2.3.5}$$
\[ \text{LHV}_{\text{fuel}} = \text{HHV}_{\text{fuel}} - \Delta H_{\text{vap}} \] (2.3.6)

Equation 4 simply calculates the energy required for each product where the right hand side represents the change in the internal energy of the system while the left-hand side represents the energy that is required to be transferred to (or from) the system node. It should be noted that equation 4 can further be classified as thermal and electrical energy load calculations. Equation 5 calculates the amount of fuel required \( (F_{\text{int}}^{\text{req}}) \), where \( \text{LHV}_{\text{Fuel}} \) is the lower heating value of a unit of input fuel. The LHV is the amount of net heat that is released from the combustion of one unit of a given fuel source and is derived using the higher heating value (HHV) of a fuel which is the gross amount of heat that is released from the combustion of one unit of a fuel source; the HHV is especially important for solid fuel sources as it contains implicitly the heat of vaporization of any water \( (\Delta H_{\text{vap}}) \) that is present in the fuel source. The correlation between the LHV and the HHV of a fuel source is provided in equation 6. Depending on the fuel source, these values may be equal to each other (for gaseous fuels) or different from each other (for solid fuels) based upon the moisture content of the solid fuel These equations are integrated with material balances using equations of the form given in equation 7.

\[ E_{\text{int}}^{\text{req}} = G_{\text{int}} \cdot \Delta H_j \] (2.3.7)

Here \( \Delta H_j \) in is synonymous to the heat of reaction for a single reaction. In this case it represents the total energy that is produced or required to produce a single unit of material j.

2.3.3 Design Constraints

These constraints pertain to the design variables, more specifically feedstock, technology, product selection, and capacity design for each node, n, of a renewable product supply and demand network. Additionally, structural design considerations can also be added.
to include design solutions for biomass supplier(s) selection, site location, and product market selection. The selection sub-problems are represented by integer variables with 1 representing the selection of choice while 0 representing otherwise (equation 8).

\[ BV_{int} = \begin{cases} 1 & \text{if design parameter } i \text{ at node } n \text{ is selected} \\ 0 & \text{otherwise} \end{cases} \]  

(2.3.8)

Where \( BV_{int} \) is the binary variable for design parameter \( i \) at node \( n \) during time \( t \).

The next issue is to determine how much quantity of each design parameter would be optimal. In order to maintain model linearity, each design parameter is given a maximum value (\( DP_{\text{Max}}^{\text{int}} \)) representing some physical constraints that prevented the design parameter from exceeding this (equation 9). These physical limits might be availability constraints for feedstocks, capacity constraints for equipment capacity, or demand constraints for products.

\[ DP_{\text{Val}}^{\text{int}} \leq BV_{int} \cdot DP_{\text{Max}}^{\text{int}} \]  

(2.3.9)

\( DP_{\text{Val}}^{\text{int}} \) is the value of design parameter \( i \) during \( t \). Hence if \( BV_{int} \) is equal to 1, the constraint is active, otherwise the \( DP_{\text{Val}}^{\text{int}} \) equals zero (passive constraint).

Finally, in order to force the optimizer to select only one parameter from each set of parameter choices, we can put restrictions on the binary variable (equation 10). This can imply choosing one feedstock out of a set of \( N \) different feedstock or choosing one production technology out of an available set.

\[ \sum_{i=1}^{N} BV_{int} \leq 1 \]  

(2.3.10)

Additional logic constraints describing real world restrictions can also be formulated, involving process system layouts for technological superstructure design, and restrictions on
product selection; the case for processing network design using integer programming is specifically useful, as multiple processing configurations for different product groups can be characterized using yield, cost, and energy parameters, following which integer programming can be used to design an optimal processing network. A generic example to illustrate processing superstructure design is presented below.

In figure 2-4, there are multiple process routes for different products (p1-p2) which can utilize different feedstocks. The optimal superstructure problem here entails selecting the optimal product and feedstock portfolios and the appropriate processing route(s) and technologies to process the feeds to final products. We first need to define integer variable sets to represent each node in the process superstructure; BVF is the binary variable for feedstock selection, BVPT are the binary variables for technology selection for technology t at each node of superstructure feeding to technologies t’ at successive downstream nodes.

**Figure 2-4: A hypothetical technological structure for systems optimization using integer programming**
and $BVP_p$ is the binary variable for product selection. We can set up a rule based equation formulation framework to design the processing network. For example, let’s consider from figure 10 that there are multiple processing routes to get to products P1 and P2:

1. $(F1, F2) \rightarrow PTA \rightarrow PTB \rightarrow PTD \rightarrow P1$
2. $(F1, F2) \rightarrow PTA \rightarrow PTC \rightarrow PTD \rightarrow P1$
3. $(F1, F2) \rightarrow PTA \rightarrow PTB \rightarrow PTE \rightarrow P2$
4. $(F1, F2) \rightarrow PTA \rightarrow PTC \rightarrow PTE \rightarrow P2$

We can derive a few general rules just by observing the processing network:

1. **If** product P1 is produced, **then** system node PTD has to be selected

   $$\sum_{p=P1} BVP_p = \sum_{t'=TD} BVPTB_{tt'} + \sum_{t'=TD} BVPTC_{tt'} \quad (2.3.11)$$

2. **If** product P2 is produced, **then** system node PTE has to be selected

   $$\sum_{p=P2} BVP_p = \sum_{t'=TE} BVPTB_{tt'} + \sum_{t'=TE} BVPTC_{tt'} \quad (2.3.12)$$

3. **If** route “AB” is established, then at least one downstream route, “BD” or “BE”, has to be established

   $$\sum_{t'=TB} BVPTA_{tt'} \leq \sum_{t'=TB} BVPTB_{tt'} + \sum_{t'=TE} BVPTB_{tt'} \quad (2.3.13)$$

4. **If** route “AC” is established, then at least one downstream route, “CD” or “CE”, have to be established

   $$\sum_{t'=TC} BVPTA_{tt'} \leq \sum_{t'=TC} BVPTC_{tt'} + \sum_{t'=TE} BVPTC_{tt'} \quad (2.3.14)$$
These types of binary selection rules can be generated, if a clear understanding of the processing system is described qualitatively. Furthermore, the binary decisions that are made by an optimization model can be controlled by quantitatively describing each processing node by its yield to its output (unit output per unit input), cost ($ per unit input/output), and revenue parameters ($ per unit output). Additionally, instead of having a single technology choice for each node of the processing network, we can populate the input technology set for each node by multiple technologies, thus empowering the decision model with the ability to not only design the optimal processing network, but also select the optimal technology sets to implement the processing routes. In this way it is possible to evaluate intrinsically, multiple processing routes and corresponding conversion technologies that can convert resources to value-added products without having to model each processing route and technology individually. This is especially true for a new products’ industry, such as those converting renewable resources to energy and chemicals, as extensive research during the initial phases of industry development usually yields a significant (often superfluous) number of processing configurations and technologies. Having such a selection tool can prevent wasteful investments in technological routes that lead to more value destruction as opposed to long term value creation, thus enabling more efficient capital allocation (in an aggregate economy for individual enterprises). A methodology to integrate such design and production models and incorporate process decisions within a business valuation framework is provided next.

2.3.4 Waste Accounting Model

Waste accounting generally refers to the process of measuring and/or estimating the net waste (solid, liquid, or gas) released (or sequestered) by an entity; an “entity” can broadly
include a single functional unit of a system, such as a motor vehicle, or can include an entire network of functional units such as a renewable/non-renewable product’s supply and demand chain. Accounting for net waste from a product’s supply and demand chain essentially implies the calculation of the waste footprint of an enterprise.

For the case of renewable product value chains, life cycle analyses should be conducted to create an inventory of waste sources and sinks from the functional units of the supply/demand chains. Waste accounting starts with an inventory analysis where waste generation and sequestration data can be classified into three broad categories; (1) transportation-related waste, (2) production-related emissions, and (3) Consumption-related waste (Figure 2-5).

**Figure 2-5:** Simplified environmental life cycle analysis methodology

Transportation-related waste specifically pertains to emissions that are released to the atmosphere from the movement of raw materials and finished products between nodes, while production related emissions accounts for releases/sequestrations generated during production of finished goods. Consumption-related waste generally accounts for the final fate of a product (disposal) after usage by consumers. It is important, before LCA, to define
clearly the goal, scope, and system boundaries for case study. LCA can not only account for carbon emissions, but also account for SOx, NOx, and particulate matter emissions, along with solid and liquid wastes that are generated throughout the construction and operation of a representative value chain. System boundaries can include only the production facilities (gate-to-gate analysis), include raw material production and processing plants (well-to-gate), or raw material production to final production consumption (cradle-to-grave). The results of the inventory analysis can be quantified in terms of production throughput and normalized to common units, such as Global Warming Potential (GWP) of a substance in terms of CO₂-equivalents.

While the methodology for LCA is not a subject of concentration for this dissertation, literature estimates for a representative renewable product system case study are used later on in this dissertation to demonstrate the incorporation of carbon accounting and valuation into the decision support framework. In this section, we will formulate a single accounting model to calculate the net waste from multiple value chain design configurations. The model is incorporated into the design and operating formulations described in the previous sections. Two consecutive functional nodes in a generic value chain are defined, and using the node-pair as an example, we will then propose the extension of the model developed here to an entire system of nodes.
In the process described above, waste data can be collected for each node in the value chain; system boundaries should be defined for the system to collect appropriate data. For example, data for the nodal system only would imply collecting data that is directly a consequence of the operation of the value chain nodes, while if the system is expanded to include the life cycle of the inputs that are used in each node’s operation, the data inventory would include the emissions/sequestrations that result from the production and transportation of those inputs to downstream nodes. Additionally, the waste data is quantified in terms of one unit of the nodal decision variables, that is, waste per unit of decision variable. Furthermore, given multiple network configurations, characterized in terms of distances between supply, production and demand points, emissions data can also be collected for inter-nodal transportation of outputs for different transportation modes and fuel types used. The waste accounting model for optimization purposes is formulated as follows:

**Figure 2-6: A generic methodology to quantify environmental impacts of a value chain**
Equation 15 calculates the total waste of type \( w \) that is generated at node \( n \) for the production of output \( j \) from input \( j' \). Here, \( \rho_{wj'j} \) is the amount of waste of type \( w \) that is generated per unit of material \( j' \) processed to nodal output \( j \). Equation 16 calculates the total waste of type \( w \) that is required for the production of output \( j \), where \( \rho_{wj} \) is the amount of waste required per unit output \( j \) produced. Equation 17 calculates the net waste of type \( w \) that is output (or sequestered) at node \( n \); here \( W_{wnt}^{\text{reqd}} \) is the total waste that is required for the production of all system outputs. Equation 18 constrains the total waste that is recycled by the total waste that is required for the production of all nodal outputs. Finally equation 19 calculates the total emissions of type \( e \) that are generated for the transportation of material \( j \) to node \( n \) using transportation mode \( x \); here \( \rho_{ex} \) represents the amount of emissions released per unit mass per unit distance travelled for mode \( x \), and \( D_{nn'} \) represents the distance between all origination nodes \( n' \) and destination node \( n \).

2.3.5 Financial Model and Constraints

We derived a financial model by reformulating an enterprise’s income, cash flow, and balance sheet statement into an equation-oriented format. The equation format allows the
A cash balance equation (equation 20) can be used as the basis of the financial formulation. The balance equation is identical in form to the material balance equation (equation 4). The accumulation term is the change in the cash position from one period to another. Cash inflows (equation 21) are represented by money raised through equity ($E_t$) and debt financing ($B_t$) while cash outflows (equation 22) are represented by taxes ($tax_t$), interest and loan payments ($int_t$). Cash generation (equation 23) is represented by revenue created by sale of products ($R_t$) while cash consumption (equation 24) is represented by the capital ($Capex_t$) and operating expenses ($Opex_t$).

\[ C_{t}^{acc} = C_{t}^{in} - C_{t}^{out} + C_{t}^{gen} - C_{t}^{cons} \]  
\[ C_{t}^{in} = B_t + E_t \]  
\[ C_{t}^{out} = int_t + tax_t \]  
\[ C_{t}^{gen} = R_t \]  
\[ C_{t}^{cons} = Capex_t + Opex_t \]  

The objective function and the integration of the production, design and financial models is provided next.

2.3.6 Integration of Design, Production and Financial Models

We enlisted some operating (mass and energy balances) and design (capacity design and technology selection) modeling equations in the previous subsection. Here we will
discuss a simple methodology to integrate operating variables with design decisions and subsequently monetizing the decisions by incorporating these variables within the financial model. These integration equations are essential towards formulating a holistic decision framework that can represent a multitude of value-driving decisions impacting the long-term value of a renewable product venture. To integrate design and production decisions in an optimization modeling framework, an efficient yet simple methodology I employ is constraining the production decisions by the net capacity of a processing and/or network node. To illustrate this point certain examples are provided:

\[
\text{Feedstock Used} \leq \text{Resource Purchased} \quad (2.3.25)
\]

\[
\text{Production} \leq \text{Processing Capacity} \quad (2.3.26)
\]

In the above equations, design variables such as total resource purchases and processing capacity design are used to constrain production variables such as feedstock utilization and final product manufacture. The cash balance equation (Equation 20) is integrated with the 1) design formulation using capital investments made in equipment (equation 27), and 2) operation formulation using revenues (equation 18) and operating expenses (equation 28). Here, \( \alpha_i \) is the unit cost of capacity addition while \( \beta_j \) is unit operating cost.

\[
\text{Capex}_t = \sum_i \alpha_i \cdot D_{it}^{val} \quad (2.3.27)
\]

\[
R_t = \sum_j \text{Sales}_{jt} \cdot \text{Price}_{jt} \quad (2.3.28)
\]

\[
\text{Opex}_t = \sum_j \beta_j \cdot (\text{Gen}_{jt} - \text{Cons}_{jt}) \quad (2.3.29)
\]

Additionally, input parameters such as product demands and enterprise budgets can be further utilized to impact investment and sales decisions. The investment and sales
decisions in turn impact the production (feed usage, product manufacture) and design (feed purchase, processing capacity) decisions thus integrating decisions made at multiple levels of an enterprise hierarchy within an optimization framework (figure 2-7).

\[
\text{Sales}_{it} \leq \min(\text{Demand}_{it}, \text{Production}_{it}) \quad (2.3.30)
\]

\[
\text{Capex}_t \leq \text{Budget}_t \quad (2.3.31)
\]

2.3.7 Objective Function Formulation

Stakeholder Value

Stakeholder value theory is a relatively new paradigm in enterprise management. As opposed to shareholder value, stakeholder value describes the value of an enterprise not only to all the equity and debt holders of a firm, but to all the stakeholders, including employees and surrounding communities and environment. Although recent attempts have been made to express the stakeholder value of an enterprise (Clift and Earl, 1999), most of these attempts have stopped short of quantifying stakeholder value, instead using qualitative analysis to
illustrate corporate social responsibility. To the author’s knowledge, this is the first attempt to quantify a stakeholder value.

We believe that developing a decision analysis system for a bioproduct enterprise merits inclusion of influences on surrounding environments and communities, since the entire purpose of bioproducts is to improve the quality and health of the our planet. In order to develop a function for quantifying stakeholder value our initial endeavor will use a shareholder valuation model (Damodaran, 2001) and mandate, within the shareholder valuation framework, waste mitigation hence including aspects of corporate social responsibility towards the local communities and environment. What follows is a discussion of the shareholder valuation model and its extension to include waste mitigation.

There are 3 major methods used for the purpose of shareholder valuation. These include dividend discount models, and free cash flow models. The dividend discount model is used very specifically for evaluating dividend strategies for dividend payments to shareholders under the assumption that the only cash flows received by the shareholders are dividends. Consequently, a free cash flow model is deemed the most appropriate to value the current biorefining enterprise case study. Amongst the free cash flow models, there are two pertinent models that can be used; 1) free-cash-flow model to equity (FCFE) and 2) free cash flow model to firm (FCFF). The FCFE model values an enterprise using residual cash flow that is leftover after meeting all debt obligations, capital expenditures, and working capital requirements. This cash is the cash available to the firm to payout as dividends to its equity holders, invest in new marketable securities, or use in adding to the cash balance of the enterprise. The FCFF model calculates the value of an enterprise after paying operating expenses, capital expenditures, and meeting working capital needs. This cash flow represents
the return to all providers of capital, whether debt or equity. It can be used to pay off debt, repurchase shares, pay dividends or be retained for future growth opportunities. The FCFE should be used for firms that have low leverage, that is, low debt ratios while the FCFF model can be used for firms that have high leverage. There are a number of loan guarantees that are available to renewable energy enterprises through current federal and state government programs. Hence we can expect a fledgling biorefining enterprise to be highly leveraged during its initial period of inception. Consequently, the firm valuation methodology that will be optimized in the present formulation will use the FCFF model. The traditional free cash flow calculation equation is shown in equation 32.

\[ \text{FCFF}_t = R_t - \text{Opex}_t - \text{Capex}_t - \text{tax}_t \]  \hspace{1cm} (2.3.32)

The enterprise value (EV, equation 33) is then calculated as weighted sum of all the future cash flow forecasts, weighted by the average cost of capital (WACC), and a terminal value for the enterprise. In the current formulation, the terminal value is calculated with an expected growth rate, \( g_T \).

\[ \text{EV} = \sum_{t} \frac{\text{FCFF}_t}{(1 + \text{WACC}_t)^t} + \frac{\text{FCFF}_T(1+g_T)}{(\text{WACC}_T-g_T)(1+\text{WACC}_T)^T} \]  \hspace{1cm} (2.3.33)

The WACC is calculated (equation 34) as a weighted function of the expected return on equity (\( E[\text{ROE}]_t \)) and the tax shielded interest rate (\( \text{ir}_t \)), weighted by a preset weight (\( \lambda \)). Here \( \lambda \) is the equity weight of the financing mix for the firm implying that \( 1-\lambda \) is the debt fraction of financing.

\[ \text{WACC}_t = \lambda_t E[\text{ROE}]_t + \text{ir}_t (1 - \lambda_t) (1 - \text{t}^{rate}) \]  \hspace{1cm} (2.3.34)

The net debt \( (D^{net}) \) at the end of the time horizon, \( T \), is the net of debt \( (D_T) \) and any liquid cash on hand \( (C_T) \). The shareholder value (SHV) is then determined as the net of the enterprise value and the debt on hand (equation 36).
In order to extend the shareholder valuation to a stakeholder valuation, we need to include mandated mitigation expenses within the formulation. Mandating waste mitigation is stating mathematically that the enterprise requires within its corporate structure to budget for waste mitigation. This is in stark contrast to the rest of the formulation wherein feedstock, technology, and product selection are modeled as binary decisions with only the most profitable options being selected. We calculate the net present value (NPV) of mitigation activities (equation 38) as the discounted sum of the cash flows as a consequence of mitigation activities (equation 37).

\[
\begin{align*}
\text{NPV}^{\text{mit}} & = \sum_t \frac{\text{CF}^{\text{mit}}_t}{(1+r)^t} \\
\text{CF}^{\text{mit}}_t & = \text{Mit}^{\text{credit}}_t - \text{Mit}^{\text{expense}}_t
\end{align*}
\]  

We use a separate interest rate for discounting the mitigation related NPV (NPV\textsuperscript{mit}), as opposed to WACC (equation 21), in order to weight waste mitigation cash flows separately for production related activities. Finally equation 39 shows how we arrive at a stakeholder value from the shareholder value.

\[
\text{SKV} = wt^{\text{SHV}} \times \text{SHV} + (1 - wt^{\text{SHV}}) \times \text{NPV}^{\text{mit}}
\]  

The next section will discuss the biorefining case study that is developed for the aforementioned model. Special emphasis will be laid on the screening of products and technologies from the initial portfolio and sensitivity analysis to determine important exogenous parameters that need to be modeled accurately when the model is extended to incorporate uncertainty.
2.4 Optimization under Uncertainty using Decision Options

2.4.1 Introduction

The growth of the renewable energy industry has been hindered by technological and market uncertainty and the lack of financial and human capital which is required to build out the infrastructure for commercial production. Research has yielded multiple technological platforms and routes that enable conversion of renewable resources to energy products, but their commercial viability is still not proven and furthermore, the choice amongst these technologies from a technical, environmental, and economic perspective is still unclear. Additionally, the absence of high margin, value-added chemical product streams to complement the low-margin production of energy has prevented seamless mitigation of market volatility in demand and prices, which are highly correlated to crude oil and fossil energy markets. These underlying uncertainties have hampered investment capital formation in the renewable sector and have deterred prospective entities from undertaking commercialization of lab- and demonstration scale technologies. For a nascent product market such as the renewables market, cost, price, and demand volatility further reduces investor and entrepreneur appetite for investing new capital in equipment and labor.

Real options analysis is a direct off-shoot of financial options, the theory of which was popularized by Black and Scholes (1973). A financial option is a common means of trading in the stock and commodity markets, and is used as an effective tool by traders and investors to decrease risks of losing large investments while maintaining as much upside as possible of asset investments. In basic terms an option is a right but not an obligation to
purchase an asset at a predetermined price; the buyer of the option pays a price to the seller of the option right now (strike price), the basic idea being, by making a smaller current investment (strike price) the buyer can wait for some underlying asset price uncertainty to resolve before making a decision to purchase or sell the underlying asset outright (at a predetermined exercise price) at or before a given date (maturity). Options are priced for various securities (called underlying assets) in dynamic markets using a formula by Black and Scholes, derived using an analytical solution to a stochastic differential equation(s) that describes the price of the underlying asset (some form of Brownian motion). An option to purchase an asset outright at the exercise price is called a Call option while an option to sell as asset is called a Put option.

Real options derive a lot of their properties from financial options but there are also many deviations from financial options. In real options the underlying asset is a capital project as opposed to a stock or commodity-based security; for the case of a biorefinery, the underlying asset is the biorefinery itself. If traditional discounted cash flow (DCF) is used to derive the Net Present Value (NPV) or the project IRR, then the investment decision to invest in constructing a biorefinery is based on the discounted value of future cash flows (or the predicted IRR) that would result if the biorefinery is constructed today. These decisions are essentially irreversible and a large investment is required in plant equipment and labor today, in order to reap possible benefits of profits in the future. These profits are highly dependent on future costs of production and future prices of biofuels and biochemicals, which are, in their current state, highly uncertain (Solomon et al., 2007) and technology platforms are expensive in their current developmental stage. If real options are used to design investment decisions for the biorefinery, then the enterprise can make a small
investment under the current market climate (the strike price), in order to give themselves the flexibility to make incremental investments in future capacity (exercise prices) as costs of production, process yields, and market prices of bioproducts become more apparent. Furthermore, the enterprise can self-prescribe flexible future dates by when they want to make a decision on increasing plant capacities (option maturity dates). Creating this kind of flexibility in investment valuation can enable an enterprise to gain a deeper control over their profits by controlling the risks that arise from uncertain cost and market structure evolutions coupled with large upfront capital investments. The option to expand, contract, or abandon production capacity at flexible dates in the future has great strategic value for any biorefinery that is looking to establish a commercially profitable and terminally sustainable facility and/or network for the production of bioproducts.

2.4.2 Literature Review

This type of analysis is a new paradigm in engineering that has been successfully applied to natural resource projects that have a high degree of uncertainty in product prices and demands along with large upfront capital investments and construction lead times. The basic motivation behind this methodology is to minimize the downside risk of uncertainty while still maintaining maximum upside potential, the idea being that capital investments and operational decisions can yield larger than normal gains by creating and valuing decision-making flexibility in the face of high uncertainty. In Real options analysis, stochastic parameter distributions are discretized using binomial trees (Wang and De Neufville, 2004) and the results are represented using a decision tree. Miller and Waller (2003) presented a detailed analysis of the advantages and shortcomings of a real-options framework and suggested an integrated approach for quantitative risk management. Rogers
et al. (2002) used this approach to generate an optimal pharmaceutical research and development product portfolio. Sekar et al. (2003) used real-options to design a carbon dioxide sequestration system for coal-fired power plants based on taxes set on emissions. Smith and Mccardle (1998) used this analysis to evaluate a portfolio consisting of various oil wells. Wang and De Neufville presented a case study where real-options were used to investigate construction of hydropower projects. A common theme in all aforementioned literature is presence of significant uncertainty in commodity availability, demand, or price, a theme abound in biorefinery ventures.

2.4.3 Theory of Decision (Real) Options

The theory behind real options analysis assumes stochastic variables following variations of Brownian motion. The theory behind BM was pioneered by a Japanese mathematician named Kiyoshi Ito as is termed as Ito’s Lemma. Ito suggested that stochastic stock prices in the markets can be described by a partial differential equation (PDE), where the PDE can be represented by a deterministic component and a stochastic component. If $S$ is the stock price, let $\partial S$ be a small change in $S$ over an infinitesimal time interval $\partial t$. If $z$ is a random variable, the change in $z$ over time $\partial t$ is then assumed to be $\partial z$. Consequently, the change in the stock price over $\partial t$ can then be described using the following PDE:

$$\partial S = A(S, t, ...) \partial t + B(S, t, ...) \partial z$$  \hspace{1cm} (2.4.1)

Where, $A$ and $B$ can be functions of multiple exogenous and endogenous factors, $\partial z$ is termed as a basic wiener process and $\partial S$ is called a generalized wiener process. The variance of $\partial z$ is calculated as the accumulated effects of independent disturbances over time interval $t$. For our case, the variance is proportional to the length of the time interval, which
in our case is $\partial t$, and consequently, the standard deviation is proportional to the square root of $\partial t$. We can then estimate the value of $\partial z$ based on this theory:

$$\text{Var}(\partial z) \propto \partial t \rightarrow \text{STD}(\partial z) \propto \sqrt{\partial t} \rightarrow \partial z = w\sqrt{\partial t}$$ (2.4.2)

Where, $w$ is a standard normal variable with mean equal to zero and standard deviation being unity. The discretization of the continuous stochastic process can be estimated as:

$$\partial z \approx z_t - z_{t-1} = w \times \sqrt{\Delta t}$$ (2.4.3)

$$\Delta t = t - (t - 1)$$ (2.4.4)

Under the assumption that $A$ and $B$ are constants, we can re-write the Equation (1) as:

$$\partial S = A \partial t + B \partial z$$ (2.4.5)

Where $A \partial t$ is termed as the (deterministic) drift rate for the stochastic process $\partial S$, while $B \partial z$ adds randomness to the path followed by $S$. Consequently, if $\partial z$ has a standard deviation of one, then $B$ times $\partial z$ has a standard deviation of $B$. Therefore, we can discretize the stochastic process, $S$, as:

$$\partial S \approx \Delta S = A\Delta t + Bw\sqrt{\Delta t}$$ (2.4.6)

Therefore, the following properties for $\Delta S$ can be derived from the above equation:

$$E[\Delta S] = A\Delta t$$ (2.4.7)

$$\text{STD}[\Delta S] = B\sqrt{\Delta t}$$ (2.4.8)

Where $S$ is the stochastic price, $A$ is the expected drift rate of the price, and $B\sqrt{\Delta t}$ is the volatility (annualized standard deviation in the stock price). To generate a decision tree based on dynamic price movements, the normal price process requires discretization. The discretization of a continuous process is merely an approximation that is carried out in order to obtain intuitive, analytical solutions to complex decision problems in the continuous time domain. The simplest of these approaches was suggested by Cox et al (1979), who
discretized a log normally distributed stochastic variable to generate a binomial lattice. A binomial lattice can be thought of as a time-varying probability tree with binary tree nodes that result from discrete, known movements in the stochastic variable. The stochastic variable is assumed to move up (u) or down (d) sequentially over time, with an estimated probability. These movements can be estimated as a function of the volatility parameter that was obtained in equation 8.

\[ u = e^{B\sqrt{\Delta T}}, \quad d = \frac{1}{u} \]  \hspace{1cm} (2.4.9)

Probabilities are usually obtained as follows:

\[ p_{\text{up}} = \frac{e^{r\Delta t} - d}{u - d} \]  \hspace{1cm} (2.4.10)

\[ p_{\text{down}} = 1 - p_{\text{up}} \]  \hspace{1cm} (2.4.11)

Here, \( r \) is a known risk-free discount rate equal to the yield on a 10-year treasury bond. The entire discretization process is shown in Figure 2-8.

**Figure 2-8: Stochastic parameter discretization and forecasting process**
A key point of difference between financial options and real options, is the path dependency of real options (Wang and Neufville, 2004); in financial options, the sequential, time-dependent path that a price process takes is immaterial. Path dependency here is referred to the trajectory that a stochastic process follows sequentially over time. In the figure above, the value of the stochastic process at the final time step for the second and the third scenarios are the same but they arrived there taking different evolutionary paths (up→down for the second scenario, down→up for the third). This path dependency is irrelevant in financial options while in real options, it is extremely important, especially when sequential capacity is being designed. For example, if capacity is established in period two for an up move while it is deferred for a down move, and then no further capacity is established for any scenario, we end up with different capacities for scenarios 2 and 3 at the third time period, even though the final value of the stochastic process (price for example) is the same for either scenario.

To impose the idea of path dependency on a model, non-anticipativity constraints are necessary when designing models for certain cases of real options, especially sequential capacity design. Non-anticipativity refers to the concept that the sister branch node for any scenario that originates from a common root node previously, should have the same value at the root node. Therefore, all scenarios will have the same value at time t=1, scenarios 1-2, and 3-4 will each have the same value at the second time step, while scenarios can have different values at the final time step.
2.4.4 Types of Decision Options in Strategic Planning

Within real options, it is important for the project manager to determine what type of options are currently available for project investment and what options may be available in the future. From a modeling perspective, there are various types of options that are described in literature that provide multiple decision trajectories for project design. Some of these options are described hereafter (Schwartz and Trigeorgis 2001).

- **Deferral Option**: An initial investment is made to acquire rights to develop in the future, a natural resource. These types of options are very common in the oil and gas and mining industries where resource lands are purchased and the enterprise holds the option to develop these resources given favorable market conditions. A rival model for a hypothetical biorefining supply chain would be acquisition of lands (even nutritionally marginal lands) to develop dedicated energy crops to supply biomass refineries (Wang, 2003; Hajek, 2009).

- **Abandonment or Contraction Options**: An enterprise may chose to abandon (or contract) the construction (or operation) of a project as market (or process operating) conditions deteriorate and possibly, sell some fixed assets for a salvage value. These options can be exercised if the salvage value of a project is greater than the expected benefit of operating the plant. Such options hold significant value for startup biorefineries as market and yield uncertainties can evolve unfavorably as commercial production comes online in the future (Dezen and Morooka, 2001; Schmit et al, 2008).

- **Embedded Growth Options**: These options enable an enterprise to stage capacity investments into smaller increments, thus losing the initial benefits of economies of
scale, but mitigating the risk of having a large plant with very little production and large fixed costs, in cases where market or process operations do not evolve favorably. We believe that these options are one of the most valuable options to possess for biorefineries; with rapidly evolving technologies and markets, it may make sense from a competitive angle to start investing in developing a platform now to produce biofuels and biochemicals, but from a risk perspective it is prudent to stage entry into market with smaller capacity additions so as to ascertain if market conditions and process operations yield expected outcomes (Kulatilaka, 1998; Panayi and Trigeorgis, 1998).

- Learning Options: Similar in structure to growth options, these options can be used to model research and development or pilot plant investments, wherein, the investment in the proof of concept stage enables revelation of uncertain variables (such as process yields) based upon which further investment decisions can be tailored. These types of options also hold significant intellectual merit for emergent technologies where commercial yields are highly uncertain. Furthermore, for proprietary technologies such as enzymes, process designs, and/or micro-organisms for bioproducts production, successful investment in the proof-of-concept stage can also yield licensing revenue possibilities (besides just capacity expansion options), thus providing an enterprise with multiple avenues for profit appreciation; these should be aptly reflected in the options models in order to clearly reflect the future value of the investment in the proof of concept stage (Turvey, 2001; Tsui, 2005; Huchzermeier and Lock, 2001, Kumbaroglu et al, 2005).
• Flexibility options: These options can be used to design multi-product plants, where an investment in a flexible technology platform that has the ability to switch production between multiple products, can help an enterprise mitigate market volatilities in one product’s market, by switching production to a more favorable mix. We believe that flexible production platform for biofuels production, wherein, the plant has the ability to switch its production mix between high volume-focused biofuels and high-margin focused biochemicals will be important determinant of the long-term sustainability and profitability of biorefineries (Adkins and Paxson, 2011; Hem et al 2011).

2.4.5 Integer Modeling of Decision Options

It should be noted that although there are other, more exotic real options that can be incorporated into investment decision modeling, the aforementioned ones are the most prevalent options that are recommended in literature, and furthermore, a blend of these can be conjured to create more exotic, hybrid formulations. The aforementioned decision options techniques will be utilized in this dissertation to develop capacity design plans under uncertain price conditions for renewable fuels and chemical markets. As opposed to analytical models (combined with dynamic programming) that are utilized extensively in literature, this dissertation will utilize integer-programming based optimization models to select optimal timing and design of capacity establishment and expansion; the optimal nodes that are selected manually in a dynamic program can be reformulated as an integer programming problem with binary integers mirroring the selection of optimal nodes in dynamic programming. The strategy aims to evaluate and optimize multiple decision options
simultaneously while modeling the implicit physical and impact-based correlations amongst different decisions. The strategy to build the integer programming model for decision options is presented in figure 2-9.

Figure 2-9: Strategy to incorporate uncertainty in the strategic decision making process

This method is utilized over dynamic programming as it intrinsically eliminates unprofitable decision nodes by setting the binary variables for those nodes to zero. Additionally, the nature of a dynamic planning problem where a swath of decisions can be made at any given decision nodes lends itself very favorably towards the utilization of an integer-optimization framework as opposed to analytical techniques.

2.5 Monte Carlo Analysis

Monte Carlo simulations will be developed as a part of the risk quantification and analysis of the decision analysis system. Since most renewable energy ventures involve large
capital investments while serving markets where product demands are highly uncertain and prices volatile, it is essential that any major capital investment be analyzed from the perspective of the value the enterprise is risking while undertaking a venture. It is plausible that optimal solutions obtained from discrete options optimization may also involve substantial risk that a renewable enterprise may not be willing to partake in. Consequently, given the parameter (price and demand) distributions from the forecasting module, a simple cash flow model can be used to simulate the overall stakeholder value. Monte Carlo sampling techniques can be used to generate histograms of the simulated stakeholder value. The cash flow model should not involve any decision variables or integer restrictions and the design alternatives that are yielded by the optimization processes should be used as inputs. Finally risk curves for each scenario can be developed using cumulative distribution functions in order to determine the stakeholder value at risk. This may amend management decisions as risk-averse management may prefer a sub-optimal portfolio profile in order to mitigate capital and/or environmental risks associated with the optimal design.

![Figure 2-10: A methodology to simulate flow equations and objective functions using Monte Carlo methods](image)

In order to develop the content, one first needs to choose a supply chain and corresponding production processes that need evaluation. For this dissertation, a lignocellulosic biorefinery that converts energy crop-derived biomass to value-added
biofuels (cellulosic ethanol) and biobased chemicals (succinic acid) has been selected. While we have selected a lignocellulosic biorefinery to demonstrate the efficacy of SDSS, its applicability to other renewable fuel and chemical chains is apparent. The content will need some adaptation to describe accurately a particular production chain, but the broad tasks and methodologies developed as a part of this case study can definitely be applied across multiple industry verticals. The next section introduces a challenging decision problem for the design of a multi-product biorefinery and utilizes the aforementioned framework to systematically design a technological superstructure, select an optimal feedstock and product portfolio, and design the spatial network structure throughput capacities to process lignocellulosic biomass to value-added biofuels and biobased chemicals.
3. APPLICATION CASE STUDY – AN SDS SYSTEM FOR MULTIPRODUCT LIGNOCELLULOSIC BIOREFINERIES

3.1 Introduction

The population in the emerging market countries has seen a remarkable rise in their income levels leading to, amongst others, upward mobility in their societies. A consequence of social upward mobility is increasing consumer demand for transportation vehicles, which in turn leads to greater demand for transportation fuels. The major source of supply for transportation fuels is crude oil. By its very nature, the supply therefore is derived from a finite resource constraining the plausible amount that can be supplied while the demand theoretically has no ceiling. This supply-demand imbalance has been a primary driver of the consistent rise in oil prices over the past decade. Additional causes, such as speculation, are in some form a manifestation of this imbalance; market prices for crude oil are composed not only of the current supply-demand balance but there is a forward looking component in them that tries to gauge what the supply-demand equation is going to look like in the coming years. A final, and recently more prominent, driver for oil price shocks has been the geopolitical risk premium that is built into the pricing, owed in large part to regions most of the world’s crude supplies are derived from. The confluence of these factors has brought into prominence the need for diversifying our energy, and more specifically, our transportation fuels portfolio.

Development of a sustainable energy portfolio has been recognized as a top priority by governments and enterprises around the United States to wean the country off our dependence on foreign oil. A significant portion our foreign oil imports are utilized in the production of transportation fuels, such as gasoline, and petrochemicals that are processed through value-added operations to produce commodity and high-value chemicals and
polymers. A rise in demand for these foreign energy resources will indirectly imply that we send a significant portion of our money to politically unstable regions of the world, which are the primary suppliers of crude oil in the world markets. Renewable transportation fuels derived from local resources appear increasingly to be a viable, long term solution to complement crude oil-derived fuels to supply our energy needs for decades to come. The development of renewable transportation fuels has focused primarily on the development of ethanol as a replacement for gasoline fuel or as an oxygenate for gasoline; as an oxygenate, ethanol replaces fossil-derived Methyl tertiary butyl ether (MTBE), which has been used traditionally to increase the octane number of reformulated gasoline. A higher oxygenate content in gasoline implies more complete combustion of gasoline during vehicle operation thus reducing the carbon emissions that result from fuel combustion and providing a larger output of energy per unit of fuel combusted. In the United States, MTBE is manufactured by reacting methanol, derived from natural gas, with isobutylene, a crude oil derivative. Besides being derived from fossil resources, MTBE has also been suggested as being a human carcinogen at high doses (EPA.gov). In lieu of the aforementioned drawbacks, MTBE has been progressively banned for use as a gasoline oxygenate in multiple states across the country, with ethanol replacing it as a safer, more environmentally benign alternative. Additionally, ethanol also has the potential of replacing gasoline as a fuel, although pure ethanol fuel (85-100 percent) cannot be used as a drop-in fuel in current engine designs due to potential damage to fuel tanks caused by fugitive moisture from ethanol phase separation in the fuel storage system. Currently, ethanol and gasoline mixtures (5-15 percent ethanol by volume), also known as gasohol, are commonly utilized. The commercialization of economically feasible flex-fuel vehicles, that can utilize larger percentages of fuel ethanol, is
the next expected wave of technological change that will dramatically shift the composition of our country’s transportation fuel portfolio.

For ethanol to be truly sustainable as an environmentally beneficial and economically viable fuel source, significant attention needs to be given to the supply side of the fuel; aspects of ethanol production such as feedstock supply and costs, conversion efficiency and costs, and distribution infrastructure need to developed and executed commercially. All these “front-end” design needs require a focused strategy that builds towards enabling private enterprises to commercially produce ethanol in a sustainable and cost-competitive manner.

For example, first generation ethanol derived from corn was plagued by the “food versus fuel” debate, and impacted food markets around the world thus diminishing some its potential environmental benefits. A better, more prudent alternative to corn ethanol is cellulosic ethanol; cellulosic ethanol is produced from biomass that can be derived from a range of wastes including agricultural wastes and commercial wastes. This type of ethanol has the advantage of being derived from waste material that does not compete with the food value chains, and is available in large amounts at much lower relative costs.

While feedstock supply is undoubtedly an essential component in determining the future sustainability of cellulosic ethanol production, equally important is the economical processing of biomass and its conversion to value-added fuels and chemicals. Two different conversion platforms have been suggested to produce cellulosic ethanol from biomass; (1) a biochemical platform that utilizes biochemical process operations to convert biomass to ethanol, and (2) a thermochemical platform that utilizes thermal operations to convert biomass to ethanol. Biochemical production of ethanol is based on the fermentation of sugars contained in cellulosic biomass to yield ethanol; all biomass contains variable amounts of
polymeric sugars that can be converted to a multitude of fuels and chemicals based to metabolism products of fermentative organisms that are utilized. The major systems operations that are utilized in the conversion chain from feedstock to value-added fuels and chemicals include, (1) fractionation of polymeric sugar-containing lignocellulosic feedstock to yield five- and six-carbon chained carbohydrates (xylose and glucose respectively), (2) fermentation of sugars using genetically engineered micro-organisms to yield value added fuels and chemicals, (3) separation, recovery, and purification of fermentation effluent containing the desired product to yield commercial quality final product, (4) treatment of wastewater and management of water utilities for plant use, (5) generation of process steam using unutilized lignin, leftover proteins and sugars, and biogas generated from waste digestion, and (6) cogeneration of power using steam turbines for plant use and sale of excess power to district power distributors.

Thermochemical production of ethanol and associated higher alcohols is based on a gasification technology (Aden et al) that involves conversion of biomass in a steam and oxygen rich atmosphere to produce a carbon rich gas known as syngas, which is a mixture of carbon monoxide, carbon dioxide, and hydrogen. This gas is subsequently upgraded catalytically to a mixture of alcohols including methanol, ethanol, propanol, and butanol that are then separated and distributed for end-use fuel and chemical applications. A heat and power recovery and distribution system is usually integrated with the entire process to design a self-sustaining plant in terms of power and enthalpy requirements. Between the two technology platforms, there are multiple points of distinction in terms of process complexity, prospects of process intensification, and capital and operating costs needed to build and operate each platform. The selection of the most appropriate platform by a prospective entity
should be based ideally on metrics that compare not only capital and operating costs per unit of revenue generated, but also on competencies of the prospective entity to design and implement a particular platform, regional incentives given for a particular technology, and market transformation potential of each platform.

Currently, process technologies and technological platforms are in their developmental stage with a primary focus on technology development, systems design, and unit testing. These analyses generally occur during the pre-commercialization phase of a technological development curve and are usually carried out with a ±50 percent accuracy target with respect to desired results. Given that there are multiple fractionation technologies, conversion (fermentation) equipment configurations, and concentration and recovery methods, we believe that a structured approach is necessary to select the most optimal process configuration and technology portfolio that has the potential to maximize the strategic value and the environmental benefits of ethanol projects over the next few decades. Ideally, a framework should be designed that is able to simulate different process configurations and conversion technologies yielding estimates for product-wise feed, raw materials, water, and energy requirements for each process design permutation. Additionally, the framework should be able optimize economic objectives to provide users with estimates for capacity design, operating levels, and expected market penetration rates, along with financial metrics such as cost-benefit ratios, NPVs, and capital structure to execute the optimal design.

In this part of the dissertation we exemplify such a framework for its application to the strategic design and operation of a multi-product biomass-based refinery. The next chapters will demonstrate the development of a decision support framework to select the
optimal technological platform, feedstocks, and final products for the conversion of biomass resources to biofuels and value-added biochemicals, and design an optimal spatial network to move feedstock to processing plants and finished products to end markets. Additionally, the framework will also suggest a forecasting methodology to generate market forecasts for input costs and product prices and demands that impact the operation of the biorefinery. Finally, we will suggest a dynamic, decision tree based methodology to design processing capacity for biomass to ethanol processing networks that incorporates uncertainties in input costs and product markets before making investment decisions in capacity.

3.2 Case Study Description

This section describes the sample biorefinery case study that was optimized. While the case study is hypothetical, we believe that such a structure will be possible to implement on a bench, pilot, and commercial scale. We tried to impart as much realism to the sample biorefinery as possible. The prospective biorefinery was assumed to be located in Louisiana; consequently, the biomass sources studied for their energy resource potential are grown extensively in the state. The overarching reason for the selection of Louisiana as a potential location of a biorefinery is discussed below.

Overall, for the State of Louisiana, agricultural employment has declined up to 18% within the past decade due to socio-economic factors. As farmers retired their land, enrollment in programs such as the Conservation Reserve Program (CRP) has risen. These programs have helped to restore lands such as alluvial bottomland hardwood mixtures displaced by agriculture, but in some regions the maximum allowable land area to be enrolled in such programs has been reached. Additionally, while these reserve programs
provide land rental payments to landowners there is no added-value industry as in conventional agricultural and wood products land uses that enhance rural economies. As such, identification of economically and ecologically optimum regions of the state for sustainable biomass resource production can attract a multitude of industrial practitioners to the area, in fields ranging from the production of bio-based fuels and chemicals, to the generation of bio-electricity. This can, in turn, help the rural landscape by converting poorly managed and unmanaged agricultural land into forest and establishing a value-added industry in the region to provide sustainable employment to its citizens. Some facts about Louisiana’s supply potential biomass resources are provided below (Jackson and Mayfield, 2007):

1. Louisiana has approximately 250-300 thousand acres per year of conservation reserve program (CRP) land available currently that can be used for herbaceous energy crop production;
2. Additionally, about $4.35 \times 10^6$ tons of agriculture residues are produced in the state primarily composed of sugarcane bagasse and grain residues;
3. A significant portion of these residues (96 percent of bagasse and 50-60 percent of grain residues) are already utilized for energy production (on farm or by utility companies);
4. Louisiana also produces $3.38 \times 10^6$ tons of forest residues and $3.58 \times 10^6$ tons of saw mill residues annually;
5. Again, a significant portion of these residues (98 percent saw mill residues) are already utilized for energy production (biopower);
6. Additionally, forest residues are also utilized for pelletization and export, specifically to Europe, with planned expansions coming online in subsequent years;
The next subsections of this chapter are organized as follows:

1. **Biomass Resources** – here we will describe the prospective resource portfolio and describe in some detail the characteristics of each resource that enable their efficient conversion to cellulosic bioproducts.

2. **Feedstock supply and product demand network** – here we will describe the particular locations for feedstock sources, processing facility sites, end product markets, and the transportation network that is used to study the optimal design of the biomass-to-bioproducts supply/demand network.

3. **Conversion Platforms** – here we will describe the characteristics of each platform and compare the attractive features and drawbacks of each for the purpose of converting biomass to cellulosic bioproducts.

4. **Technological Superstructure** – here the specific unit operations for each conversion platform will be described and the different technologies that are used for each operation will be compared.

5. **Product Portfolios** – here the possible products that are evaluated from each conversion platform and the corresponding unit operations necessary to recovery and purify them (following fermentation) will be described along with the long-term technical and market potential for each.

### 3.2.1 Biomass Resources

Government agencies including US DOE and USDA are strongly committed to expanding the role of biomass as a viable feedstock of the future to supply our energy needs. Biomass has been identified as a promising source to reduce the country’s dependence on
foreign oil imports by supplanting some of the crude oil demand for transportation fuels and petrochemicals. Biomass is a broad category used to describe plant-derived materials. Already, it is the largest domestic source of renewable energy, passing hydropower; yet biomass only forms about 3 percent of the total energy resource supply. The long-term goal of the United States is to displace 30 percent of the total domestic energy fossil resource demand by biomass resources equating to approximately 1 billion tons of biomass feedstock utilization. Recent studies have found that the United States has about 1.3 billion tons of biomass potential (Perlack et al, 2005), enough to supply about 33 percent of the domestic energy demand currently. The resource potential is derived from forest and agricultural lands with 33 percent of the total potential from forestlands and the balance from agricultural lands. Forest resources can provide biomass in the form of harvested trees, residues from wood processing, urban wood wastes, and residues from logging operations. Agricultural resources for biomass include annual crop residues, dedicated energy crops, grains, and animal manures.

All biomass resources have one thing in common; they are primarily composed of carbon, oxygen and hydrogen. Each resource has differing compositions of these elements and different compounds that incorporate these materials into the biomass. Essentially all biomass-derived energy is through the cellulosic, hemicellulosic and lignin fractions of the resource. Additional materials that are contained in the plant structure include amino acids, lipids and other organic compounds. Usually, C6 sugars are derived from the cellulosic fraction of biomass while C5 sugars are derived from hemicellulose; lignin is a complex polymeric compound that surrounds the cellulosic and hemicellulosic fractions in the plant. In order to access the C5 and C6 fractions, this lignin structure has to be broken apart before
further processing can be accomplished. This is usually accomplished using mechanical, thermal, catalytic, and/or enzymatic process whose purpose is to fractionate the compact biomass structure to release its components. Figure 3-1 shows a simplified representation of a common biomass resource’s structural composition pre- and post-fractionation.

Figure 3-1: A general representation of a biomass structure, pre- and post-fractionation; Source: www.ecn.nl

While forest resources are more “woody”, that is, are larger percentage of its composition is in the form of lignin, agriculture resources are more “starchy”, that is, their composition is more in the form of cellulosic and hemicellulosic materials. The choice of an appropriate process to convert biomass to energy is heavily dependent on the type of biomass that will be processed; thermal and catalytic processes are more suited to utilize woody biomass while biochemical and enzymatic processes are better suited for starchy biomass. Additionally, site location for a biofuels producer will govern what biomass resources and the appropriate processing technologies are selected.
In the next few sections we will discuss different conversion platforms that can convert biomass to value-added fuels and chemicals, complete with a description of possible product and technological configurations.

3.2.2 Spatial Network Description

To design an appropriate supply and demand network, three major input data sets are required:

1. Appropriate sites to locate processing facilities within the state of Louisiana;
2. Prospective feedstock source locations around the potential processing facilities with given transportation resources to move feedstock from sources to processing facilities;
3. Potential markets for finished products along with appropriate transportation mediums to move finished products from processing facility to final demand points.

As the purpose of this case study is to demonstrate the formulation of a strategic decision support system for renewable product enterprises, the exact datasets to characterize each node in the potential biomass-to-biofuels supply and demand network is not deemed necessary; rather we utilize approximate distances from feedstock sources to processing facilities and from processing sites to final markets, as inputs to an optimization model. The optimization model will utilize these (hypothetical) node-specific datasets to select the appropriate locations for processing facilities, select feedstock sources to supply the site(s), and choose the optimal set of markets as demand points for finished products. Figures 3-2 shows images sourced from online resources that describe a layout of the rail and road
networks that are existent in Louisiana. We assume that these are the transportation mediums that will be utilized to move materials across the potential network.

![Rail and Highway networks in Louisiana](image)

**Figure 3-2: Rail and Highway networks in Louisiana; Sources: www.mapsofworld.com; www.sitesatlas.com**

The selection of an appropriate site location(s) for processing biomass to biofuels and biobased chemicals will depend on a multitude of factors including:

1. Cost of land acquisition and preparation;
2. Capital costs of construction including delivery of major unit operations to site;
3. Contractor’s fees and legal/permitting expenses for acquiring land and erecting a processing facility;
4. Cost of process raw materials including delivery costs to site;
5. Availability and cost of producing and delivering appropriate (optimally chosen) feedstock(s) to the processing site;
6. Labor and related fixed charges based on regional labor rates and availabilities;
7. Proximity and access to major end product markets (optimally chosen);
8. Availability of local incentives to invite industrial participants to community.
As can be seen from the aforementioned list there are a multitude of factors that affect the choice of an optimal site for locating a processing facility, most of which interact with each other; the optimal choice will not only depend on the cost of production at a particular site, but also on the availability of an optimal set of feedstock(s) in close proximity to the site (to reduce input costs), the availability and proximity of process chemical and ancillary resource suppliers to the site, and efficient access to markets (optimal set based on local prices and demands) for final products (in order to drive higher profits). Additional to these considerations, the modeling and optimization endeavors in this dissertation also incorporate environmental sustainability considerations; specifically the emissions impact of designing an appropriate supply and demand network will also factor into the decision(s) for selection an optimal set of processing facility locations and supply and demand nodes.

All these considerations make the formulation of an appropriate optimization model an attractive prospect to optimally select and study network nodes that will supply and process feedstocks and act as end markets for final products. Figure 3-3 shows the hypothetical network structure that was used as an input to the optimization model with appropriate highway and rail distances between prospective upstream and downstream nodes. Ideally, GIS-based software can and, in real life should, be employed to get accurate distances between supply, processing, and demand points for a potential biomass-to-biofuels network. But for the case of demonstrating the utility of a model-based decision support system, as is the exercise for this dissertation, we will utilize approximate distances between network nodes; these distances will be based on Google searches for distances between two network nodes and the transportation costs and the optimal mode of transportation (railway or road) will be based upon these distances and standard cost functions for transporting...
materials (on a mass basis) using each mode. Additionally, in order to represent the “centralization” and/or “remoteness” of a particular network node, a scaling factor will be used to increase/decrease the calculated transportation costs to account for aspects such as road weight limits, tortuosity, and transportation service providers’ willingness to provide mediums for pickup/delivery of material at a certain network node. For biomass transportation, we assumed that storage facilities are maintained at the site of feedstock harvest where harvested feedstock is stored and trucks can pick up biomass shipments and transport it to processing facilities. For final product transportation, we assume that biofuels can be shipped to blending facilities at regional blending centers using either rail or road transport; the distances from the processing site to the blending center are again obtained using Google map searches for distances while the standard cost functions (on a mass basis) are utilized to model the cost of freight movement. While we fully understand that the datasets generated using the aforementioned methodology may not be fully accurate, we are confident that these estimation techniques are adequate to give readers and users a feel for the utility of a model-based, strategic decision support system for renewable product systems.
Figure 3-3: Hypothetical value chain for a biomass-to-bioproduct enterprise in Louisiana

In figure 3-3, the green boxes represent the possible market locations; we assume 2 separate markets in Louisiana with northern Louisiana being a blending station and southern Louisiana being a petroleum refiner blending on site; the markets in Arkansas and Mississippi represent blending stations while the market in Texas is assumed to be a refinery. These markets are assumed based on actual existence of blending stations and refineries in these areas, but the establishment of a contractual supply agreement will depend, in real life, on a multitude of factors not modeled in this case study. We will work under the assumption that a supply agreement can be established with a 100 percent probability. The demand for ethanol in the state (www.fhwa.dot.gov) was used as the aggregate demand of the state and it is assumed that a percentage of this demand can be served by the bioproducts enterprise. The triangular boxes in the figure represent possible locations for setting up processing facilities.
with the circular regions representing the area from where biomass can be sourced. The northern region of the state is assumed to be able to produce switchgrass as a feedstock, the delta region (south-central) is assumed to produce energy cane, while the southwestern region is assumed to be able to produce both energy cane and switchgrass. It is assumed that the biomass processor can sign long term supply agreements with farmers and landowners of CRP land, the exact structure of which is described later in the model and data description section. Finally, for the movement of biomass from sources to the processing facility, it is assumed that diesel trucks with a capacity of 13 dry tons can be utilized, for the movement of ethanol single railcars with a 60,000 gallons capacity and/or trucks with a 30,000 gallon capacity can be utilized, while for the movement of biobased chemicals, freight rail or trucks can be utilized with capacities of 110 and 25 tons respectively. The railway and highway networks are approximations of actual routes that are available in Louisiana and their distances (see data description section for numbers) are extracted using Google maps. We assumed that weight limitations for biomass movement will not be a bottleneck, especially on highways, since sugarcane is already transported across the state from fields to sugar processing mills. Nevertheless, further investigation into the road networks, especially near the field and processing sites (non-highway parts), should be carried out in order to ensure resolution of any weight/volume limitations before the actual network is established. The next sections will describe the decision processes and models that are used to select the appropriate conversion platform, feedstocks and sources, products and technologies and product markets.
3.2.3 Conversion Platforms

There are two major conversion pathways that process biomass into value-added fuels and chemicals (figure 3-4); (1) a biochemical pathway that uses biological processes to achieve the requisite conversion, and (2) a thermochemical pathway that utilizes thermal and catalytic processes to yield the desired outputs. Each pathway has its own advantages and disadvantages, which are discussed further in the sections following this introduction.

**Figure 3-4: Conversion platforms that convert biomass to biofuels and biobased chemicals**

Thermochemical Pathway

Thermochemical pathways for the conversion of biomass to biofuels and biochemicals utilize heat and chemical catalysis to convert the carbohydrates in biomass to value-added fuels and chemicals. The major processes that can be utilized for
thermochemical conversion include combustion, pyrolysis, and gasification (thermal part of thermochemical). Each process is described in brief below:

1. Combustion: thermally convert biomass in the presence of an oxidant to produce thermal and electrical energy along with carbon dioxide and water.

2. Pyrolysis: Thermal conversion of biomass (at low temperatures) in the absence of an oxidant to produce liquids as the primary product (fuels and chemicals).

3. Gasification: Thermal conversion of biomass at elevated temperatures and reductive conditions to produce gases, char, water and other condensable matter.

Combustion is technically the easiest process to execute, but the energy yield and its applicability to transportation fuel production are low. While combustion is a process that has been historically studied over the past decades, pyrolysis and gasification deserve some discussion here.

**Pyrolysis:** pyrolysis in its most basic form is defined as the heat-induced chemical changes in organic matter in the absence of oxygen. For biomass pyrolysis, the major products include water, oils, tar, and charcoal. Pyrolysis reactions are endothermic reactions whose energy efficiency, defined as the heat output (in terms of product) per unit of heat input, depends in large part to the moisture content of biomass feedstocks. Before the advent of petroleum as a feedstock, wood pyrolysis, also referred to as the destructive distillation of wood, was utilized for ages to derive charcoal and important chemicals such as methanol, with the majority of the heat value of wood retained in the charcoal. Additionally, some gases including oxygen, hydrogen, methane, and carbon mono- and dioxide are also produced. The ratios in which these products are produced depend on the biomass particle
size, the operating temperatures, the length of reaction time, and the heat rates during pyrolysis. Usually, lower operating temperatures and slower heat rates will yield solid materials including charcoal, while higher temperatures and faster heat rates will yield a larger percentage of gases and bio-oil (liquid), which can be refined to obtain transportation fuels and chemicals. This process of deriving bio-oils from lignocellulosic biomass is known as fast pyrolysis and the processes for the production of bio-oils have only recently been discovered and studied.

**Gasification**: gasification is a modern conversion method (an extension of pyrolysis) to obtain gaseous fuels from biomass. The major difference between gasification and traditional pyrolysis is that gasification is optimized to produce high yields of gaseous fuels and energy, rather than producing charcoal and liquids. These gaseous fuels can be utilized in their native forms or liquid transportation fuels and chemicals can be manufactured from them using value-adding unit operations. Some value-added operations for the gaseous fuels include the use of Fischer-Tropsch catalysts to produce synthetic gasoline and diesel, their fermentation to yield cellulosic biofuels such as ethanol and higher alcohols, and the catalytic reforming of gases to produce hydrogen fuel. A major advantage for gasification is that the process itself can utilize a multitude of feedstocks including urban, industrial and agricultural wastes, and dedicated energy crops and forest wood. The majority of gasifiers work with partial oxidation reactions where just enough air or steam (oxidizing agent) is introduced for the biomass to provide sufficient heat for the gasification reactions to occur. The amount of oxygen is a major driver of the calorific value of the resultant products from gasification. A major product post gas cleaning from gasification is synthesis gas (syngas), which is composed of carbon monoxide and hydrogen. Syngas is a flexible feedstock that can be upgraded to a
multitude of products through downstream processing operations including biofuels (ethanol and higher alcohols) and hydrogen fuel, and biobased chemicals such as ammonia.

**Biochemical Pathway:** biochemical conversion of biomass to biofuels and biobased chemicals is based on fermentation and digestion processes. Based on the operating conditions and micro-organisms utilized, the fermentative processes have the potential to produce a range of biobased fuels including fermentative hydrogen and fermentative ethanol, butanol, and a range of biobased chemicals. Anaerobic and aerobic digestion of biomass, on the other hand, produces gaseous fuels primarily consisting of methane referred to as biogas. Additionally, fermentation of organic matter such as glycerol also has the potential to yield value-added biofuels and biochemicals. The biomass inherently contains a large amount of complex and simple carbohydrates that can be converted enzymatically to value-added fuels and chemicals using fermentative organisms. The final product concentrations that result from fermentation are dependent on the organisms that are utilized and the operating conditions of the fermentation reactors. Some salient features of a biochemical production platform that are worth mentioning here follow:

1. Biochemical conversion involves the fractionation of biomass into sugars using thermal, chemical, biological, or a mixture of these processes;
2. These sugars provide significant flexibility to processors, in terms of what portfolio of products can be produced;
3. The portfolio of products will usually require genetically engineered micro-organisms that have the ability to yield a particular product through a fermentation process;
4. Lignin and other waste components (unfermented sugars, unutilized proteins, and ancillary biomass components) provide a rich fuel source to generated heat and power for the processing plant, enabling a self-sustaining (energy basis) plant design;

Within each conversion pathway, there are multiple permutations of unit operations and process configurations that can be utilized to convert biomass to biofuels and biobased chemicals. This subsection will describe qualitatively some unit operations that are considered during technology selection. We will focus our efforts on gasification technologies for thermochemical conversion that produce syngas which can then be upgraded to cellulosic biofuels and fermentative technology for biochemical conversion that produce liquid biofuels such as ethanol and butanol. The driving force behind this selection is two-fold: (1) liquid biofuels have the most attractive market potential in the near-to-medium term to become a commercially viable replacement for crude oil derivatives, and (2) the market size for liquid biofuels, at least theoretically, is the size of the crude oil markets, while market sizes for hydrogen fuel is still in question specifically for its use as a transportation fuel (based on safety, efficacy, and portability issues). This is not to say that hydrogen and methane in the future will not be major parts of a sustainable energy portfolio, but that the commercial development curve for hydrogen is much steeper currently than that for liquid biofuels, while production of methane for use as a transportation fuel requires significant infrastructure upgrades and the competition from lower priced natural gas from petroleum drilling remains a significant barrier to overcome.
Thermochemical Platform Technologies

A systems representation of the production chain to convert biomass to liquid transportation fuels via gasification is provided below (figure 3-5).

![Thermochemical conversion system via biomass gasification](image)

**Figure 3-5: Thermochemical conversion system via biomass gasification**

Preprocessing operations are used to reduce the biomass to consistent particle size, and reduce the moisture content. As mentioned previously, these are important drivers that determine the energy yield of the conversion processes, as smaller particles have larger surface area per unit mass thus enabling better heat transfer. Milling and grinding are common unit operations that are utilized for size reduction. Drying is usually carried out to reduce moisture content of the feedstock; drying is an energy-intensive unit operation that can reduce the overall energy yield of the process.

For gasification, multiple reactor designs have been suggested in order to optimize the energy efficiency of the process including fixed and moving bed reactors (multiple flow patterns for feed and oxygen source), and fluidized bed gasifiers. The process can also be classified, on the basis of their heat supply processes, as direct and indirect gasifiers. In direct gasifiers, biomass is combusted in the gasifier (exothermic), which then provides the heat for the endothermic gasification reactions. During indirect gasification, part of the biomass is combusted in a separate chamber and heat exchangers are utilized to provide heat for downstream gasification. For fixed and moving bed reactors, co-current and counter-current
flows can be used for preprocessed biomass and oxygen sources; in counter-current flow the feed enters the top of the reactor while the oxygen source is fed at the bottom, while for co-current both streams enter from the top of the reactor. The product gas stream for counter-current flow exits the top of the reactor which is the lowest temperature zone of the reactor; this yields a large amount of tar in the product stream decreasing the overall energy efficiency of the process. For co-current flow the product stream exits the reactor through the highest temperature zone (bottom) thus consuming a majority of the tar in the product stream. However, energy recovery through process integration is still required to improve the energy efficiency of the process. For fluidized bed reactors, the feed is input at the bottom of the reactor and fluidized using air (also the oxygen source). Fluidization improves the heat transfer and conversion efficiencies of the overall process thus improving the overall energy yield. Catalysts can also be added as fluidization medium to further improve the conversion efficiency, but catalysts are susceptible to poisoning, especially at higher temperatures, consequently increasing catalyst regeneration (operating) costs.

Following gasification, efficient production of biofuels and biobased chemicals requires intermediate processing of the product gas in order to remove contaminants, such as tar, from it. Operations including cyclone separators (particulate removal), barrier filters (alkali removal), and hot/wet gas scrubbing (NO$_x$ removal). Tar removal is an essential process in order to efficiently produce bioproducts from the product gas; tar formation can be minimized by optimizing the design and operating variables of the gasification reactor and by using catalysts in the reactor itself (primary methods) or by hot/wet gas scrubbing and catalytic removal in a separate downstream reactor (secondary methods).
Following cleanup, the product gas is ready for conversion to value added transportation biofuels and biochemicals. Multiple biofuels production routes are possible from the product gas including catalytic methanol/higher alcohol synthesis, Fischer-Tropsch synthesis of synthetic diesel and gasoline, and fermentative production of cellulosic ethanol. Methanol/higher alcohols can be used as gasoline oxygenates or as esterification agents for biodiesel production. Usually, metallic catalysts are utilized for alcohol synthesis and the choice of the catalyst will determine the mix of the alcohols obtained. Fischer-Tropsch (FT) synthesis utilizes iron, cobalt, and ruthenium based catalyst to produce higher chain alkanes and alkenes from the product gas. In order to obtain consistent products in the gasoline/diesel hydrocarbon ranges, the FT product requires downstream hydrocracking to break up the unsaturated hydrocarbons. Alternatively, catalysts with higher selectivities can be used to produce gasoline/diesel during the FT reaction. Ethanol can be produced from syngas by using fermentative micro-organisms; the high selectivity of micro-organisms towards ethanol production makes this a very attractive process for commercial biofuel production. Additionally, lower operating temperatures imply that the energy load of the fermentative processing much lower than for the production of methanol/higher alcohols or FT gasoline/diesel. The major challenge for this production route is the efficient cleanup of syngas post gasification; impurities in the product gas can severely impact the fermentation efficiency thus reducing the overall process yields. Energy recovery post gasification can also increase the energy efficiency of the overall production process.

Biochemical Platform Technologies

A systems representation of the production chain to convert biomass to liquid transportation fuels via fermentative production is provided below (figure 3-6).
Figure 3-6: Biochemical conversion route via sugar fermentation

For each operating system in the biochemical production route, there are multitude of choices in terms of preprocessing and fractionation technologies that can be used, fermentation configurations that can be designed, and concentration and recovery technologies that can be employed to yield products within acceptable specifications for different end-use applications. Preprocessing, unlike thermochemical conversion, is not necessary to obtain a consistent sized feedstock in order to efficiently convert it to the desired products. This is primarily due to the fact that downstream fractionation can “double-up” as a preprocessing unit operation also. The choice of the appropriate fractionation technology, consequently, is absolutely necessary for maximizing the overall process yields over the biochemical production route. Usually, biomass fractionation is carried out in order to release the cellulosic material which, in its native form, is surrounded by branched chain hemicellulosic material and polymeric lignin. Besides size reduction, there are several characteristics that define a good fractionation technology; these include maximized sugar yields (including the preservation of the hemicellulosic fraction of the feedstock), minimizing the production of inhibitory compounds that may decrease the downstream fermentative efficiency, and optimization of energy utilization. Fractionation technology can be categorized into 3 broad categories; (1) physical pretreatment that do not utilize any chemical agents such as steam explosion and hot water fractionation, (2) chemical pretreatment that are usually chemically catalyzed such as dilute acid pretreatment (acid-catalyzed) and ammonia fiber explosion (AFEX, base-catalyzed), and (3) biological pretreatment that involve the utilization of fungi and/or bacteria to modify the lignocellulosic structure of
biomass, which can then be digested enzymatically to release the sugars contained in the biomass. Each fractionation technology has its advantages and disadvantages, and the combined costs and yields of each technology, along with their impact on downstream unit operations are a major determinant of the overall yield and efficiency of the biochemical production route. Table 3-1 lists the various fractionation technologies described above.

Table 3-1: Qualitative comparison of different biomass pretreatment technologies;
*Source: Lau et al (2009); Kazi et al (2009)*

<table>
<thead>
<tr>
<th>Fractionation Technology</th>
<th>Advantages</th>
<th>Disadvantages</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dilute Acid</td>
<td>Well Understood</td>
<td>Reactors susceptible to corrosion (high capital costs)</td>
</tr>
<tr>
<td></td>
<td>Wide applicability to biomasses</td>
<td>Degradation of sugars especially hemicellulosic fraction</td>
</tr>
<tr>
<td></td>
<td>High glucose yields</td>
<td>Large waste formation → fermentation efficiency</td>
</tr>
<tr>
<td>AFEX</td>
<td>Negligible inhibitors</td>
<td>Not very well understood</td>
</tr>
<tr>
<td></td>
<td>No particle size reduction</td>
<td>Does not work well with high lignin biomasses</td>
</tr>
<tr>
<td></td>
<td>Preserves hemicellulose structure</td>
<td>Ammonia recovery essential for control operating costs</td>
</tr>
<tr>
<td>Hot Water</td>
<td>Enhances cellulose digestibility</td>
<td>High pressure equipment required → high capital costs</td>
</tr>
<tr>
<td></td>
<td>Very little inhibitor formation</td>
<td>High water requirements → high operating costs</td>
</tr>
<tr>
<td></td>
<td>Little waste formation</td>
<td>Hemicellulose solubilisation → Low overall sugar yield</td>
</tr>
</tbody>
</table>

Following the release of the cellulosic fraction of biomass, the cellulose needs to be converted to glucose sugars that can then (along with xylose derived from hemicellulose during pretreatment), be fermented to a whole host of final products. It should be noted that depending on the pretreatment process used, the hemicellulosic fraction of biomass may be available for fermentation (AFEX) or may need additional recovery if it is solubilized and removed along with the liquid effluent (Acid, Hot water). Cellulose can be hydrolyzed to glucose, wherein, the carbon-oxygen linkages holding the cellulosic structure together are broken up to yield monomeric glucose sugars. This process can be carried out either catalytically using acids such as sulfuric acid, or enzymatically using cellulase enzymes. Following the release of glucose and xylose sugars, fermentative organisms can be utilized to
yield a range of products as fermentation broth effluent. There are multiple configurations of hydrolysis and fermentation that are possible; some of these are shown in figure 3-7 with their advantages and disadvantages discussed in table 5.

**Figure 3-7: Different hydrolysis and fermentation configurations that can be used to convert biomass starches to final products**

**Table 3-2: Qualitative comparison of different fermentation and hydrolysis configurations; Source: Zheng et al (2009)**

<table>
<thead>
<tr>
<th>Hydrolysis + Fermentation Configuration</th>
<th>Advantages</th>
<th>Disadvantages</th>
</tr>
</thead>
<tbody>
<tr>
<td>Separate + Separate (SHSF)</td>
<td><strong>Best</strong> control of hydrolysis and fermentation conditions ⇒ <strong>Highest</strong> overall process yields</td>
<td><strong>Highest</strong> Capital and Operating Costs (more unit operations)</td>
</tr>
<tr>
<td>Separate + Co-fermentation (SHCF)</td>
<td><strong>Better</strong> control of operating conditions ⇒ <strong>higher</strong> overall yields</td>
<td><strong>Higher</strong> capital and operating costs (more unit operations)</td>
</tr>
<tr>
<td>Simultaneous + Separate (SSSF)</td>
<td><strong>Lower</strong> overall process yield due to <strong>poorer</strong> control of operating conditions leading to product inhibition</td>
<td><strong>Lower</strong> Capital and Operating Costs</td>
</tr>
<tr>
<td>Simultaneous + Co-fermentation (SSCF)</td>
<td><strong>Lowest</strong> overall process yield due to <strong>poorest</strong> control of operating conditions leading to product inhibition</td>
<td><strong>Lowest</strong> Capital and Operating Costs</td>
</tr>
</tbody>
</table>
Table 3-2 enlists the advantages and disadvantages of various hydrolysis and fermentation configurations; the major driver of glucose yields (from cellulose) and product yields from sugars are the operating temperatures, with optimal hydrolysis temperatures being 50ºC while that for fermentation is 32ºC. Consequently, when the hydrolysis and fermentation unit operations are combined, the overall product yields are sub-optimal as the operating conditions for either process are not optimal. Additionally, for xylose and glucose fermentation in separate tanks, wash water is required to remove xylose (hydrolyzed in liquid stream) from the cellulose-containing solid stream. This leads to highest overall process yields, but the capital and operating costs are also significantly higher in order to purchase and operate additional process equipment. This is not the case for simultaneous hydrolysis and fermentation, as both processes are carried out in the same set of reactors although this impacts overall process yields as inhibitory compounds formed during cellulose hydrolysis reduce the fermentative action of micro-organisms. More robust micro-organisms that can withstand hydrolytic compounds (inhibitory) are a viable way to circumvent this drawback. Finally, consolidated bioprocessing, where pretreatment, hydrolysis, and fermentation are carried out in the same set of reactors should be the final goal of technological development as this has the potential to significantly reduce capital and operating costs; the current state of technology makes this process unattainable commercially.

3.2.4 Product Portfolios

This subsection discusses the product portfolios that are considered for each conversion platform. While multiple permutations of products are possible from each pathway, we will limit our analysis to similar products from each pathway in order to legitimize an “apples to apples” comparison. Designing an optimal portfolio individually for
each platform is something that is readily achievable using the proposed DSS framework, but it is not the goal of this demonstration.

Choosing an optimal portfolio of products to produce is not a trivial task, as the choices are themselves determined by the choices for processing options, their respective yields, and capital and operating costs incurred. One of the goals of this dissertation is to demonstrate a methodology that enables choice of a product portfolio for a multi-product biorefinery and concurrently selects the optimal process configuration to convert biomass feedstock to the optimal products. Ideally, a biorefinery should be composed of a diversified product portfolio with a judicious balance of high-volume fuel production and high value chemical production. This structure has been proven to be an effective hedge against season variations in individual product markets in various industry verticals such the petroleum refining industry. A mix of volume-based and margin-based products produced on a flexible production platform can enable product switching to navigate input cost and market variability; in a high input cost environment it may make sense to switch to a higher value product mix to maintain profitability, while in a low input cost environment fuel production can be emphasized to driven revenue growth. Similarly, product mixes can be adjusted to match market demands and production levels can be controlled given the market pricing environments for each product in a respective portfolio.

Thermochemical Products

The major product that results from thermochemical gasification of biomass is syngas. Syngas is a mixture carbon mono- and dioxide gases along with hydrogen and trace amounts of other combustion products. Syngas provides a valuable platform compound that
can be converted to a variety of finished products by applying appropriate processing operations on the effluent. For comparison between the biochemical and thermochemical platforms, I wanted to maintain consistency amongst the products that will be evaluated from each platform. Specifically, the biofuel that is produced from each should be similar, while other co-products can be different. Consequently, cellulosic ethanol is chosen here as the common biofuel that can be produced from each conversion pathway. Additionally for thermochemical production, higher alcohols including propanol and butanol are produced. These higher alcohols can be used to either serve the chemical markets as feedstocks or as additives to fossil fuels such as gasoline. According to NREL, the market for higher alcohols as chemical feedstocks is relatively small and fairly competitive; consequently higher alcohols will be assumed to serve the transportation fuel additive markets.

Biochemical Products

The product portfolio for biochemical conversion of biomass consists of three products; 1) cellulosic ethanol, which is a low-margin high volume fuel source and additive, 2) lactic acid, which is a low-margin platform chemical that is used as, amongst others, a food additive and a monomer for value-added biopolymer production (Polylactic Acid), and 3) succinic acid, which is a high-margin chemical with a variety of uses as a platform chemical for specialty chemicals and biopolymers. These products can all be produced via the fermentation of C5 and C6 sugars; the enzyme/micro-organism used along with the operating conditions shifts the fermentation equilibrium towards the maximization of one of these products. Given this structure, we assumed that the same pretreatment and fermentation equipment (a battery of fermentors) can be used to yield the desired product after which
product-specific recovery and purification equipment can be used to reach desired purity targets (Lynd, 2005).

3.3 Portfolio and Spatial Design Optimization

3.3.1 Model Architecture

This chapter describes the formulation of an assessment and optimization framework that we used to design the technological and supply chain structure that can process biomass feedstocks to value-added fuels and chemicals. Specific functions of the framework include selection of the appropriate conversion platform (thermochemical vs. biochemical), feedstock selection, conversion technology and corresponding product portfolio design, and supply and demand network design. There are different ways the framework can be formulated, for example, a single mathematical optimization model can perform all selection and design tasks or parts of the selection process can be carried out analytically and optimization models can be utilized for certain specific tasks. For the purpose of this case study the task of platform selection will be carried out qualitatively with the utilization of simple comparative statistics. Once the platform is selected a process superstructure will be formulated to convert biomass sources to bioproducts; an inventory of data describing potential feed sources and products with greatest market and environmental potential will be discussed. An integer-based optimization model will then be utilized to design the optimal feedstock, technology, and product portfolio along with an appropriate supply and demand network for a hypothetical biorefining enterprise operating in Louisiana and serving regional markets in Southeastern United States. Finally energy efficiency and environmental metrics will be used
to describe the potential performance of the optimal design. The entire process of selection and analysis is shown in figure 3-8, with green boxes representing system inputs, blue boxes representing the decision processes, and green boxes representing the results that are obtained from the decision processes.

Figure 3-8: DSS architecture for site, technology, feedstock, and product portfolio selection

We can see from the block flow diagram that there are significant complexities involved with designing the entire conversion technology superstructure; embedding these features into a single model, although novel, may become too computationally burdensome, with model granularity being sacrificed. Additionally, the selection of a platform should ideally be a mutually exclusive task following which tasks such as detailed process superstructure design and product and feedstock selection can be carried out. The next
subsections will describe the formulation of the platform selection and process design optimization problems.

3.3.2 Platform Selection

For platform selection, we utilized aggregate cost, yield, and market potential estimates for the thermochemical and biochemical platforms. The purpose of this exercise is to gauge the long-term potential of each conversion platform to generate economic and environmental value for an enterprise. Detailed technological intricacies are not considered and this exercise is merely used to pick a platform to carry out further modeling and analyses on. The platform selection exercise is usually not a math-intensive exercise, and a lot of times, the regional location of a facility and the types of biomass feedstocks available for processing will determine the appropriate platform to choose for commercialization. Important qualitative characteristics that should also be considered while selecting the appropriate platform are the human capital that is available for designing and operating a platform, customer relations to sell the final products to, and the enterprise business model; issues such as capital availability and budgetary constraints will undoubtedly also impact the choice of an appropriate platform for conversion. A brief description of each platform was presented in the previous chapter. Here we will utilize literature derived quantitative and qualitative metrics to compare the two platforms from the perspective of a commercial ethanol facility (50-75 MM gallons annually) and legitimize our selection of a particular platform. Once an appropriate platform is selected, feedstock selection, product and technology portfolio design and process superstructure optimization can be carried out on the selected platform.
Table 3-3: Comparative metrics of biochemical and thermochemical production platforms; Source: Wright and Brown (2007)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Biochemical</th>
<th>Thermochemical</th>
</tr>
</thead>
<tbody>
<tr>
<td>Feedstock Flexibility</td>
<td>Herbaceous (starchy) feed</td>
<td>Woody biomass</td>
</tr>
<tr>
<td>Capital Investment</td>
<td>~$400 million</td>
<td>~500 million</td>
</tr>
<tr>
<td>Operating Costs</td>
<td>~$2.15 per gallon of ethanol</td>
<td>~$2.05 per gallon of ethanol</td>
</tr>
<tr>
<td>Ethanol Yields</td>
<td>60-80 gallons per ton biomass</td>
<td>60-80 gallons per ton biomass</td>
</tr>
<tr>
<td>Co-product Potential</td>
<td>High potential for value added, biobased chemicals</td>
<td>High potential for fuels (higher alcohols)</td>
</tr>
<tr>
<td>Process Energy Loads</td>
<td>Self-sufficient using co-produced lignin</td>
<td>Portion of biofuels (higher alcohols) produced to be diverted back as energy input</td>
</tr>
<tr>
<td>Wastes</td>
<td>Dependant on pretreatment, significant amounts of waste is digested during waste treatment</td>
<td>Catalyst, Olivine, ash, and sulphates which require handling</td>
</tr>
<tr>
<td>Environmental Emissions</td>
<td>Flue gas, fermentation gas</td>
<td>Flue gas, CO₂ vent</td>
</tr>
</tbody>
</table>

From Table 3-3 we see that the comparative metrics between biochemical and thermochemical production routes are very similar. A few points of difference lie in the feedstock types that are suitable for each process, the total capital investment required for a commercial scale facility, and the co-products that can be produced from each platform. This is not to say that high value chemicals cannot be produced from syngas (thermochemical), or that other transportation fuels cannot be produced from biochemical conversion (ex. butanol); this just suggests that the current state of technologies and R&D is focused on generating these product streams from each conversion platform. Another point to note about each process is that the thermochemical platform utilizes some portion of the resultant biofuel products in order to satisfy the heat requirements for gasification (endothermic reaction), while the biochemical platform utilizes lignin (~20-25% of feedstock) to generate heat and power for the processes. Given these metrics for comparison, it is very difficult to arrive at an objective selection for the platform I wanted to study. We refer back to the quantitative metrics that were provided for selecting Louisiana as a prospective location for erecting a biorefinery. From the factoids, we noticed that a significant fraction of the state’s biomass resources are already utilized by existing industries for electricity generation and other niche
applications. For a commercial scale biorefinery to remain in operation for any period of time, it is essential that a consistent supply of feedstock be secured, preferably before any new capital is invested in site preparation, permitting and equipment purchasing. Given the resource supply constraints for currently grown biomass resources, the only true viable and consistent source of feedstock in the state seems to be cultivation of herbaceous energy crops on CRP lands, nutritionally-marginal lands, or contractually obligated land; this is not to say that residue supplies (forest and agriculture) cannot be used for biofuels production, but that the competition for these resources can put upward pressure on pricing and lead to erratic supplies over the long term. Development of CRP land for biomass production is not a trivial task though, and R&D for production methods and logistical support is necessary to drive a sustainable resource supply over the next few decades. Nevertheless, CRP land is a very promising resource nexus for biomass feedstocks. The question then becomes, what feedstocks are most attractive; significant government research has provided estimates for uses of CRP lands and the answer emphatically has been shown to be dedicated energy crops. Given that the biochemical production route is amenable to energy crops’ processing, this production route will be expounded on in this dissertation. Additionally, in an economic environment constrained by capital availability, the 25 percent additional capital requirement for a commercial thermochemical conversion plant can prove to be a significant budgetary constraint. Finally, the skilled labor available in Louisiana for crop production and the logistical infrastructure already established can significantly shorten the learning curve for energy crop harvesting and collection. The biomass source choices that I will investigate for their efficacy to produce biochemically-derived fuels and chemicals comprise of switchgrass and energy cane. Further analysis on this feedstock portfolio will be conducted through
modeling and optimization endeavors. The purpose of this dissertation is less to design an appropriate supply infrastructure for resources, and more to design an appropriate conversion process to utilize the resource. Nevertheless, some time will be invested in modeling important characteristics of feedstock production and supply, but more importantly the impact of feedstock characteristics on technology selection and process design will be studied in greater detail. As an extension to the framework, the integration of an appropriate methodology to model and optimize feedstock production and supply in sufficient detail is an endeavor that we are currently working on at the PSE group at LSU.

The next section provides a description of a detailed design optimization model that can systematically design and optimize a spatial and technological superstructure, and select appropriate feedstocks to process and convert to an optimized product portfolio.

3.3.3 Spatial and Technological Superstructure Design

The overall portfolio design problem was shown previously in figure 3-8. While platform selection was carried out qualitatively to select a biochemical processing platform, we chose to formulate a single model to design spatial network to supply feedstock and distribute products, and select the optimal portfolio of feedstock(s), technologies, and products that maximize the strategic value of the biorefining enterprise. A joint model was chosen as opposed to separate models as it was realized that these selection problems are not mutually exclusive; for example, the choice of an appropriate technological configuration for processing biomass to value-added fuels and chemicals will depend on the yields and costs of the technologies which in turn will determine the resource loads (feedstocks, chemicals, water, process fuel) for the facility which then will determine the appropriate location for the...
processing facilities given these resource constraints. A decision made to select an appropriate product portfolio will be determined by not only the demand and price prospects of the product, but also by the accessibility of the facility to end markets and the resultant freight costs that arise for their distribution. With such interdependencies prevalent through the network and process design decision problem, it then makes sense to formulate a single model that recognizes all these relationships and optimizes the enterprise decisions based on the appropriate resource, capital, and supply/demand constraints for the representative network and enterprise.

To design the spatial network and technological portfolios from an enterprise perspective, a vertically integrated biorefinery was assumed that undertakes the costs involved with biomass production and processing including establishment of the biomass producing crops. It was assumed that the biorefiner can rent contractually expiring CRP land from regional farmers within the network studied (figure 3-3) by compensating them appropriately for opportunity costs that arise from the farmers foregoing rental payments from the government through the CRP enrollment program. For biomass source selection it was assumed that the prospective biorefinery is located in Louisiana. The feedstock-related reasons for selecting Louisiana were mentioned in the previous subsection (Platform Selection). For end product markets (biofuels and biochemicals) the following inferences can be made to further legitimize Louisiana for site location:

1. Good end markets to sell into including refining plants (ethanol blending) and downstream processors for biobased chemicals (polymer, specialty chemical plants);
2. Availability of distribution channels for multi-modal movement of final products to end markets (rails and barges for out of state transport, Gulf of Mexico for international trade);

3. The presence of state tax incentives and grants to promote the production of renewable fuels and chemicals.

For spatial nodes, the supply and demand chains were divided into the following nodes:

1. Feedstock sources where energy crops can be grown, harvested, and stored;
2. Site selection for processing facilities where biomass inventories can be maintained and processed to final products;
3. Market selection where final products can be shipped, stored, and sold to end customers.

For technology selection, a systems optimization approach (figure 3-9) was adopted where the technologies were allocated between the feedstock nodes and feedstock processing nodes and input/output models were formulated for each technology at each node:

1. Harvesting and Densification technology (feed production node) that harvested land (input) to yield biomass feedstock (output);
2. Transportation technology (feed production node) to move biomass feedstock (input and output) from CRP land to processing nodes;
3. Fractionation technology (processing node) that converted biomass (input) to carbohydrates (output);
4. Fermentation technology (processing node) that converted carbohydrates (input) to higher-value fuels and chemicals (outputs);
5. Concentration and recovery technology (processing node) that recovered and purified the final products (input) from fermentation broth to a marketable form in terms of purity (outputs);

6. Boiler technology (processing node) using a lignin and solid residue feed (input) to produce process steam (output);

7. Turbine and generator technology (processing node) to use high pressure steam from boiler (input) to produce electricity (output);

8. Utilities and wastewater technology (processing node) to purify process effluent water (input) to yield process water (output).

9. Transportation technology (processing node) to move final products (input and output) from processing facility to markets (demand node);

Figure 3-9: Systems representation of the technological superstructure used for optimization
The system input to each operating section is provided in the Table 3-4.

**Table 3-4: System input to each operating section in the value chain**

<table>
<thead>
<tr>
<th>Operating System</th>
<th>System Input</th>
</tr>
</thead>
<tbody>
<tr>
<td>Harvesting and Preprocessing</td>
<td>Land (acres)</td>
</tr>
<tr>
<td>Biomass Transportation</td>
<td>Biomass (tons)</td>
</tr>
<tr>
<td>Fractionation</td>
<td>Biomass (tons)</td>
</tr>
<tr>
<td>Fermentation</td>
<td>Fermentable Sugars (tons)</td>
</tr>
<tr>
<td>Concentration and Recovery</td>
<td>Final Product (gallons fuel or tons chemicals)</td>
</tr>
<tr>
<td>Steam Generation</td>
<td>Kilograms Steam × Steam Enthalpy</td>
</tr>
<tr>
<td>Power Generation</td>
<td>Kilowatt-hours of Electrical Energy</td>
</tr>
<tr>
<td>Wastewater and Utilities Management</td>
<td>Total wastewater treated + make-up water load</td>
</tr>
<tr>
<td>Product Transportation</td>
<td>Final Products (gallons fuel, tons chemicals)</td>
</tr>
</tbody>
</table>

Figure 3-10 provides a system dynamics based layout for the modeling framework that is formulated in the next section. We employ a bottom-up modeling methodology, wherein, process models for each node in the value chain are blended in with a financial cost and profit model to generate a holistic framework that can (theoretically) be employed to model not only renewable product value chains but any process or manufacturing operation. In this dissertation, the modeling framework is adapted to fit renewable product value chains with special attention paid to government grants, tax subsidies, and environmental considerations that are essential in determining the profitability of an emergent renewable product.
In figure 3-10 process models for resource production and processing are government by material and energy balances that describe the flow of material and energy across each processing node in the value chain. Additionally, yield equations (rate of reaction) are used to describe the conversion of an input to a requisite output. The process model outputs are utilized by a financial model to describe the costs and revenues that are incurred (generated) through decisions made at a processing node. The profit and cash flow for a particular value of a process output (decision variable) is governed by financial and market parameters such as capital availability in the form of loans, grants, and equity capital, tax rates and subsidies, and market prices and demands for each product. The financial outcomes (revenue, cost, profit, cash flow) of each process decision in then fed into the objective function model where the discounted value of the projected cash flows (Net Present Value) is optimized under resource, capacity, demand, and capital availability constraints. The entire framework is formulated as one single model with special attention paid to the integration aspects of the financial formulation with the process model for each node in the value chain.

The next sections describe the optimization model that was used to provide decision support for the tasks of portfolio design and the data that was used to populate the model inputs. The modeling equations are tailored specifically to the biochemical platform case study, and require minor tweaking to execute the same framework for other renewable product value chains. A significant amount of data for unit operations’ was derived from Kazi et al (2010) that provided detailed cost analysis of different cellulosic biorefinery process configurations. We are currently working with researchers at the PSE group at LSU to develop dynamic simulations and equipment costing reports using ASPEN Plus and
ASPEN ICARUS to supplement the need for using literature estimates to run the optimization models.

Before we embark on defining the optimization model for the purpose of spatial network design, and feedstock, technology, and product selection, we wanted to briefly mention the concept of Stakeholder Value. A stakeholder in an enterprise is any person, entity, or ecology that is impacted by the enterprise operations. A modern-day enterprise has expanded from focusing just on its shareholders to focusing on all stakeholders as a means to generating the highest long term value. Stakeholders for a biorefining enterprise can be comprised of feedstock suppliers (farmers and land owners), transportation service providers, customers, capital providers including debtors and equity investors, the surrounding environment, and local communities. The modeling framework proposed here is formulated so as to incorporate the stakeholders’ needs and obligations during the design and planning process.

3.3.3.1 Biomass Production Model

Biomass constraints are utilized to develop a systems model for crop production and collection operations at representative land locations; it is assumed that switchgrass can be produced on CRP landed that is expiring while energy cane can be produced on sugarcane producing land. In order to incentivize farmers to switch from sugarcane production to energy cane, we assume that the biorefiner can make opportunity cost payments to farmers, while also compensating land owners for the cost of crop establishment and variable operating expenses. It is assumed that CRP locations represent 20,000 (annually) acres of aggregate land area while sugarcane land is represented by 10,000 annual acres of aggregate area per region. Each location has its own cost structure including fixed upfront payments for
contracting land, amortized payments for crop establishment, rent payments for energy cane harvesting and collection equipment, capital costs for purchase of switchgrass harvesting equipment, and transportation payments for biomass logistics services. The costs are discussed further in the production cost model. The formulation is used to model a biorefinery’s decisions to select types, quantities, and locations of feedstock to purchase. Additionally, the model also calculates the total acreage of land to contract.

Equation 1 models the total biomass \( b \) that is harvested (\( BM_{b,l,h,t}^{hvest} \)) at a given source \( l \) using a given harvesting and preprocessing technology \( h \). The total biomass is available for purchase (\( BM_{b,l,h,sto,t}^{purch} \)) is modeled as a function of the type of feedstock selected, the total land (\( Land_{b,l,h,t}^{hvest} \)) that is harvested and the expected biomass yields (\( BYLD_{b,l,t} \)) from the harvest operations adjusted for harvest losses (\( Hvst_{b,h}^{loss} \)). Equation 2 is a material balance on roadside storage facilities where harvested and preprocessed biomass is stored for pickup; here \( BMFI_{b,l,h,t} \) denotes the inventory of biomass while \( S_{p,b,h}^{BM} \) denotes the annual storage loss.

Equation 3 is an area balance on the land that is held under contract by the biomass processor (\( Land_{b,l,h,t}^{contr} \); this model assumes that the biorefiner can contract new land (\( Land_{b,l,h,t}^{new} \)) by making up-front payments to land owners in order to secure a steady supply of feedstocks in the future. To model the growth cycle for each energy crop (\( GC(b) \)), equation 4 is used to
mandate that land be released \((\text{Land}_{b,l,h,t}^{\text{release}})\) once a crop has run the course of its production cycle, following which the crop needs to be re-established.

\[
(\sum_{t'=t}^{t_{\max}} \text{BVHVST}_{h,l,t'}) \times \text{Land}^{\text{max}}_t \geq \sum_{b=\{b,l\}} \text{Land}_{b,l,h,t}^{\text{contr}}
\]  
\hspace{1cm} (3.3.5)

\[
\text{Land}_{b,l,h,t}^{\text{contr}} \geq \text{Land}_{b,l,h,t}^{\text{hvst}}
\]  
\hspace{1cm} (3.3.6)

\[
\rho_l^{\text{minutil}} \times \text{Land}_{b,l,h,t}^{\text{contr}} \leq \text{Land}_{b,l,h,t}^{\text{hvst}}
\]  
\hspace{1cm} (3.3.7)

Equation 5 constrains the area of land that can be contracted at one time \((\text{Land}^{\text{max}}_t)\); here \(\text{BVHVST}_{h,l,t'}\) is a binary variable that is used to denote the technological choice for harvesting and preprocessing operations. Finally, equations 6 and 7 are used to constraint the maximum land that can be harvested during a time period and the minimum land that is required to be harvested, respectively. The minimum utilization constraint represents a stakeholder consideration, wherein, if land is contracted by a processor, a minimum percentage \((\rho_l^{\text{minutil}})\) has to be utilized in order to provide land owners with consistent income by minimizing unutilized land area under contract.

3.3.3.2 Process Systems Model

3.3.3.2.1 Mass Balances

Material balances were performed for each node in the supply and conversion chains of biomass production and conversion to ethanol and succinic acid; these nodes include feedstock sources, biomass fractionation to sugars, sugar conversion to final products, product concentration and recovery, and product sales in end-use markets.
Equation 8 is a mass balance on the biomass that is transported to the biorefinery; here BMI_{bt} denotes the inventory levels of biomass type b that are maintained at the processing facility, BM^{used,prod}_{b,p,pt,ft,st,t} is the biomass quantity that is used for the production of product p, and BM^{used,Elec}_{b,ft} is the amount of biomass that is co-fired along with process fuel in order to generate electricity; biomass procured can be allocated towards production of electricity and/or value-added biofuels and biobased chemicals in order to make up for any energy/power deficit that may arise during their production. Additionally, Loss_{b} is used to represent dry matter losses in biomass quantities during storage.

\[ \sum_{b,h} BM^{\text{purch}}_{b,l,h,\text{st,t}} + BM_{b,st,t-1} \times (1 - \text{Loss}_{b}) = \sum_{p,pt,ft} BM^{\text{used,prod}}_{b,p,pt,ft,st,t} + BM^{\text{used,Elec}}_{b,ft,t} + BMI_{b,ft,t} \]  

Equation 9 is a reaction rate equation of the conversion of biomass to sugars of type s (glucose or xylose); here Sugar^{\text{Cont}}_{b,s} is the theoretical amount of fermentable sugar s that can be obtained from biomass b and SYLD_{b,s,pt,ft} is used to adjust the theoretical amount to an actual obtained value (Sugar^{\text{prod}}_{s,b,p,pt,ft,t}) based on the fractionation unit operations (prehydrolysis and enzymatic hydrolysis) that are employed. These yield adjustments, along with several other cost and energy factors will be used by the optimizer to obtain the optimal process.

\[ \text{Sugar}^{\text{prod}}_{s,b,p,pt,ft,t} \times \text{SYLD}_{b,s,pt,ft} \times BM^{\text{used,prod}}_{b,p,pt,ft,st,t} = \text{Sugar}^{\text{prod}}_{s,b,p,pt,ft,t} \]  

\[ \text{Sugar}^{\text{prod}}_{s,b,p,pt,ft,t} \times \text{E}[\text{YLD}]_{ps}^{\text{theoretical}} \times \text{FYLD}_{s,b,pt,ft,p}^{\text{actual}} = \text{Product}^{\text{broth}}_{p,s,b,pt,ft,t} \]  

\[ \sum_{b,s} \text{Product}^{\text{broth}}_{p,s,b,pt,ft,t} = \text{Product}^{\text{total}}_{p,pt,ft,t} \]  

\[ \text{Product}^{\text{final}}_{p,i,cr,pt,ft,t} = \text{RCYL}_{p,i,cr,pt,ft} \times \text{Product}^{\text{total}}_{p,pt,ft,t} \]
configuration and technology portfolio. Equation 10 employs the same theoretical yield \((E[YLD]_{p_s}^{\text{theoretical}})\) and actual yield \((FYLD_{s,b,pt,ft,p}^{\text{actual}})\) adjustment methodology to the fermentation unit operations, where the final product is obtained in the fermentation broth \((\text{Product}_{p,s,b,pt,ft,t}^{\text{broth}})\) that is effluent from the tanks. Finally, Equation 12 is used to adjust the final, concentrated and purified product quantity based on the separation yields of the concentration and recovery unit operations of type \(cr\) for product \(p\); here, subscript \(i\) is introduced to categorize final products based on their purity. For bioproducts such as ethanol and succinic acid, the target markets, and consequently the demands and prices, are dependent on product purity levels. The amount of energy and cost expended on reaching a certain purity level will vary and so will the final yield to product (from product recovery and purification) for that product category. Consequently, equation 12 is used to provide the optimization model a choice to target different product markets for the same bioproduct based on the purity level reached after the purification section of the plant. The choice of final product amounts that are sold into each demand category, for each purity level, will depend on not only the total demand and price levels for each category, but also on the capital cost for the purification equipment, and the input and energy costs expended to reach the purity level.

\[
\sum_{m, tr} \text{Sales}_{p,i,m,st,tr,t} + \text{FPI}_{p,i,sta} = \sum_{cr,pt,ft} \text{Product}_{i,cr,pt,ft,sta}^{\text{final}} + \text{FPI}_{p,sta-1} \times (1 - \text{Loss}_p) 
\]  

(3.3.13)

Equation 13 is a material balance on the final product storage containers, where the product from the container is sold to end-use market \(m\), under the product category \(i\), from site \(st\), using transportation mode \(tr\) \((\text{Sales}_{p,i,m,sta,tr,t})\), and \(\text{FPI}_{p,sta,t}\) denotes the final product inventories adjusted for product losses during storage.
3.3.3.2.2 Emissions Accounting Model

The next set of equations is used to model the net carbon emissions, biogenic and non-biogenic, that result from (1) biomass production, harvesting, and transportation, (2) processing chemical production and transportation to processing facilities, (3) bioproduct processing, (4) final product distribution, and (5) final product consumption. These equations are essentially used to represent the Life cycle analysis (cradle-to-grave) for the production of biofuels and biobased chemicals using biomass derived from energy crops. These equations are a manifestation of the waste accounting model that was proposed in Chapter 2 (Section 2.3.4). Additional emissions such as NO\textsubscript{x} and SO\textsubscript{x} are not modeled here due to the scarcity of data for each operation of the value chain, but the proposed model can easily be extended to include other emissions, and even solid waste products. Biogenic sources of carbon include CO\textsubscript{2} produced from ethanol fermentation and heat and power generation through the combustion of lignin and residual organic material post-product recovery. Additionally, biogenic carbon is also consumed during succinic acid production; we ensure that only fermentation gas based carbon dioxide is used for succinic acid fermentation (due to purity concerns of flue gases), while flue gases are assumed to be released to the atmosphere without any impact on the carbon balance of the value chain (biogenic carbon released that is previously sequestered by energy crops during production). For final product consumption, it is assumed that ethanol can replace gasoline (E5, E10, and E85 blends) thus having a positive impact on the carbon balance of the bioproduct value chain. Additionally, succinic acid is assumed to replace (a) petroleum-derived succinic acid in niche markets comprising of coolants, plasticizers, and fuel additives, or (b) replace maleic acid derived succinic acid which is again derived from crude oil (through the use of butane or benzene as a feedstock).
Equations 14-19 are used to track the total biogenic carbon that is released (sequestered) during biomass production and conversion to final products; equation 14 calculates the total soil carbon that is released to the atmosphere from the use of land (specifically CRP land) to produce energy crops; equations 15 and 17 calculates the net biogenic carbon that is released and sequestered during the production of ethanol and succinic acid, respectively; equation 16 calculates total biogenic carbon released via combustion of residual plant solids and any makeup biomass feedstock used to generate electricity and heat for the plant; equation 18 is a balance on the emissions flow in and out of the processing unit operations, while equation 19 constrains the total emission recycle by the minimum of the total emissions required for optimal production and emissions produced during unit operations (not biomass combustion).

\[
\begin{align*}
EmSequestered_{b,t} &= EmSeq_{b,t} \times \sum_h Land_{b,h,t}^{hyst} \quad (3.3.14) \\
EmProd_{st,t}^{production} &= \sum_p EmProd_p^{unit} \times \sum_{pt,ft} \text{Prod}_{pt,ft,st,t}^{total} \quad (3.3.15) \\
EmProd_{st,t}^{power} &= \sum_b EmProd_b^{unit} \times \sum_{pt,ft} \text{Fuel}_{pt,ft,st,t}^{used} + \sum_b EmProd_p^{BM,Comb} \times BM_{b,st,t}^{used,Elec} \quad (3.3.16) \\
EmReqd_{st,t}^{production} &= \sum_p EmReqd_p^{unit} \times \sum_{pt,ft} \text{Prod}_{pt,ft,st,t}^{total} \quad (3.3.17) \\
EmVent_{st,t}^{total} &= EmProd_{st,t}^{production} + EmProd_{st,t}^{power} - EmRecyl_{st,t}^{production} \quad (3.3.18) \\
EmRecyl_{st,t}^{production} &\leq \min[EmReqd_{st,t}^{production}, EmProd_{st,t}^{production}] \quad (3.3.19)
\end{align*}
\]

Equations 20-26 calculate the total fossil-based carbon that is released to the atmosphere during feedstock production and transport, feedstock conversion to final products, and product transportation to markets. For feedstock production it is assumed that
the major sources of carbon are the establishment and harvest machinery (diesel fuel) and fertilizer inputs. For biomass conversion it is assumed that carbon sources comprise of the production (in terms of energy used) of process chemicals that are utilized during the conversion ($\varphi_{\text{pt,ft,stat}}^{\text{PChem}}$) and purification ($\varphi_{\text{cr,fr,ist}}^{\text{PChem}}$) processes. For biomass transportation, we assume that biomass can be transported in its preprocessed form using trucks whose carbon impact is calculated based on:

1. Its diesel fuel efficiency ($\text{MPG}_{\text{truck}}^{\text{truck}}$),
2. Emissions factor for diesel ($\varphi_{\text{CO}_2}^{\text{Diesel}}$), and
3. The amount of preprocessed biomass that can be fitted into a truckload ($\tau_{b,h}$)

For final product distribution, a similar methodology is utilized; except I assume that final products can be distributed using multiple transportation modes (an optimization variable).

\[
\text{EmProd}^{\text{B,lt}}_{b,lt} = \left\{ \text{Diesel}^{\text{hvest}}_{b,lt} \times \varphi_{\text{CO}_2}^{\text{Diesel}} + \text{Fert}_{b,lt}^{\text{N,P,K}} \times \varphi_{\text{CO}_2}^{\text{N,P,K}} \right\} \times \sum_n \text{Land}^{\text{hvest}}_{b,lt,h}\lt \tag{3.3.20} \right.
\]

\[
\text{EmProd}^{\text{PChem}}_{\text{pt,ft,stat}} = \left( \sum_{\text{Chem,pt,ft}} \varphi_{\text{pt,ft,stat}}^{\text{PChem}} \times \sum_{b,p} \text{BM}_{b,p,\text{pt,ft,stat}}^{\text{hased,prod}} \right) + \left( \sum_{\text{Chem,cr,ip}} \varphi_{\text{cr,ip,ist}}^{\text{PChem}} \times \sum_{\text{pt,ft}} \text{Product}_{\text{final},p,i,\text{cr,pt,ft,stat}} \right) \tag{3.3.21} \]

\[
\text{EmProd}^{\text{BM,import}}_{b,lt,h} = \text{Distance}_{b,lt} \times \sum_n \left( \frac{\text{Diesel}_{\text{CO}_2}^{\text{MPG}_{\text{truck}}^{\text{truck}}}}{\tau_{b,h}} \right) \times \text{BM}^{\text{purch}}_{b,lt,h,\text{stat}} \tag{3.3.22} \]

\[
\text{EmProd}^{\text{prod,Dist}}_{p,\text{st,m,fr,stat}} = \text{Distance}_{p,\text{st,m,fr,stat}} \times \left( \frac{\text{Diesel}_{\text{CO}_2}^{\text{MPG}_{\text{truck}}^{\text{truck}}}}{\tau_{p,fr}} \right) \times \sum_i \text{Sales}_{p,i,\text{m,fr,stat,fr,stat}} \tag{3.3.23} \]

The total fossil based carbon is calculated using equation 24. Equation 25 then calculates the total fossil carbon that is avoided assuming biomass-derived products will displace their fossil-
derived counterparts (including green electricity), while equation 26 yields the net fossil-based carbon that is avoided (or emitted) due to the operation of the biomass-to-bioproducts value chain.

\[
\text{EmProd}_{t}^{\text{tot,fossil}} = \sum_{b,l} \text{EmProd}_{b,l,t}^{BM} + \sum_{st} \text{EmProd}_{st,t}^{PChem} + \sum_{b,l,st} \text{EmProd}_{b,l,st,t}^{BMX} + \sum_{p,m,st,tr} \text{EmProd}_{p,m,st,tr,t}^{Sale}.
\]  

(3.3.24)

\[
\text{EmAvoided}_{t} = \sum_{p,l} \left( \text{GHG}_{p,l}^{\text{savings}} \times \sum_{m,st,tr} \text{Sales}_{p,i,m,st,tr,t} \right) + \text{GHG}_{\text{elec}} \times \sum_{st} \text{Elec}_{st,t}^{\text{excess}}.
\]  

(3.3.25)

\[
\text{NetEm}_{t} = \text{EmAvoided}_{t} - \text{EmProd}_{t}^{\text{tot,fossil}}.
\]  

(3.3.26)

3.3.3.2.3 Steam, Power and Utility Balances

Simplified heat and power load calculations were used to estimate the design capacities for boilers and turbogenerators. The total fuel produced is a combination of (1) insoluble lignin solids that are obtained using a solid-liquid separation system (filter press unit operation), (2) unused proteins in biomass, and (3) unused sugars and oligomers in the fermentation broth. While lignin is sent directly to the boilers for combustion, the other waste streams are sent to the wastewater treatment facility, where anaerobic and aerobic digesters are utilized to convert these streams to biogas and sludge. These streams are then used as fuel sources for combustion (\(\text{Fuel}_{pt,ft,t}^{\text{produced}}\)). The fuel yield value (\(\text{YLD}_{b,p,pt,ft,t}^{\text{fuel}}\)) used in equation 27 is the combined total of the aforementioned sources that is obtained per ton of biomass processed using a particular process configuration. We also claim that all fuel produced (\(\text{Fuel}_{pt,ft,t}^{\text{produced}}\)) does not have to be used for steam generation (\(\text{Fuel}_{pt,ft,t}^{\text{used}}\)) as some solid fuel
can be sent to a landfill if plant (Fuel\textsubscript{\textit{pt,ft}}\textsuperscript{\textit{disposed}}) heat and power requirements are satisfied, but in such a scenario a waste disposal cost is associated with fuel that is disposed.

\[
\left( \sum_{b,p} BM_{b,p,pt,ft,stt}^{\text{used,prod}} \times YLD_{b,p,pt,ft}^{\text{fuel}} \right) = \text{Fuel}_{pt,ft,stt}^{\text{produced}} \quad (3.3.27)
\]

\[
\text{Fuel}_{pt,ft,stt}^{\text{used}} + \text{Fuel}_{pt,ft,stt}^{\text{disposed}} = \text{Fuel}_{pt,ft,stt}^{\text{produced}} \quad (3.3.28)
\]

The next 4 equations calculate the energy and the consequent steam loads of all possible process configurations; we assume that the main sinks for energy in the conversion processes are the fractionation unit operations for biomass and the concentration and recovery unit operations for the final purified product streams. While other, minor energy sinks are present, for pre-feasibility designs such as this, we assert that our formulation provides a sufficient level of detail. All unitary energy loads for fractionation technology sets (EReq\textsubscript{\textit{unit,Frac}}\textsubscript{\textit{pt,ft}}) and concentration and recovery technologies (EReq\textsubscript{\textit{unit,Rec}}\textsubscript{\textit{p,cr,pt,ft}}) were obtained from the process simulations that were carried out for each permutation of the processes. All unitary quantities are in the form of kilojoules per unit system input for that system. The total steam load (SLoad\textsubscript{\textit{total}}\textsubscript{t}) of a process configuration is obtained by assuming a representative steam enthalpy (H\textsubscript{steam}) at a known temperature (125C) and pressure (4 atmospheres). Finally, the total steam produced (Steam\textsubscript{\textit{pt,ft}}\textsuperscript{\textit{produced}}\textsubscript{t}) is calculated, assuming a boiler efficiency (Eff\textsubscript{boiler}), an average LHV for the fuel inputs (LHV\textsubscript{\textit{fuel}}\textsubscript{\textit{pt,ft}} or LHV\textsubscript{BM\textit{b}}), and adjusting the energy for sensible heat of water and heat of vaporization of steam (H\textsubscript{steam} – H\textsubscript{water}).

\[
\text{ELoad}_{b,pt,ft,stt}^{\text{Frac}} = \text{EReq}_{\textit{pt,ft}}^{\text{unit,Frac}} \times \sum_{p} BM_{b,p,pt,ft,stt}^{\text{used,prod}} \quad (3.3.29)
\]

\[
\text{ELoad}_{p,cr,pt,ft,stt}^{\text{Rec}} = \text{EReq}_{\textit{p,cr,pt,ft}}^{\text{unit,Rec}} \times \text{Product}_{\textit{p,cr,pt,ft,stt}}^{\text{final}} \quad (3.3.30)
\]
The power requirements are calculated in a manner similar to the thermal energy load calculations (equations 37-39), the only difference being, the total steam produced is converted to electrical energy using equation 22 through a steam turbine unit operation. An electrical efficiency value is used to adjust for energy losses during the Rankine cycle (conversion of thermal energy to electrical energy). Finally, equation 23 is used to estimate the expected excess amount of electricity that can be obtained using a particular process configuration; this electricity can then be sold to regional power distributors to create an additional value added revenue stream.

\[
\text{ELoad}_{\text{st,t}}^{\text{total}} = \sum_{b, \text{pt,ft}} \text{ELoad}_{b, \text{pt,ft,stat}}^{\text{Frac}} + \sum_{p, \text{pt,cr}} \text{ELoad}_{p, \text{cr,pt,ft,stat}}^{\text{Rec}}
\]  

(3.3.31)

\[
\text{SLoad}_{\text{st,t}}^{\text{total}} = \frac{\text{ELoad}_{\text{st,t}}^{\text{total}}}{H_{\text{steam}}}
\]  

(3.3.32)

\[
\text{Steam}_{\text{produced,pt,ft,stat}} = \frac{\text{Eff}_{\text{boiler}} \times \text{Fuel}_{\text{used,pt,ft,stat}} \times \text{LHV}_{\text{fuel,pt,ft}}}{H_{\text{steam}} - H_{\text{water}}}
\]  

(3.3.33)

\[
\text{Steam}_{\text{st,t}}^{\text{Tot}} = \sum_{\text{pt,ft}} \text{Steam}_{\text{produced,pt,ft,stat}} + \left( \sum_{b} \alpha_{b}^{\text{Steam}} \times \text{BM}_{\text{b,stat}}^{\text{used,Elec}} \right)
\]  

(3.3.34)

\[
\text{Steam}_{\text{st,t}}^{\text{Tot}} - \text{SLoad}_{\text{st,t}}^{\text{total}} = \text{Steam}_{\text{st,t}}^{\text{excess}}
\]  

(3.3.35)

\[
\alpha_{b}^{\text{Steam}} = \frac{\text{Eff}_{\text{boiler}} \times \text{LHV}_{b} \times \text{BM}_{b,\text{stat}}^{\text{used,Elec}}}{H_{\text{steam}} - H_{\text{water}}}
\]  

(3.3.36)

The power requirements are calculated in a manner similar to the thermal energy load calculations (equations 37-39), the only difference being, the total steam produced is converted to electrical energy using equation 22 through a steam turbine unit operation. An electrical efficiency value is used to adjust for energy losses during the Rankine cycle (conversion of thermal energy to electrical energy). Finally, equation 23 is used to estimate the expected excess amount of electricity that can be obtained using a particular process configuration; this electricity can then be sold to regional power distributors to create an additional value added revenue stream.
The next set of equations is used to estimate a prospective load for water for each
process configuration. Each operating system was assumed to have a unitary water load
based on the system input being processed. The water to be purchased included the operating
systems’ water loads plus the steam requirements for each configuration. The final purchased
quantity was adjusted for a loss factor under the assumption that water losses will be a
consequence of real operating scenarios. It was also assumed that the total water used in
facility will be treated for impurities and recycled to the fractionation section to mix with the
dry biomass inputs to the facility.

\[
\sum_{pt,t} E\text{lec}_{pt,ft,tt}^{\text{produced}} - P\text{Load}_{st,tt}^{\text{total}} = E\text{lec}_{st,tt}^{\text{excess}} - E\text{lec}_{st,tt}^{\text{purch}} \tag{3.3.41}
\]

\[
W\text{Load}_{st,tt}^{\text{Frac}} = \sum_{b,p,pt,ft} W\text{Load}_{b,p,pt,ft}^{\text{unit,Frac}} \times B\text{M}_{b,p,pt,ft,tt}^{\text{used,prod}} \tag{3.3.41}
\]

\[
W\text{Load}_{st,tt}^{\text{Steam}} = \text{Steam}_{st,tt}^{\text{Tot}} \tag{3.3.42}
\]

\[
W\text{Load}_{st,tt}^{\text{Ferm}} = \sum_{p,pt,ft} W\text{Load}_{p,pt,ft}^{\text{unit,Ferm}} \times \sum_{b,s} \text{Product}_{b,s,b,pt,ft,tt}^{\text{broth}} \tag{3.3.43}
\]

\[
W\text{Load}_{p,cr,pt,ft,tt}^{\text{Rec}} = \sum_{p,cr,pt,ft} W\text{Load}_{p,cr,pt,ft}^{\text{unit,Rec}} \times \text{Product}_{p,cr,pt,ft,tt}^{\text{final}} \tag{3.3.44}
\]

\[
W\text{Load}_{st,tt}^{\text{total}} = W\text{Load}_{st,tt}^{\text{Frac}} + W\text{Load}_{st,tt}^{\text{Ferm}} + W\text{Load}_{st,tt}^{\text{Rec}} + W\text{Load}_{st,tt}^{\text{Steam}} \tag{3.3.45}
\]

\[
\text{Water}_{st,tt}^{\text{purch}} = (1 + \text{loss}_{\text{water}}) \times W\text{Load}_{st,tt}^{\text{total}} - \text{Water}_{st,tt}^{\text{Recyl}} \tag{3.3.46}
\]

\[
\text{Water}_{st,tt}^{\text{treated}} = W\text{Load}_{st,tt}^{\text{total}} = \text{Water}_{st,tt}^{\text{Recyl}} \tag{3.3.47}
\]
3.3.3.2.4 Capacity Design

The following model equations were used to design capacity of each operating system:

\[ BVCI \times \text{CAP}^{UB} \geq \text{CapExp} \]  \hspace{1cm} (3.3.48)

\[ BVCI \times \text{CAP}^{LB} \leq \text{CapExp} \]  \hspace{1cm} (3.3.49)

\[ \text{Cap}_t = \text{Cap}_{t-1} + \text{CapExp}_{t-CD} \]  \hspace{1cm} (3.3.50)

\[ \text{Cap} \geq \text{SystemInput} \]  \hspace{1cm} (3.3.51)

\[ \text{MinUtil} \times \text{Cap} \leq \text{SystemInput} \]  \hspace{1cm} (3.3.52)

The first two equations provide bounds to capacity expansion, where BVCI is the increment binary variable. Equation 50 is used to update to processing capacity of each operating system, adjusting for a construction delay of 2 years. Equation 51 provides a lower bound to total established capacity based on the respective input to the operating system, and equation 52 imposes minimum equipment utilization bound on the established capacity.

3.3.3.2.5 Demand Constraints

To constrain the sales levels for each product demand constraints were employed. It was assumed that the enterprise can sign 5-year contracts to serve product demands in local markets, which is represented by a binary variable (BVSales). Once a contract is signed, a minimum percentage of the demand has to be satisfied every year (Customer Service level, CSL). The annual sales levels were also constrained by a maximum demand that is available to be fulfilled. Finally, to force the optimizer to recognize market share as a competitive
advantage, a constraint was employed to force sales growth to be greater than the demand growth, year-over-year. The demand constraints are presented below (Equations 53-56).

\[
\sum_{st, tr} \text{Sales}_{p, i, m, st, tr} \leq \text{Demand}_{p, i, m, t} \times \left\{ \sum_{t'=t}^{t+PSC} \text{BVSales}_{p, i, m, t'} \right\}
\] (3.3.53)

\[
\sum_{st, tr} \text{Sales}_{p, i, m, st, tr} \geq \text{CSL} \times \left\{ \sum_{t'=t}^{t+PSC} \text{BVSales}_{p, i, m, t'} \right\} \times \text{Demand}_{p, i, m, t}
\] (3.3.54)

\[
\text{Demand}^{\text{growth}}_{p, i, m, t} = \frac{\text{Demand}_{p, i, m, t} - \text{Demand}_{p, i, m, t-1}}{\text{Demand}_{p, i, m, t-1}}
\] (3.3.55)

\[
\sum_{st, tr} \text{Sales}_{p, i, m, st, tr} \geq (1 + \text{Demand}^{\text{growth}}_{p, i, m, t}) \times \sum_{st, tr} \text{Sales}_{p, i, m, st, tr, t-1}
\] (3.3.56)

3.3.3.2.6 Binary Constraints

Binary variables are used to control a yes or no decision in the entire model. Specifically, network/feedstock/technology/configuration choices, facility establishment, capacity expansion, and biomass purchase and product distribution contract agreement decisions were controlled using binary variables. Equation 57 and 58 are employed to select a feedstock source and corresponding harvesting and preprocessing technology once every production cycle of a particular feedstock. Equation 59 is used to drive the optimization model to select a facility site (LANDBVE_{st,t}) only once over the entire time horizon, while equations 60-62 are used to constrain the selection of only one fractionation (FRBVE_{pt,ft,st,t}), fermentation (FERMBVE_{p,s,pt,ft,st,t}), and recovery and purification (RCBVVE_{p,cr,pt,ft,st,t}) technology per site, respectively. Equations 63-65 imply that technologies cannot be established without the purchase of land at a particular site, while equations 66-68 state that capacities for fractionation (FRBVC_{pt,ft,st,t}), fermentation (FERMBVC_{p,s,pt,ft,st,t}), and recovery (RCBVC_{p,cr,pt,ft,st,t}) cannot be expanded without the establishment of a particular technology. Additional binary constraints (using the same binary variables) were employed to impart
more realism to the model. The model uses separate binary variables for technology selection (__BVE type variables) and capacity expansion (__BVC type variables) as one needs to constrain technology choice to only one per site (equations 63-65), while capacity expansion for that technology can happen multiple times over the planning horizon depending on the state of the input parameters (optimally). Finally, contractual obligation constraints for biomass purchase and final product supply (to markets) are used in order impart a greater degree of realism to the optimization problem that is being modeled. Some examples include the signing of a Biomass Supply Contract (BMSC$^{BV}_{b,l,h,t'}$) once for the entire growth cycle (GC) of a particular feedstock (Equation 69), and the signing of a Product Distribution Contract (PDC$^{BV}_{p,l,m,t'}$) once every five years (Equation 70).

\[
\sum_{t'=t}^{t+G_{b}} BMSC_{b,l,h,t'}^{BV} \leq 1 \quad (3.3.57)
\]

\[
\sum_{t'=t}^{t+G_{b}} BMSC_{b,l,h,t'}^{BV} \leq 1 \quad (3.3.58)
\]

\[
\sum_{t} LANDBVE_{s,t} \leq 1 \quad (3.3.59)
\]

\[
\sum_{p,t} FRBVE_{p,t,s,t} \leq 1 \quad (3.3.60)
\]

\[
\sum_{p,t} FERMBVE_{p,s,t,s,t} \leq 1 \quad (3.3.61)
\]

\[
\sum_{p,t,c} RCBVE_{p,c,t,s,t} \leq 1 \quad (3.3.62)
\]

\[
FRBVE_{p,t,s,t} \leq \sum_{s} LANDBVE_{s,t} \quad (3.3.63)
\]

\[
FERMBVE_{p,s,t,s,t} \leq \sum_{s} LANDBVE_{s,t} \quad (3.3.64)
\]

\[
RCBVE_{p,c,t,s,t} \leq \sum_{s} LANDBVE_{s,t} \quad (3.3.65)
\]

\[
FRBVE_{p,t,s,t} \leq \sum_{s} FRBVE_{p,t,s,t} \quad (3.3.66)
\]

\[
FERMBVE_{p,s,t,s,t} \leq \sum_{s} FERMBVE_{p,s,t,s,t} \quad (3.3.67)
\]

\[
RCBVE_{p,c,t,s,t} \leq \sum_{s} RCBVE_{p,c,t,s,t} \quad (3.3.68)
\]

\[
\sum_{t'=t}^{t+G_{b}} BMSC_{b,l,h,t'}^{BV} \leq 1 \quad (3.3.69)
\]
3.3.4 Financial Model

The financial model is broken into 5 salient aspects that describe the financial impact of resource procurement, technology selection, network design, production of final products, and sales:

1. Capital costing of equipment;
2. Financing of capital expenditures;
3. Estimation of operating expenses and revenues;
4. Calculation of income and cash flow statement line items;
5. Calculation (optimization) of the objective function.

The next sub-section describes the methodologies used to formulate each one of the models with special attention given to the integration of operating and design variables (from previous sections) into the financial formulation.

The methodology for deriving the capital cost structure was adapted from Kazi et al (2010) that exemplified NREL’s n<sup>th</sup> plant cost analysis. The capital expenses are broken up into six components:

1. Land acquisition charges for facility establishment and biomass production,
2. Equipment costs for biomass production and processing,
3. Construction and Engineering costs,
4. Legal and permitting costs
5. Contingency fund,
Considering the time value of money, these charges are distributed over the construction period as opposed to being charged all at once in order to mitigate their impact on the balance sheet. While land acquisition and feedstock establishment costs are charged the same period, equipment costs are charged the subsequent period, and construction and engineering costs are charged 2 years following land acquisition. All capital costs were calculated using the following methodology:

1. Land acquisition charges for processing facilities ($\text{Capex}_{\text{st,t}}^{\text{Land}}$) were based on estimates derived from online sources (http://www.landandfarm.com) for given rates in Louisiana for 1000 acres of industrial land:

$$\text{Capex}_{\text{st,t}}^{\text{Land}} = \text{LANDBVE}_{\text{st,t}} \times Fc_{\text{st,t}}^{\text{Land}}$$

(3.3.71)

2. Harvest and preprocessing equipment charges were derived from literature (Chen, 2011) and charged to the biorefiner’s budget assuming that the processor aims to set up a vertically-integrated value chain where control over upstream and downstream nodes of the value chain exists:

$$\text{Capex}_{\text{b,l,h,t}}^{\text{H&P}} = \text{BMSC}_{\text{b,l,h,t}}^{\text{BV}} \times Fc_{\text{b,l,h,t}}^{\text{H&P}}$$

(3.3.72)

3. The base costs for each operating section was obtained from literature for that given capacity (Kazi et al 2010; Lynd et al, 2002; Bailly, 2002);

4. The capacity was varied between ±75 percent from the base capacity;

5. The resultant costs were scaled using the following cost exponent formula:

$$\text{NewCost} = \text{OldCost} \times \left( \frac{\text{NewCapacity}}{\text{OldCapacity}} \right)^{\theta}$$

(3.3.73)

6. These costs were then plotted against the calculated capacities;
7. A linear approximation was fitted to the cost curve to obtain the equation of a line:

\[
\text{Capex}_{\text{eqp}}^{\text{st,t}} = \_BVC \times FC + \text{Capacity}^{\text{Exp}} \times VC
\]  

(3.3.74)

8. Here, \_BVC denotes the binary variable representing the expansion of capacity of a particular operating node (equations 3.3.66-68), FC is the fixed capital level (also the constant of the linear approximation), Capacity^{Exp} is the level of capacity expansion (in terms of units of input to the operating section), and VC is variable capital in terms of unit cost of capacity expansion (also the slope of the linear approximation).

9. Construction and Engineering (Capex^{C&E}_{\text{st,t}}) were assumed to be 32 and 35 percent of total equipment costs, respectively;

10. Legal and permitting expenses (Capex^{L&P}_{\text{st,t}}) were varied between 20-30 percent (of equipment costs) depending on the location of a facility;

11. The total direct and indirect capital (Capex^{TDIDC}_{\text{st,t}}) was then calculated as the sum of the equipment, C&E, and permitting charges.

\[
\text{Capex}^{\text{TDIDC}}_{\text{st,t}} = \text{Capex}^{\text{land}}_{\text{st,t}} + \text{Capex}^{\text{eqp}}_{\text{st,t}} + \text{Capex}^{\text{C&E}}_{\text{st,t}} + \text{Capex}^{\text{L&P}}_{\text{st,t}}
\]  

(3.3.75)

12. The contingency fund (Capex^{cont}_{\text{st,t}}), usually put aside to manage cost overruns during the construction period was estimated to be 20 percent of total direct and indirect capital investment;

13. The startup working capital (Capex^{WC}_{\text{st,t}}), usually put aside to provide for initial startup expenses once construction is completed, was then estimated to be 15 percent of total fixed capital investment (FCI_{st,t}).

\[
\text{FCI}_{\text{st,t}} = \text{Capex}^{\text{cont}}_{\text{st,t}} + \text{Capex}^{\text{TDIDC}}_{\text{st,t}}
\]  

(3.3.76)
\[ \text{Capex}_{st,t}^{WC} = 0.15 \times \text{FCI}_{st,t} \]  

(3.3.77)

14. Finally the total growth-oriented capital investment was calculated as the sum of the fixed capital investment, the harvest and preprocessing equipment cost, and the startup working capital.

\[ \text{TCI}_{t}^{\text{growth}} = \sum_{st} \left( \text{FCI}_{st,t} + \text{Capex}_{st,t}^{WC} \right) + \sum_{b,l,h} \text{Capex}_{b,l,h,t}^{H&P} \]  

(3.3.78)

15. Depreciation of equipment was assumed to be on a straight line basis for a 7 year period for processing equipment, 10 years for harvest and preprocessing equipment, and 20 year period for steam and power equipment, with no salvage value;

The operating costs for the value chain were broken into 7 parts that utilize system outputs from each node in the value chain to calculate the total cost of operation:

1. Feedstock costs \( \left( C_{b,l,t}^{\text{feed}} \right) \) including amortized establishment costs \( \left( C_{b,l,t}^{\text{EstblAmort}} \right) \), rental payments to land-owners \( \left( \pi_{b,l,t}^{\text{Rent}} \right) \), maintenance costs \( \left( \pi_{b,l,t}^{BM} \right) \) of equipment, harvesting and preprocessing costs \( \left( \pi_{b,l,h,t}^{Hvst} \right) \), and storage and transportation costs \( \left( \pi_{b,l,h,t}^{store} \right) \);

2. Water purchase \( \left( \pi_{st,t}^{\text{water}} \right) \) and treatment costs \( \left( \pi_{st,t}^{\text{treat}} \right) \);

3. process chemical costs for biomass pretreatment \( \left( \pi_{pt,ft,st,t}^{\text{PT}} \right) \);

4. enzyme, nutrient, and micro-organism costs for fermentation \( \left( \pi_{p,s,pt,ft,\text{st,t}}^{\text{PT}} \right) \);

5. operating charges \( \left( C_{st,t}^{\text{S&P}} \right) \) for steam \( \left( \pi_{st,t}^{\text{Steam}} \right) \) and power plant operation \( \left( \pi_{st,t}^{\text{Power}} \right) \);

6. labor costs \( \left( C_{st,t}^{\text{Lbr}} \right) \) for the entire processing facility broken up into a fixed labor cost \( \left( \pi_{st,t}^{\text{Lbr,Fixed}} \right) \) not dependent on capacity and a variable charge based on biomass throughput capacity \( \left( \pi_{st,t}^{\text{BM,\text{Cap}}} \right) \);
7. selling, general and administrative costs ($C^S_G A_t$) for product distribution ($\pi^P r o d D i s t_{p,m,st,tt}$) and value chain operation ($\pi^F r e d, M k t_{m,t}$);

Each cost equation is described below.

\[ c^\text{feed}_{b,lt} = (\sum_h B M^\text{hyst}_{b,l,h,t} \times \pi^\text{BM}_{b,lt}) + \sum_h (\pi^\text{Hvst}_{b,l,h,t} \times \text{Land}^\text{hyst}_{b,l,h,t}) + \sum_h (\text{Land}^\text{contr}_{b,l,h,t} \times \pi^\text{Rent}_{b,lt}) + \]

\[ \sum_h (\pi^\text{store}_{b,l,h,t} \times B M^\text{hyst}_{b,l,h,t}) + \sum_h (\pi^\text{Xport}_{b,l,h,tt} \times B M^\text{purch}_{b,l,h,tt}) + \]

\[ c^\text{EstblAmort}_{b,lt} = c^\text{EstblAmort}_{b,lt-1} + \left( \frac{c^\text{Estbl}}{G C_b} \right) \times c^\text{Estbl}_{b,lt} \]  

(3.3.79)

\[ c^\text{water}_{st,tt} = \pi^\text{water}_{st,tt} \times \text{Water}^\text{purch}_{st,tt} + \pi^\text{treat}_{st,tt} \times \text{Water}^\text{treated}_{st,tt} \]  

(3.3.80)

\[ c^\text{PT}_{st,tt} = \sum_p \pi^\text{PT}_{p,tt} \times \sum_{b,p} P \text{Chem} \times B M^\text{used}_{b,p,pt,tt} \]  

(3.3.81)

\[ c^\text{FT}_{st,tt} = \sum_{p,s} \pi^\text{FT}_{p,s,pt,tt} \times \{ \rho^\text{FTChem}_{p,s,pt,tt} \times \sum_b \text{Sugar}^\text{prod}_{s,b,pt,tt} \} \]  

(3.3.82)

\[ c^\text{S&P}_{st,tt} = \{ \pi^\text{Steam}_{st,tt} \times \text{Steam}^\text{Tot}_{st,tt} \} + \{ \pi^\text{Power}_{st,tt} \times \sum_{p,tt} \text{Elec}^\text{produced}_{p,tt} \} \]  

(3.3.83)

\[ c^\text{Lbr}_{st,tt} = (\sum_{st} \text{LAND} \text{BVE}_{st,t-cD_{st}} \times \pi^\text{Lbr,Fixed}_{st,tt}) + \pi^\text{BMCap}_{st,tt} \times \sum_{c,p,tt} \text{Cap}_p \text{pt,tt} \]  

(3.3.84)

\[ c^\text{SGA}_{tt} = \sum_{p,i,m,tt} \{ \text{Sales}^\text{prodDist}_{p,i,m,tt} \times \pi^\text{prodDist}_{p,i,m,tt} \} + \sum_m \{ \sum_{p,i} P D c^{BV}_{p,i,m} \times \pi^\text{Fixed,Mkt}_{m} \} \]  

(3.3.85)

(3.3.86)

It should be noted that the labor costs were derived from Kazi et al (2010) for different process configurations (based on biomass throughput capacity); a 3/10 rule was used to scale up variable labor costs similar to capital cost scaling:
\[
\text{NewCost}^{\text{Lbr}} = \text{OldCost}^{\text{Lbr}} \times \left( \frac{\text{Capacity}^{\text{BM,New}}}{\text{Capacity}^{\text{BM,Old}}} \right)^{0.3}
\] (3.3.87)

Once a curve was plotted using the above equation a linear approximation was made yielding a fixed labor cost component and a variable labor cost component based on biomass throughput capacity \((\text{Cap}_{\text{pt,ft,stat}}^{\text{Biomass}})\). Additionally, the costs mentioned above were further grouped into direct costs (cost of goods sold or COGS), and indirect costs (IDC); this was done for analysis of gross and operating margins that will result from the optimization of the model.

\[
\text{COGS}_t = \sum_{b,t} c_{b,t}^{\text{feed}} + \sum_{s,t} (c_{s,t}^{\text{water}} + c_{s,t}^{\text{PT}} + c_{s,t}^{\text{PT}})
\] (3.3.88)

\[
\text{IDC}_t = \left( \sum_{s,t} c_{s,t}^{\text{S&IA}} + c_{s,t}^{\text{Lbr}} \right) + c_t^{\text{SGA}}
\] (3.3.89)

Following the calculation of these costs, the income statement of a general enterprise was stated in equation form to calculate line items such as gross profit, earnings before interest taxes and depreciation (EBITDA), earnings before interest and taxes (EBIT), earnings before taxes (EBT), taxes, operating profit after taxes (NOPAT), and net income (NI). Additionally, the cash flow statement of an enterprise was derived (in equation form) using the outputs of the income statement along with the capital investment charges that were calculated previously. The financial model was designed to assess the impact of project operation on the enterprise’s capital structure; specifically, the cash balance of the enterprise was assumed to be composed of operating (CFO), financing (CFF), and investment cash flow (CFI). While the operating cash flow was derived from the income statement, the investment cash flows were projected as a function of total capital expenses. Finally, the capital structure of the enterprise was represented as the debt and equity capital that can be raised in order to
fund current operations and further network capacity growth. Finally, the objective function
(Net Present Value, NPV), also termed as the discounted value of free cash flow (FCFF) was
derived using the operating cash flow statement. All the equations are listed in table 3-5.

<table>
<thead>
<tr>
<th>Line Item</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gross Profit</td>
<td>Total Revenue – COGS</td>
</tr>
<tr>
<td>EBITDA</td>
<td>Gross Profit – IDC</td>
</tr>
<tr>
<td>EBIT</td>
<td>EBITDA – Depreciation</td>
</tr>
<tr>
<td>EBT</td>
<td>EBIT – Interest</td>
</tr>
<tr>
<td>Taxes</td>
<td>0.40 × EBIT - Tax Credits</td>
</tr>
<tr>
<td>NOPAT</td>
<td>EBIT – Taxes</td>
</tr>
<tr>
<td>NI</td>
<td>NOPAT - Interest</td>
</tr>
<tr>
<td>CFO</td>
<td>NI + Interest + Depreciation</td>
</tr>
<tr>
<td>CFF</td>
<td>Net Debt\text{new} + Net Equity\text{new}</td>
</tr>
<tr>
<td>CFI</td>
<td>TCl\text{growth} + TCl\text{maintenance}</td>
</tr>
<tr>
<td>FCF</td>
<td>CFO – CFF</td>
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<td>NPV</td>
<td>[\sum_{t} FCF_{t} (1 + WACC_{t})^{t}]</td>
</tr>
<tr>
<td>Δ Retained Earnings (Δ RE)</td>
<td>NI – Dividend</td>
</tr>
<tr>
<td>Δ Cash</td>
<td>CFO + CFF – CFI</td>
</tr>
<tr>
<td>Δ Debt</td>
<td>Interest + Net Debt\text{new}</td>
</tr>
<tr>
<td>Δ Equity</td>
<td>Net Equity\text{new}</td>
</tr>
</tbody>
</table>

Besides the aforementioned income and cash flow equations, a minimum interest
payment constraint, positive cash balance constraint, and maximum debt level constraints
were employed. Additionally, a pre-defined debt to equity ratio was assumed and capital
expenditures were assumed to be funded either through a mix of debt and equity (constrained
by the debt to equity ratio) or through retained earnings from previous years (in the cash
balance). Finally, maximum demand and minimum customer service level constraints were
employed to limit the total product sales that were possible.

Cost of Capital Derivation

Once the model was formulated and tested, I quickly realized that the discount rate was a
major determinant of project profitability; consequently some effort was spent to derive a
theoretically sound cost of capital figure that would be used to discount the projected cash
flow from the biorefinery. The cost of capital model is provided below. Some underlying assumptions regarding the enterprise’s capital structure are also listed.

1. It was assumed that capital investments in plant and equipment could be funded through a mix of debt and equity;
2. The debt to equity mix was constrained by a firm-specific ratio;
3. The debt was assumed to be raised through bond issuance and will be traded in the markets (floating interest rate);
4. Interest payments on debt are required annually for bond holders;
5. Equity providers do not require annual payments but tax-related cash flows are automatically channeled to the investors;
6. Both equity and debt interest rates are calculated using a risk free rate (10 year treasury bond yield), an expected risk premium (based on historical S&P returns), and a volatility scaling factor to represent the project risks.

\[ i_{t}^{\text{debt}} = RFR_{t} + \beta^{\text{debt}} \times (MR - RFR_{t}) \]  
(3.3.90)

\[ E[\text{ROE}]_{t} = RFR_{t} + \beta_{L}^{\text{equity}} \times (MR - RFR_{t}) \]  
(3.3.91)

\[ \lambda_{t} = \frac{\text{Equity}_{t}^{\text{tot}}}{\text{Equity}_{t}^{\text{tot}} + \text{Debt}_{t}^{\text{tot}}} \]  
(3.3.92)

\[ \beta_{L}^{\text{equity}} = \beta_{\text{base}}^{\text{equity}} \times \left(1 + (1 - \text{tax rate}) \times \frac{1 - \lambda_{t}}{\lambda_{t}}\right) \]  
(3.3.93)

\[ \text{WACC}_{t} = \lambda_{t} \times E[\text{ROE}]_{t} + (1 - \lambda_{t}) \times i_{t}^{\text{debt}} \times (1 - \text{tax rate}) \]  
(3.3.94)

In the cost of capital model beta is used to represent the project specific risk for debt and equity investors. Equation 50 calculates the interest rate on floating debt while equation 51 represents the return of equity required by equity investors; RFR is the risk free rate while MR is the market returns from the S&P 500 (previous year). Lambda is the equity fraction of financing which is determined by the enterprise (equation 52). Equation 53 calculates the
impact of leverage (debt) on the project risk; $\beta^\text{equity}_L$ is the levered project risk representation, calculated as a function of the unlevered beta ($\beta^\text{equity}_\text{base}$) and the debt fraction of total capital financing. The WACC is calculated (equation 54) as a weighted function of the expected return on equity and the tax shielded interest rate, weighted by the financing mix for the firm.

3.3.5 Key Performance Indicators

In addition to the project NPV, other key performance indicators (KPI) are suggested as dashboard metrics to analyze the performance of the optimal design plans. The KPIs are divided into three categories:

1. Financial Valuation;
2. Carbon Efficiency;

The financial valuation metrics are as follows:

Terminal Value: $TV = \frac{E[CFO] \times (1+E[GR]) - E[Reinvestment]}{E[WACC] - E[GR]}$ (3.3.95)

Debt Value: $DV = \text{Debt}_{T}^{\text{net}}$ (3.3.96)

Cash Value: $\text{Cash}_{T}$ (3.3.97)

Stockholder’s Equity: $\text{SKE} = \text{Equity}_{T}^{\text{net}} + \text{RE}_{T}$ (3.3.98)

Firm Value: $\text{FV} = \text{NPV} + \text{TV}$ (3.3.99)

Shareholder Value: $\text{EV} = \text{FV} + \text{CV} - \text{DV}$ (3.3.100)

Stakeholder Value: $\text{SKV} = \text{EV} + \text{Carbon}^{\text{value}}$ (3.3.101)

The terminal value is the value of continuing operations beyond the planning horizon of 20-years under the assumption that the project will continue operating past 20 years with re-investments made into the plant to upgrade equipment efficiencies. The TV estimates how
much the operating assets of an enterprise are worth beyond the planning horizon value (NPV). Usually, for new firms, the terminal value can be up to 90 percent of the total enterprise value. The debt and the cash values are simply the debt and cash balances that remain at the end of the planning horizon. The stockholder’s equity calculates how much capital the enterprise possesses at any given time which can be claimed by equity investors in a firm, which in turn is composed of the initial capital outlay (principal) by investors and the earnings that are retained (cumulative) by the enterprise; it should be noted that the percentage of retained earnings that (technically) belong to equity investors depends on what percentage of an enterprise is owned by the investors. The firm value (FV) is the sum of net present value and the terminal value and denotes the gross value of a firm’s operating assets. Finally, the sum of the firm value and the net of debt and cash represent the total shareholder value, that is, if a firm is bought out or traded publically, the value on the books for a firm is represented by the shareholder value. These metrics, while not used directly during model optimization, are used to shape the objective function (Net Present Value); for example positivity constraints are employed for each one of these terms in order to drive higher value creation for stakeholders while maximizing the project NPVs.

The energy metrics that are used to characterize the energy efficiency of the biomass-to-bioproducts value chain are as follows:

\[
\text{GER} = \frac{E_{\text{out, gross}}}{E_{\text{in, gross}}} \tag{3.3.102}
\]

\[
\text{NEV} = \frac{E_{\text{out, net}} - E_{\text{in, fossil}}}{\text{Total Fuel Output}} \tag{3.3.103}
\]

\[
\text{EROFEI} = \frac{E_{\text{out, net}}}{E_{\text{in, fossil}}} \tag{3.3.104}
\]
In the above equations, GER is defined as the gross energy ratio, which simply calculates the ratio of the gross energy outputs from the system to the gross energy inputs to the system. NEV is the net energy value of a production chain, that is, the amount of fossil energy that is displaced per unit of fuel output. EROFEI, defined as the energy return on fossil energy invested calculates the ratio of the net energy outputs from the system (fuel and co-products) to the net energy inputs from fossil fuels only. Qualitatively, GER describes the energy efficiency of the supply and production chains in adding energy value to all form of input energy that is expended in the feedstock production, transportation, and conversion processes including recycled streams; this value has very little to do with comparison of renewable resources with fossil sources, rather it should be used to analyze the efficiency of the supply and production chains to convert input energies (all sources) to output energies (all sources). NEV and EROFEI on the other hand describe specifically, the displacement potential of an energy output for fossil fuel inputs only. For the optimal design, the GER values are obtained by dividing the gross totals for energy outputs by the gross totals for energy inputs, while the NEV and EROFEI considers the net energy outputs embodied in the value chain products and the net fossil energy inputs; the net fossil energy inputs are considered assuming that all biomass production and transportation, and product transportation will require fossil energy while all process operations utilize energy that is generated using renewable fuels (lignin, biogas, sludge).

The carbon efficiency metrics are described as follows:

\[
NCR = \frac{C_{\text{fossil,out}}^{\text{gross}}}{C_{\text{fossil,in}}^{\text{gross}}} \]  
(3.3.105)

\[
NCS = \frac{C_{\text{fossil}}^{\text{net}}}{\text{Total Fuel Output}} \]  
(3.3.106)
Net Carbon Ratio (NCR) represents the ratio carbon savings that are achieved from fossil product displacement and the fossil carbon that is emitted while operating the renewable product value chain; Net Carbon Savings (NCS) per gallon of biofuel which represents the carbon savings that are achieved by displacing fossil fuels with biofuels; Land efficiency of carbon which represents the net carbon savings per acre of land that is planted with energy crops. Finally, the last carbon metric used is Carbon Savings on Fossil Carbon Emitted (CSOFCE) which represents the net carbon savings that are achieved per unit of fossil carbon that is emitted to operate the optimal value chain.

3.3.6 Some Additional Stakeholder Considerations

We had previously mentioned the concept of a Stakeholder Value (SKV); it is not just the value of the enterprise to its shareholders, but also to its debtors, suppliers, customers, and surrounding environment. In order to engender better, the SKV concept, we have imposed certain constraints during model optimization that force the decision processes to recognize aspects of corporate social and market responsibility, that would be hard to otherwise model mathematically.

1. Minimum interest and dividend payments are used to return capital to debtors and equity providers;
2. A customer satisfaction level constraint is imposed by mandating that a minimum percentage of total customer demand is satisfied if a product is selected;
3. For feedstock production, the biorefinery is assumed to bear the capital and operational risk of feedstock production;

4. If a particular feed source is selected, minimum land utilization constraints are imposed over the entire growth cycle of the crop, which in theory, provides farmers with a reliable income source over the lifetime of the crop.

5. A waste treatment and carbon capture facility is mandated if production of any kind is established essentially integrating corporate environmental responsibility with process conception, design, budgeting, and planning.

3.3.7 Data Inventory and Trend Forecasting

Any sound decision analysis system has to be supported by a robust forecasting system that can accurately forecast, especially for long decision time horizons as is the case with strategic planning, the input and output parameter values that affect the decisions and objectives of the biomass refinery.

In order to complete the optimization model mentioned previously (and the ones that will be suggested later), input data is required for model implementation. Given the breadth of input data that is required (costs, yields, market, financial) for each technology, different strategies can be utilized for data collection and aggregation. The data types can be broadly classified into two major categories (figure 3-11); (1) business data that includes costs and prices along with supply-demand balances for inputs and outputs, and (2) process data (including environmental implications) that includes yields, energy and water loads, and waste production and consumption estimates.
For a real enterprise, a significant portion of the process data can be derived from in-house experiments and market data can be either derived from in-house market research or purchased from marketing firms in specific industry verticals. Either way, it is essential to collect, aggregate, and store data in a common source as decision guidance is heavily dependent on the quality of data that is utilized for predicting performance (garbage in, garbage out). For the purpose of this dissertation, we want to demonstrate the design of a decision framework; the purpose is not to attain 100 percent accuracy in predicted results, but to design a framework and demonstrate its efficacy with some reasonable accuracy. Consequently, most data that is utilized here is garnered from literature sources. All data that is collected are current estimates and for decision support in future decision making, current data needs to be forecasted into the future. A key factor in generating future forecasts, especially for renewable fuels and chemicals, is the nascency of the markets; since renewable product markets (fuels and chemicals) are relatively new in their existence, historical data is not available in any scale to use for future predictions. Add to that the long-term horizon of the forecasts, it safe to assume a significant amount of uncertainty in the forecasted data.
Under this premise, it is important to evaluate multiple scenarios of data evolution and test their impacts on crucial enterprise decisions. A strategy to incorporate this uncertainty in data and study their impact on enterprise decisions is proposed later in this dissertation. Here we will describe the sources of data and aggregation techniques utilized, along with the forecasting methodologies.

A Note about Logistic Curves

A number of cost components used as inputs are projected to decrease over time. For long-term planning, it becomes important that cost trends are adequately represented in order to gauge how decisions are affected by these trends. All technology related capital and operating costs are assumed to follow a logistic distribution as a function of time. These curves (known as experience or S-curves) have been used to describe costs associated with technologies that are new to the market (Woerlen, 2004; Sandor et al, 2008, Alberth, 2008). The costs for technology are assumed to be the highest initially, when the overall R&D investment and production capacity of the economy for cellulosic products are low. As more R&D and capacity investments are assumed to come online with time, the unit technology costs decrease due to learning effects and increased market penetration leading to more competitive pricing for equipment. Operating cost reductions are assumed due to standardization of operating procedures, and general increases in production efficiency during facility operation. One can also model the decrease in per unit operating costs as an increase in the process yields yielding the same effect; Cost trends were modeled as opposed to process yield trends to describe an improvement in general operating efficiency which may or may not improve product yield. Additionally, biomass costs are also modeled using an S-curve; such a treatment implies that the procurement costs for biomass are going to rise
with increasing input costs and a rise in demand for the commodity (with rising processing capacity).

We have used the logistic distribution curve extensively to forecast the price and yield trends for input data. Figure 3-12 shows the different phases of a logistic distribution curve (S-curve) for a hypothetical scenario where technology costs (capital and/or operating) are initially high owing to relatively low market penetration and usage. As technology diffuses through the economy, R&D spend increases, more capacity comes online, and consequently technology costs reduce significantly. Finally during the mature phase, that particular technology has saturated its market share, and costs associated approach a constant floor asymptotically.

**Figure 3-12: Generic representation of an experience curve to represent cost and yield evolutions dynamically**
To generate such a curve some nomenclature is introduced; the ceiling is defined as the maximum value the parameter is expected to achieve (either at the beginning or at the end of the time horizon). The floor consequently, is defined as the minimum value the parameter is expected to reach. Progress ratio (PR) is defined as the relative cost after doubling of cumulative capacity of the economy for a given technology. For energy related technologies, regression analysis has yielded a progress ratio of approximately 80 percent, that is, there is a 20 percent (1-PR) reduction in costs for every doubling of cumulative capacity. We assume that the cumulative biomass processing capacity for biofuels and biochemicals will double every 10 years, which implies that given a PR of 20 percent, all costs are going to change by approximately 40 percent over a planning horizon of 20 years. While capital and operating expenses are going to reduce, feedstock costs are assumed to increase by 40 percent over the planning horizon implying a PR value of 80 percent. The equations used to generate all curves used in the model are provided below.

\[ P_t = p_{\text{max}} - \frac{p_{\text{max}} - p_{\text{min}}}{1 + e^{\Delta(t-t_{\text{avg}})}} \]  
\[ P_t = p_{\text{min}} + \frac{p_{\text{max}} - p_{\text{min}}}{1 + e^{\Delta(t-t_{\text{avg}})}} \]

\( T_{\text{avg}} \) represents the year when 50 percent of the maximum (or minimum) value of the forecasted parameter is achieved. \( P_t \) is the parameter in question and \( \Delta \) is used to control the annual rate of change of the curve and has a maximum value at 50 percent of market potential. For technology costs in the model, \( \Delta \) describes the rate of accumulation of experience (market penetration) over time. It is set at 40 percent for the current case study. For product demand and prices, \( \Delta \) describes the rate of adoption of the product over time. The rate of market penetration parameter for product prices is set at 40 percent. The market
penetration parameter for demand will depend on the price elasticity of demand and was calculated as follows:

\[
\Delta_p = \varepsilon_p \left( \frac{\text{Price}_{\text{initial}} - \text{Price}_{\text{final}}}{\text{Price}_{\text{initial}}} \right)
\] (3.3.111)

Where, \(\varepsilon_p\) is defined as the price elasticity of product demand. The demand for the product is then calculated as follows:

\[
\text{Demand}_{t+1} = \text{Demand}_t \left( \frac{\text{Price}_{t+1}}{\text{Price}_t} \right)^{-\Delta_p}
\] (3.3.112)

3.3.8 Case Study Data

The next data presented is assumed to be known a priori. This data will appear in the model in the form of inputs.

Financial Data:

- Cost estimates for raw material acquisition, storage, handling, and transportation.
- Cost estimates for final product storage, handling, and transportation;
- Demand-price forecasts for finished products;
- Capital expenditure estimates for capacity design;
- Initial investment required for land acquisition and overhead for setting up a new facility;
- The interest rate on the debt held by the enterprise;
- Fixed and variable charges associated with the operation of a facility;
- The prevalent tax rate and depreciation;
- The tax breaks earned from producing renewable energy related products;
• A minimum debt-to-equity ratio to be maintained throughout;
• The time value of money;
• The risk-free interest rate and the risk premium on the debt and equity held by the enterprise;

Physical/Operational data:
• The planning horizon;
• The set of potential feedstock and their corresponding yields to products;
• The expected loss of raw materials due to spoilage;
• The set of potential products that can be manufactured;
• The set of potential technologies available to manufacture the final products;
• Physical bounds on capacity increments;
• Construction time (during which there can be no production);
• Emissions data related to production using all potential technologies in the portfolio;
• The minimum and estimated capacity utilization of production facility
• Utility requirement estimates for each processing technology.

Decision Variables yielded by the model:
• Preliminary raw material portfolio for the enterprise;
• Preliminary product and technology portfolio for the enterprise;
• Capacity design for production;
• Semi-annual production and sales forecasts for each facility;
• Integration scheme for utilities generation;
• Debt and equity mix for financing;
• Emissions-related estimates and costs.

3.3.8.1 Biomass Source Description

In order to incentivize energy crop production over traditional crops, the biorefinery has to assume the establishment costs, overhead expenses, and operating costs for crop production. For the growth and harvest cycles, energy cane is assumed to have a 5-year production cycle with 4 stubbles and a one year delay from land contracting to biomass harvest; sweet sorghum is harvested annually with no growth delay, while switchgrass is assumed to have a 12-year production cycle with a one year delay. The biomass yields are assumed to increase by 1.5 percent every year, while the cost for producing biomass is modeled using a logistic distribution, where the operating costs for production are projected to double over the time horizon.

Table 3-6: Yield and composition parameters for energy crops studied; Source: Lee et al, Kim and Day (2011)

<table>
<thead>
<tr>
<th>Biomass</th>
<th>Availability (1000 Ac)</th>
<th>Biomass Yield (tons per acre)</th>
<th>Composition</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>Cellulose</td>
</tr>
<tr>
<td>Switchgrass</td>
<td>50</td>
<td>5</td>
<td>0.37</td>
</tr>
<tr>
<td>Energy Cane</td>
<td>20</td>
<td>10</td>
<td>0.43</td>
</tr>
</tbody>
</table>

Table 3-7: Cost parameters for energy crops; Mark et al (2009); Chen (2011)

<table>
<thead>
<tr>
<th>Biomass</th>
<th>Establishment ($/ac)</th>
<th>Fixed Overhead ($/ac)</th>
<th>Variable Payment ($/ton)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Switchgrass</td>
<td>320</td>
<td>00</td>
<td>80</td>
</tr>
<tr>
<td>Energy Cane</td>
<td>275</td>
<td>160</td>
<td>85</td>
</tr>
</tbody>
</table>

The biorefinery can contract land to produce any feedstock in order to supply biomass to the refinery. Once contracted, the biorefinery assumes the costs associated with biomass production over each crop’s respective production cycle. For energy cane, only 20 percent of
the total land contracted can be utilized at a time (stubble). We assume that a vertically integrated enterprise can assure a consistent annual supply of biomass in order to take advantage of economies of scale for capacity design. Additionally, having a mix of sources with differing production cycles can help hedge against supply irregularities of one particular feedstock during operation. This formulation can decrease inventory costs of holding biomass while increasing capacity utilization.

3.3.8.2 Process Description

The technology selection problem is comprised of selecting the optimal pretreatment-fermentation-recovery configuration to process biomass to final products. The pretreatment technologies included 1) Dilute Acid (DA), 2) Ammonia Fiber Explosion (AFEX), and 3) Liquid Hot Water (LHW). These pretreatment option selections were driven by the availability of literature data to accurately represent their characteristics during optimization. Additionally, the choice of downstream hydrolysis and fermentation operations are also driven the choice of the pretreatment technology as effluents from pretreatment have a significant impact on enzymatic and micro-organism conversion efficiencies. The different pretreatment, hydrolysis and fermentation configurations were mentioned previously and are used as model inputs here. Out of the different fermentation configurations mentioned, we have chosen to ignore process designs that utilize separate hydrolysis with a downstream fermentation layout (SH_ _); this is in part because the capital and resource loads to execute these configurations are very high with only marginal yield benefits in term of conversion efficiencies. Additionally, the current state of biological innovation boasts of many strains of micro-organisms that can operate in a simultaneous hydrolysis and fermentation (SS_ _) process setup. While I have only used the configurations that are currently being investigated
by researchers and industry, the technological inputs can readily be expanded to include more configurations, such is the model and framework flexibility:

1. Dilute acid pretreatment produces a significant amount of inhibitory compounds during fractionation which can reduce overall fermentative efficiencies. Additionally, the hemicellulosic fraction is solubilized and can be washed away with wash water (~40% total input sugar); consequently SSSF and SSCF configuration can be combined with dilute acid pretreatment.

2. AFEX pretreatment maintains the structural integrity of hemicellulose with approximately 90 percent of total input sugar maintained in solid form. Consequently, we will only investigate the SSCF hydrolysis and fermentation configuration with AFEX;

3. LHW pretreatment also dissolves the hemicellulosic fraction of biomass thus reducing the total sugars that can be utilized for downstream fermentation. Additionally, the pretreatment hydrolyzate tends to inhibit glucose fermentation at certain solids concentration in the pretreatment process effluent. Consequently SSSF and SSCF configuration can be combined with dilute acid pretreatment.

Table 3-8: Fractionation process parameters; Source: Kazi et al (2010)

<table>
<thead>
<tr>
<th>Pre-treatment</th>
<th>Total Sugar yield (% total in biomass)</th>
<th>Thermal Energy (KJ / ton biomass)</th>
<th>Hydrolysis &amp; Fermentation</th>
<th>Potential Product yield per unit sugar</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dilute Acid</td>
<td>89</td>
<td>1150</td>
<td>SSSF</td>
<td>0.080 gal ET, 0.30 kg Succinic</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>SSCF</td>
<td>0.075 gal ET, 0.25 kg Succinic</td>
</tr>
<tr>
<td>AFEX</td>
<td>87</td>
<td>1300</td>
<td>SSCF</td>
<td>0.100 gal ET, 0.40 kg Succinic</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>SSSF</td>
<td>0.070 gal ET, 0.25 kg Succinic</td>
</tr>
<tr>
<td>LHW</td>
<td>75</td>
<td>2000</td>
<td>SSCF</td>
<td>0.065 gal ET, 0.20 kg Succinic</td>
</tr>
</tbody>
</table>
For product concentration and recovery multiple technologies have been proposed for each product. Upon carrying out a literature search, a few technologies were noticed to be prominent for each product’s concentration and recovery unit operations; these technologies are discussed below.

For ethanol recovery and concentration, two technologies were investigated; (1) conventional distillation followed by molecular sieve purification, and (2) pervaporative separation followed by sieve based purification. While conventional distillation is a well understood unit operation, it should be stated that the ethanol-water mixture that is effluent post fermentation, form an azeotrope at approximately 94 percent purity of ethanol; consequently molecular sieves have to be utilized to further purify ethanol to fuel quality (~99 percent). For our case two columns in series were assumed with approximately 33 percent pure ethanol from the first column. Pervaporative separation replaces the first column in the distillation configuration by a membrane-based separation technology yielding 60 percent pure ethanol and consequently reducing the thermal load on the second column (downstream). Nevertheless, molecular sieves are still required due to the azeotropic mixture. The choice between the two technological configurations will take into the yields, energy loads, and cost tradeoffs; while distillation requires a large energy input, pervaporative recovery requires lower energy but the membrane requires replacement and costs approximately $500 per square meter bi-annually.

For succinic acid recovery and purification operations, three different technologies were investigated; (1) cell filtration (of fermentation broth) followed electrodialysis, (2) cell filtration followed by ionic adsorption, and (3) cell filtration followed by chemical precipitation. In all cases, to achieve reasonable purity levels (≥ 95 percent) evaporative
crystallization was assumed to be used downstream from each purification operation. Each technology is briefly discussed below:

1. **Electrodialysis**: This is well known method of separating organic acids in the food industry and is widely used for purification of citric acid from citric juices. There are two steps involved in electrodialytic recovery of organic acids; (1) desalting electrodialysis separates trace ionic acids (such as acetic acid) from the fermentation broth in order to provide a product rich stream for the second (downstream) unit operation, and (2) water splitting electrodialysis where a current is passed through water to break it up into hydrogen and hydroxyl ions. The hydrogen ions are then supplied to the organic acid ion (at the anode) to yield pure organic acids in water (which is separated using downstream evaporative crystallization). Usually, the desalting membranes are charged with anionic (or cationic) species that selectively allow the organic acid ions (or the sodium ions) to pass by while repelling the other ion. The approximate yield post water splitting electrodialysis is approximately 60 percent of organic acid from the fermentation broth.

2. **Ionic Adsorption**: also known as ion exchange, this method is fairly similar to electrodialysis except in this case, the membranes utilized in the unit operations are ionic and supply the organic acid salts with the necessary hydrogen ions as the fermentation broth solution passes though the membranes. The membranes have an affinity for the positive ions that are initially attached to the organic acid; consequently after several runs of acid separation, the membranes require regeneration (usually with a strong acid) in order to replenish the membrane’s ability to provide organic salts with the necessary hydrogen ions. In order to maintain a
continuous process, I assumed that two batteries of membrane vessels will be purchased; as one set of membranes are regenerated, the fermentation effluent can be switched to the spare set and vice versa. Additionally, three vessels were assumed in series for each battery, wherein the yields from each vessel were incrementally higher (0 → 25% → 50% → 60%).

3. **Chemical Precipitation:** this method relies on two physical attributes of succinic acid that include low solubilities in water (presence of sulfuric acid) and higher solubilities in methanol (Lynd et al, 2002). For chemical precipitation, the fermentation broth is filtered to remove any cell mass (which is recycled back to the fermentation tanks), following which, ammonia is added to the effluent to form ammonium succinate, sulfuric acid is added to form ammonium sulfate and succinic acid and finally succinic acid is recrystallized from the solution using methanol. Although simple in operating procedure, significant waste products are formed throughout this process resulting in higher operating costs (of waste mitigation). Additionally, the use of ammonia and sulfuric acid also contributes to the input costs of the process.

Capital Costing

The equipment costs for dilute acid processes are high since corrosion resistant materials have to be used for constructing the tanks. Additionally, cellulose hydrolysis and fermentation with separate C5 and C6 fermentation (SSF) has higher capital expenses (processing equipment) due to separate tanks for fermentation but lower costs for product recovery due to separate fermentation effluent streams. The AFEX process also spells
significant capital expenses on product recovery as equipment is required to recover ammonia in addition to recovering products from a single effluent stream post-fermentation.

**Table 3-9: Capital Cost parameters for different plant technology configurations;**

<table>
<thead>
<tr>
<th>Primary Technology</th>
<th>Secondary Technology</th>
<th>Fixed Cost (1000$)</th>
<th>Variable Cost ($/basis)</th>
<th>Basis</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dilute Acid</td>
<td>Co-Fermentation</td>
<td>18000</td>
<td>0.0637</td>
<td>$/kg biomass</td>
</tr>
<tr>
<td>Dilute Acid</td>
<td>Separate Fermentation</td>
<td>21000</td>
<td>0.0699</td>
<td>$/kg biomass</td>
</tr>
<tr>
<td>AFEX</td>
<td>Co-Fermentation</td>
<td>19000</td>
<td>0.0601</td>
<td>$/kg biomass</td>
</tr>
<tr>
<td>Hot Water</td>
<td>Co-Fermentation</td>
<td>16000</td>
<td>0.0436</td>
<td>$/kg biomass</td>
</tr>
<tr>
<td>Distillation</td>
<td>Dilute Acid</td>
<td>4000</td>
<td>0.5080</td>
<td>$/gal Ethanol</td>
</tr>
<tr>
<td>Distillation</td>
<td>AFEX</td>
<td>4000</td>
<td>0.5711</td>
<td>$/gal Ethanol</td>
</tr>
<tr>
<td>Distillation</td>
<td>Hot Water</td>
<td>5000</td>
<td>0.7656</td>
<td>$/gal Ethanol</td>
</tr>
<tr>
<td>Distillation</td>
<td>Dilute Acid, Separate Fermentation</td>
<td>4000</td>
<td>0.5305</td>
<td>$/gal Ethanol</td>
</tr>
<tr>
<td>Pervaporation</td>
<td>Dilute Acid</td>
<td>30000</td>
<td>0.8080</td>
<td>$/gal Ethanol</td>
</tr>
<tr>
<td>Electrodialysis</td>
<td>N/A</td>
<td>1000</td>
<td>0.7862</td>
<td>$/kg Succinic</td>
</tr>
<tr>
<td>Adsorption</td>
<td>N/A</td>
<td>1650</td>
<td>0.7865</td>
<td>$/kg Succinic</td>
</tr>
<tr>
<td>Chemical Precipitation</td>
<td>N/A</td>
<td>3000</td>
<td>0.3314</td>
<td>$/kg Succinic</td>
</tr>
</tbody>
</table>

Operating Cost

For plant operations, all costs were calculated based on unit costs of inputs to each operating section of the biorefinery (fractionation and hydrolysis, fermentation, concentration and recovery, steam generation, power generation, and utilities and wastewater treatment). All ethanol costs were derived from Kazi et al. and the labor costs scaled up (or down) using a cost exponent of 0.3. Succinic acid costs were assumed to be broken up according to the following convention:

1. All biomass processing and fermentation costs were assumed to be the same as that of ethanol on a per ton biomass processed basis;
2. For concentration and recovery, solvent (reactive extraction), membrane (electrodialysis and adsorption), power, water, and chemical requirements were estimated using spreadsheet models;
3. The cost of solvent for reactive extraction was derived from Alibaba.com with a 25 percent premium assumed on the derived prices to account for exchange rates and shipping and handling;

4. The membrane and chemical costs for electrodialysis and adsorption were assumed to be 100 percent of variable capital costs assuming that the membranes and chemicals need replacement every year of operation.

Fixed maintenance costs were assumed to be 5 percent of total equipment costs. Selling, general and administrative costs were assumed considering the enterprise hires an energy marketer (for ethanol) and a chemical marketer for succinic acid; the cost structure was broken up into fixed and variable cost components, with fixed payment made upfront when market is established and variable payment assumed to be 2 percent of product prices in a given market. The cost summary for each technology is provided in Table 3-10.

<table>
<thead>
<tr>
<th>Primary Technology</th>
<th>Secondary Technology</th>
<th>Basis</th>
<th>Cost</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dilute Acid</td>
<td>Co-Fermentation</td>
<td>$/kg biomass</td>
<td>0.0824</td>
</tr>
<tr>
<td>Dilute Acid</td>
<td>Separate Fermentation</td>
<td>$/kg biomass</td>
<td>0.1134</td>
</tr>
<tr>
<td>AFEX</td>
<td>Co-Fermentation</td>
<td>$/kg biomass</td>
<td>0.0785</td>
</tr>
<tr>
<td>Hot Water</td>
<td>Co-Fermentation</td>
<td>$/kg biomass</td>
<td>0.0746</td>
</tr>
<tr>
<td>Distillation</td>
<td>N/A</td>
<td>$/gal Ethanol</td>
<td>0.0000</td>
</tr>
<tr>
<td>Pervaporation</td>
<td>N/A</td>
<td>$/gal Ethanol</td>
<td>0.1700</td>
</tr>
<tr>
<td>Electrodialysis</td>
<td>N/A</td>
<td>$/kg Succinic</td>
<td>0.1998</td>
</tr>
<tr>
<td>Adsorption</td>
<td>N/A</td>
<td>$/kg Succinic</td>
<td>0.0865</td>
</tr>
<tr>
<td>Chemical Precipitation</td>
<td>N/A</td>
<td>$/kg Succinic</td>
<td>0.0371</td>
</tr>
</tbody>
</table>

3.3.8.3 Product and Market Description

For the purpose of technology and product portfolio design, the exact correlations are not essential; the idea here is to use “best-guess” price scenarios that are conservative in
nature, to test the prospective design cases. Once a design has been decided upon, more accurate forecasts should be generated for important in order to test the performance of the optimal process structure. This methodology is utilized in this dissertation, wherein, conservative estimates are used for deterministic technology and product portfolio design, following which uncertainty is introduced in market parameters to design the capacity for the optimal process structure.

The product portfolio for the biorefinery contains 1) ethanol as the high-volume, low-margin fuel that can add to the top-line and 2) succinic acid which is the high-margin chemical that can add significantly to the bottom-line. The biorefinery serves local ethanol markets in the southeast while assuming distribution responsibilities to a regional satellite center. Biosuccinic acid is produced on a contractual basis annually implying that once a contract is signed a predefined level of the customer demand has to be satisfied subsequently. While ethanol markets are relatively mature and better understood, a market for co-products such as succinic acid are still under-developed and depend largely on the cost competitiveness of the fermentation process (Werpy and Petersen, 2004) with the petroleum counterpart. Fermentation based succinic acid has been touted as a viable replacement to its maleic anhydride derivative, where maleic anhydride is currently a petroleum derived chemical. The market for succinic acid is one of the most promising ones as succinic acid is a platform intermediate for many industrially relevant chemicals. It can be envisioned that with more biobased succinic acid supply hitting the markets in the future, prices of succinic acid will reduce significantly. Additionally, increasing crude oil prices have the potential to drive up maleic anhydride prices which in turn affects the market for petroleum derived succinic acid. We notice that the major competing factors, amongst many others, that drive succinic
acid prices include the supply of the commodity, crude oil prices, and technological advancement (cost-competitiveness) of the fermentation processing route. Even then, the degree of correlation of the prices with these factors is unclear. Furthermore, while there are very specialized niche markets for current succinic acid applications (plasticizer, coolant, additive) with a higher degree of price certainty and non-elastic behavior of demand, higher volume markets for its applications as a bulk chemical can be envisioned; one of the most attractive bulk commodity market for succinic acid application is its use as a feedstock for 1,4-Butanediol (BDO) production, which is currently derived from the esterification maleic anhydride/acid with methanol. Being a commodity market, the prices for succinic acid serving the BDO markets are predicted to come down as more supply comes online and more processors replace their petroleum-based feedstock by biobased succinic acid.

All prices for bioproducts are modeled using S-shaped curves; while not proclaiming that these price trajectories are the best representation of actual future realizations, we believe that given the confluence of regulatory uncertainty in the near term and high market potential in the long term, such price trajectories can provide a satisfactory representation for portfolio design. Regression models relating macro-economic environment, crude oil prices, and world GDP growth to describe the prices are recommended are a subject of ongoing research. S-curves are generated assuming a maximum and minimum price levels and a rate of change parameter ($\Delta P$) for each product using the S-curve model equations. While ethanol prices are assumed to be at their lowest levels currently, the chemical prices are assumed to be at their highest levels and assumed to decrease exponentially (S-curve) as a function of time. Underlying assumptions for this treatment are as follows:
1. We assumed that ethanol supply from corn will reduce over time and replaced by cellulosic ethanol. The reduction in supply will create upward pricing pressure which is compounded by the secular rise in crude oil and gasoline prices;

2. Succinic acid prices serving niche markets are assumed to increase over time driven by higher crude prices, while that serving BDO markets are assumed to reduce over the time horizon to represent the fact that larger supply of these bio-based chemicals will drive the prices down in the future. Additionally, cost competitiveness with petroleum counterparts will increase downward pressure.

To model demand trends, certain assumption were made; 1) price elasticities of demand were assumed for each product, 2) a rate of change was calculated using the initial and final prices, 3) Demand was calculated using the rate of change parameter ($\Delta_D$) as a function of the demand from the previous period. For such a treatment, the current demand was assumed to be a percentage of world gasoline and chemical demand, for ethanol and biochemicals, respectively.

Table 3-11: Price forecasting parameters used to generate price trajectories using S-curves

<table>
<thead>
<tr>
<th>Product</th>
<th>Max Price</th>
<th>Min Price</th>
<th>Rate of market penetration ($\Delta_p$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ethanol ($/gal)</td>
<td>4</td>
<td>2.5</td>
<td>0.4</td>
</tr>
<tr>
<td>Succinic Acid, Niche Markets ($/kg)</td>
<td>6</td>
<td>4.2</td>
<td>0.4</td>
</tr>
<tr>
<td>Succinic Acid, BDO Markets ($/kg)</td>
<td>3</td>
<td>2.0</td>
<td>0.4</td>
</tr>
</tbody>
</table>

Table 3-12: Demand forecasting parameters used to generate demand trajectories using S-curves

<table>
<thead>
<tr>
<th>Product</th>
<th>Price Elasticity Of Demand (%)</th>
<th>Rate Of Change of Slope ($\Delta_D$)</th>
<th>Initial Demand</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ethanol (1000 gal)</td>
<td>1.4</td>
<td>-0.808</td>
<td>75000</td>
</tr>
<tr>
<td>Succinic Acid, Niche (tons)</td>
<td>5</td>
<td>1.462</td>
<td>5000</td>
</tr>
<tr>
<td>Succinic Acid, BDO (tons)</td>
<td>5</td>
<td>2.500</td>
<td>5000</td>
</tr>
</tbody>
</table>
3.3.8.4 Financial Description

The description of the financial inputs is provided below (table 3-13). These inputs are utilized directly in the cost of capital (Equations 90-94) model provided previously.

<table>
<thead>
<tr>
<th>Phase</th>
<th>Time, Years</th>
<th>Risk Free Rate, %</th>
<th>Market Return</th>
<th>Beta, Debt</th>
<th>Beta, Equity</th>
<th>Inflation Rate, %</th>
<th>DC Ratio</th>
<th>Tax, %</th>
<th>Grant (%)</th>
<th>Producer Credit ($/gal)</th>
<th>Investment Credit (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Growth</td>
<td>5</td>
<td>2</td>
<td>7</td>
<td>0.25</td>
<td>2.50</td>
<td>2</td>
<td>0.6</td>
<td>40</td>
<td>10</td>
<td>1.01</td>
<td>30</td>
</tr>
<tr>
<td>Transition</td>
<td>11</td>
<td>3</td>
<td>6</td>
<td>0.22</td>
<td>2.00</td>
<td>2</td>
<td>0.4</td>
<td>40</td>
<td>0</td>
<td>0.56</td>
<td>10</td>
</tr>
<tr>
<td>Mature</td>
<td>5</td>
<td>3</td>
<td>5</td>
<td>0.20</td>
<td>1.50</td>
<td>2</td>
<td>0.2</td>
<td>40</td>
<td>0</td>
<td>0.00</td>
<td>0</td>
</tr>
</tbody>
</table>

It is assumed that capital expenditures in capacity for biomass production and processing can be funded using long-term debt, and private and public equity with investments in capacity allowed once every 5 years. This constraint is applied to reflect a decision process that a real enterprise would follow in the wake of a nascent technology platform and undeveloped markets. Furthermore, the long-term debt to finance investments is raised by floating coupon bonds with maturities equaling the planning horizon, that make periodic (annually) interest payments to bond holders. The debt to capitalization ratio, defined as the debt fraction of the total financing, are obtained from literature estimates for currently operating ethanol refineries (Zindler and Boyle, 2007), and used to control the financing mix of the biorefinery. Equity can be raised through government financing, the interest on which is assumed to be the 10-year Treasury bond yield (risk free rate) or through private financing, which has a higher limit available but also requires higher payment on the equity invested (Return on Equity). To issue equity, the enterprise incurs transaction costs at five percent of total equity issued. The planning horizon is divided into three growth phases characterized by their financial parameters. The first 5-year period of planning is considered to be the high growth period, where a build out of processing capacity is assumed to occur.
Due to the presence of federal loan guarantees, it is assumed that the enterprise will be highly leveraged (controlled using the debt-to-capitalization ratio) in order to take advantage of the low interest rates. On the private capital front, private investments will command a high return on equity due to the high leverage and default risk of the investment characterized by the risk premium desired and the volatility of expected return (beta) in the Capital Asset Pricing Model. During the transition phase, interest rates are assumed to normalize higher as loan guarantees are withdrawn while the expected ROE goes down with reducing leverage. Finally during the mature phase, the interest rates and expected ROE are assumed to remain stable with consistent free cash flow and a dividend payment is introduced to return capital to shareholders. The biorefinery can also receive public funding with an interest rate at the 10-year Treasury bond yield (risk free rate).

There are 3 different tax subsidies/grants that are available; 1) a $1.01 federal tax subsidy for ethanol production, 2) a state sponsored working capital grant as a percentage of working capital expenses during facility construction, and 3) a renewable energy investment credit to offset a percentage of the total facility establishment costs.

3.4 Model Results

The model presented above was solved in GAMS using a CPLEX linear solver. The results are presented below.

3.4.1 Optimal Network Structure

Figure 3-13 shows the optimal network design under a carbon trading scheme with a fixed carbon price of $5 per ton and a carbon cap set at 100,000 tons annually. We assume this
scenario as the base case, against which all other results, including variations in the carbon cap and the traded permit prices, will be tested later.

A few salient features about the optimal network are listed below:

1. Due to economies of scale, a large facility at one site is preferred over multiple facilities closer to local markets. This may be different if harder resource constraints, such as critically low availability of water, long hauling distances for feedstock, or global markets for final products are introduced. This theory will be tested in the numerical experiments section of the results.

2. Feedstock transportation is implemented using a trucking medium, with most of the feedstock sourced from local land owners (southwest region, 40 mile average hauling
distance), although additional feedstock is sourced from the south-central region (90 mile average hauling distance) to satisfy throughput capacity of the plant.

3. The ports of New Orleans and Beaumont (assumed end markets) are selected as the major markets for both ethanol and succinic acid. Additionally, the blending terminal near Shreveport is also supplied with ethanol.

4. Single car rail (60,000 gallon capacity) is selected for ethanol transportation, and bulk freight rail transportation is selected for succinic acid supply to markets. This is primarily due to the lower unit cost of transportation and lower carbon load (per unit product transported per mile), although in real life it should be noted that there is a significant backlog to acquire single car rails and rail freight capacity is very constrained (USDA). While these issues were not modeled for the hypothetical case study, it may be prudent for a real enterprise to incorporate delivery times for new railcars or capacity constraints for bulk freight transportation.

The next sections will discuss some quantitative metrics that were obtained for the optimal design including:

1. Feedstock selection and resource base utilization,
2. Capacity design and utilization rates,
3. Sales volumes and demand satisfaction rates,
4. Gross and operating margins,
5. Cash flow and NPV evolution,
6. Tax credits and effective tax rates,
7. Expected return on invested capital and equity,
8. Carbon impact and efficiency,

3.4.2 Feedstock Portfolio

Figure 3-14 show the utilization of biomass based on total availability annually. Additionally, the figure also shows the sourcing ratios of each biomass source to fulfill the processing plant demand for feedstock. Switchgrass and energy cane are both utilized extensively within a 40-mile radius of the southwest facility location. Additionally, energy cane is used from the south-central sources as makeup feedstock (90-mile hauling distance). Ideally, makeup feedstock should be sourced from around the facility, but from a modeling perspective we modeled tight constraints on maximum land availability within a 40-mile radius of each site location. Switchgrass is assumed to be grown on CRP land with expiring program contracts; this resource was modeled to have the highest availability and consequently has the highest usage. For energy cane, it was assumed that sugarcane land had to be replaced with energy cane, implying that sugarcane farmers demanded a fixed payment per acre as lost opportunity income from sugarcane sales. In real life, a few more soft skills including negotiations and a sweetened purchase agreement may be required to make sugarcane farmers switch from a stable revenue stream (sugar mills) to a relatively uncertain revenue stream (biorefinery).
Switchgrass resources are utilized completely in the southwest region despite higher establishment costs and capital investment for purchase of harvesting equipment (not the case with energy cane where I assume that sugarcane equipment can be used with a maintenance rate paid to farmers); I attribute this primarily to the feedstock demand of the biorefinery and the lack of availability (to satisfy plant demand) of energy cane. During sensitivity analysis later, I will investigate how switchgrass utilization patterns will change if more land is available for energy cane cultivation. While feedstock selection was not a major component of this case study, this by no means dwarfs the importance of this decision problem in the bigger scheme of things. Feedstock supply have been identified as a major bottleneck in the commercialization of biorefineries, and the PSE group at LSU is actively pursuing research directions to incorporate supply and logistics modeling to describe the feedstock selection problem in greater detail in the overall DSS. Nevertheless, a bit of color can be imparted
from this result; we can safely assume that marginally higher costs for feedstock should not
deter enterprises from pursuing higher yields. As this is the most upstream node in the
biomass-to-biofuels production chain, optimization of yields will have a bullwhip effect on
downstream processes by magnifying the yield improvement across the entire value chain.
This again will be demonstrated in the sensitivity analysis section.

For purchase of switchgrass harvesting and densification equipment, a mix of round
and rectangular baling was selected with a capital investment of $35 million; the impact of
such capital expenditure levels is lessened due to the provision of BCAP (biomass crop
assistance payments) from USDA. The choice of switchgrass feedstock and its impact on
project NPV therefore, hinges on the availability of such payments to offset the cost of crop
establishment and purchase of equipment. During sensitivity analysis, we will analyze the
impact of the lack of BCAP on the mix of feedstock choices and project NPV. Alternatively,
the biorefiner can choose to forego vertical integration and shift the capital cost of
establishment and equipment over to the land owner; in this case it can be assumed that a
significantly larger purchase price may have to be paid to the land owner in order to offset
their costs. Additionally, this can increase supply uncertainty of feedstock for the plant as the
biorefiner will not have control over the crop allocation and management practices. A total of
$55 million is sourced from the BCAP program (over 5 years), with $34 million allocated to
switchgrass production and $21 million to energy cane production. The sum, by no means is
a guarantee and the biorefiner should, in real life, make sure that the feedstock production is
eligible under the USDA program (USDA biomass Crop Assistance Program).
Figure 3-15: Feedstock costs and the percent cost share through the USDA BCAP program

Figure 3-15 shows the annual feedstock cost breakdown (capital and operating) for switchgrass and energy cane. Additionally, the impact of the BCAP program is also shown; one can notice that approximately $8 per ton of biomass is saved through the program totaling $55 million of capital and operating savings over the 5 years that the BCAP program is modeled to be available. The sensitivity analyses will shed more light on the impact of removal of the program on the total project NPV, network capacity design, and total enterprise value.

3.4.3 Process Analysis

Cellulosic ethanol and succinic acid are both selected as the optimal products in biorefinery portfolio. The optimal process configuration that was yielded by the model is shown in Figure 3-16. Ammonia Fiber Explosion (AFEX) was selected as the biomass fractionation technology, fitted with an ammonia recovery system. Centrifugation is utilized immediately downstream from the AFEX system to separate lignin solids from the cellulose-
and xylose-rich, aqueous effluent. The lignin is dried and directed to the combined heat and power cogeneration (CHP) facility where it will be utilized as a fuel source to satisfy the energy requirements for production. The aqueous effluent is directed to the saccharification and co-fermentation train of vessels for further processing; here the cellulose is hydrolyzed to glucose and co-fermented with xylose to yield ethanol, succinic acid, trace amounts of acetic acid.

Figure 3-16: Optimal process configuration

We assumed that xylose- and glucose-utilizing organisms are added into the fermentation vessels to maximize the utilization of all components of biomass. Additionally, A.succinoproducens, a glucose-utilizing organism that can shift the fermentation equilibrium
towards the expression of succinic acid (as opposed to ethanol) is assumed to be added to fermentation vessels that are allocated towards succinic acid production. Carbon dioxide, effluent in the fermentation gas from ethanol expression, is pressurized and siphoned to the bottom of the succinic acid vessels where it is used to control the broth acidity. This form of process integration is an innovative form of carbon sequestration where value is added to fugitive emissions as they are transformed to a usable product. Value-addition to GHG emissions, rather than simple underground sequestration, is the most efficient way to proliferate environmentally-conscious industrial production, where the fundamental concept of a capitalist economy (profit) is merged with environmentally responsible production practices. Following fermentation, membrane-based filtration is utilized to separate cell matter from the fermentation effluent (broth), which is recycled back to the fermentation tanks. The concentration section is meant to concentrate the product in the broth by separating ancillary co-products and amino-acids (from the feedstocks) present in the fermentation broth. Distillation is selected over pervaporative separation for ethanol concentration where ethanol is concentrated up to a 94.5 percent pure stream (azeotropic at this point with water). For succinic acid, a 2-stage electrodialysis configuration (desalting followed by water-splitting) is selected over ionic adsorption, and precipitation with a strong acid followed by recrystallization; a detailed discussion on the key process and economic drivers/bottlenecks for each technology is presented later. Finally, for recovery of concentrated product, it was assumed that molecular-sieves and evaporative crystallization were the only technology choices for ethanol and succinic acid recovery unit operations, respectively. Following product recovery, the residual solids are directly sent to a wastewater treatment facility, as opposed to drying of solids to obtain a syrup for the CHP section. The
wastewater treatment consequently produces a larger quantity of biogas (due to larger organic matter input for digestion) that is sent to the CHP generation plant supplementing the loss of syrup fuel. This configuration is selected due to a lower capital outlay as opposed to purchasing additional evaporators ($4.5 million lower). Additionally, the evaporators require heat which is generated by burning the very solid fuel that is generated as an output from the evaporators; unless this closed loop cycle is 100 percent energy efficient, qualitatively it makes sense to choose to divert the residual solids to a wastewater facility to drive higher gas fuel production. It should be noted that the optimal configuration increases operating expenses (for wastewater treatment), as evaporator heat load is supplied by fuel that is supplied internally, but the annualized capital cost and the corresponding interest payment ($0.50 per ton of biomass capacity) is greater than the modeled increase in operating costs ($0.007 per ton of biomass throughput). Another caveat to the optimal configuration is the loss of electricity output which was modeled to be 0.066 kilowatt-hours per ton of biomass equaling to $0.003 of lost revenue per ton of biomass (at $0.04 per kwh electricity price); the total cost of the optimal configuration is therefore $0.010 (operating cost and lost revenue). This is still orders of magnitude lower that the capital cost impact on enterprise profits hence legitimizing the optimal choice for wastewater treatment and CHP generation configuration.

Figure 3-17 shows the total biomass throughput capacity, and succinic acid and ethanol recovery capacity that were obtained as a result of model optimization. The figure also shows how pretreated biomass is allocated to succinic acid and ethanol fermentation tanks. Additionally, the capital cost per unit of product output is tabulated in the figure. While the recovery equipment cost calculation was straightforward, the calculation for the pretreatment and fermentation equipment cost allocation (for each product) was based on the
average biomass capacity allocated towards each product, the steam and power equipment
cost allocation was based on total steam and power allocated towards each product, and the
utility/wastewater equipment cost allocation was based on water loads for each products.

![Graph showing optimal biomass throughput capacity and allocation](image)

### Figure 3-17: Optimal biomass throughput capacity and allocation and succinic acid and ethanol recovery capacities

The total capital expenditure over the time horizon for processing capacity was approximately $290 million; succinic acid related cost was 19 percent while ethanol accounted for 81 percent of the capital costs. We assumed that 25 percent of the total capital cost was funded through a government cash grant (~$70 million), implying that about $220 million was the responsibility of the enterprise. Additionally, about 80 percent of the pretreatment and fermentation capacity of the plant is allocated towards ethanol production; this is primarily due to the fact that the process yield (product per unit biomass) of ethanol is
about 3.5 times lower than the process yield of succinic acid. The overall process yield for ethanol was assumed 83 gallons per ton of biomass while the yield for succinic acid was assumed to be 320 kilograms per ton of biomass. It should be noted that these numbers would be significantly lower if xylose utilization is not considered; we analyze the impact of loss of total process yield on the NPV in the sensitivity analysis section of this dissertation.

Figure 3-18 shows the flow of energy and yields of each system in the optimal process configuration.

![Diagram](image)

**Figure 3-18: Material and energy balance for the optimal technology configuration**

The next table (table 3-14) focuses on the discussion of process parameters that were yielded by the optimal design. Specifically I will analyze the technology choices that were made by the optimizer based on process yields, energy loads and total capital and operating
costs. Other parameters such as water loads and emissions factors can also be considered important for an environmental perspective, but in our case we try to focus on economic profitability, leaving environmental quality analyses as an exercise for the future.

Table 3-14: Qualitative summary of fractionation impact parameters

<table>
<thead>
<tr>
<th>Pre-treatment</th>
<th>Sugar Yields</th>
<th>Energy Loads</th>
<th>Costs</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Glucose</td>
<td>Xylose</td>
<td>Thermal</td>
</tr>
<tr>
<td>Dilute Acid</td>
<td>Medium</td>
<td>Low</td>
<td>Low</td>
</tr>
<tr>
<td>AFEX</td>
<td>High</td>
<td>High</td>
<td>Medium</td>
</tr>
<tr>
<td>Hot Water</td>
<td>Low</td>
<td>Medium</td>
<td>High</td>
</tr>
</tbody>
</table>

Table 3-14 provides a qualitative summary of fractionation (pre-hydrolysis) parameters that are analyzed to determine the economic and process drivers of the pretreatment technology selection process. We classify the parameters as [high, medium, low] based on the percent differences in the values for each technology, where a difference of more than 5 percent is set as the threshold for re-classification into a different qualitative group. AFEX was selected as the fractionation technology of choice; although the energy load and cost structures (investment and operating) are medium level, AFEX provides high xylose yields in the solid (undissolved) washed stream from pretreatment as it is able to protect the structural integrity of the hemicellulosic fraction of biomass, whereas the hemicellulose fraction from dilute acid and hot water is solubilized and removed with the liquid wash stream requiring separate fermentation tanks for fermenting them. This in turn enables a greater utilization of the total biomass leading to higher overall downstream product yields. We can infer from this that maximizing sugar yields is an important aspect of plant design for biorefineries and marginal cost tradeoffs can be acceptable given significantly higher yields are achievable through additional investment in the technology.
Table 3-15 describes the fermentation parameters that were utilized to contrast the fermentation configurations for the plant design, namely, (1) enzymatic hydrolysis followed by separate fermentation of xylose and glucose sugars or (2) enzymatic hydrolysis followed by co-fermentation of sugars.

### Table 3-15: Qualitative summary of fermentation impact parameters

<table>
<thead>
<tr>
<th>Fermentation</th>
<th>Product Yields</th>
<th>Water Loads</th>
<th>Costs</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Ethanol</td>
<td>Succinic</td>
<td>Ethanol</td>
</tr>
<tr>
<td>Co-fermentation</td>
<td>Medium</td>
<td>Medium</td>
<td>Low</td>
</tr>
<tr>
<td>Separate Fermentation</td>
<td>High</td>
<td>High</td>
<td>High</td>
</tr>
</tbody>
</table>

Since energy loads for hydrolysis and fermentation processes are negligible, here we compare only the cost structure, the process yields, and the water loads of each process. Although we modeled a higher product yield attainable from separate fermentation of C5 and C6 sugars, a co-fermentation configuration was selected based on lower capital and operating costs and water loads. Qualitatively, we can infer that marginal yield improvement in the fermentation processes (through metabolic or process engineering) may not warrant a higher capital investment level; this is in stark contrast to the fractionation technology selection where AFEX was selected based on higher process yields. A possible reason for this can be that upstream yield improvement has a direct impact on downstream unit operations’ yields thus reducing the necessity of additional capital investment for marginally better product yields. We do believe that there is a yield threshold for which it may be advisable to spend additional capital to acquire a higher quality asset; this aspect can be corroborated using sensitivity analyses, which is a current topic of development at our research group. Finally, table 3-16 tabulates the process and economic drivers for the selection of the concentration and recovery technologies.
Table 3-16: Qualitative summary of purification impact parameters

<table>
<thead>
<tr>
<th>Concentration</th>
<th>Final Product Yields</th>
<th>Energy Loads</th>
<th>Costs</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Ethanol</td>
<td>Succinic</td>
<td>Thermal</td>
</tr>
<tr>
<td>Distillation</td>
<td>High</td>
<td>--</td>
<td>High</td>
</tr>
<tr>
<td>Pervaporation</td>
<td>High</td>
<td>--</td>
<td>Low</td>
</tr>
<tr>
<td>Electrodialysis</td>
<td>--</td>
<td>High</td>
<td>Medium</td>
</tr>
<tr>
<td>Adsorption</td>
<td>--</td>
<td>Low</td>
<td>High</td>
</tr>
<tr>
<td>Precipitation</td>
<td>--</td>
<td>Low</td>
<td>Low</td>
</tr>
</tbody>
</table>

From the optimal technology structure, distillation and electrodialysis are selected for ethanol and succinic acid concentration operations, respectively. The use of pervaporative separation, where a membrane is used in a column to reduce energy costs of separating water from ethanol, does not seem to be a better option over distillation; this is almost certainly due to the high capital (membrane purchase) and operating (membrane replenishment) costs that are incurred. Additionally, all power and thermal heat requisite for traditional distillation is already produced in the cogeneration facility and the extra electricity that can be sold to the grid. If pervaporative separation is used, the additional electricity saved during the separation process does not make up for the additional capital and operating expenses that are incurred for membrane purchase and regeneration. Electrodialysis is selected for concentrating succinic acid over precipitation with a strong acid (followed by solvent re-crystallization) or membrane adsorption; this can be attributed to high product yields and a lower (relative) operating cost structure for the technology. Although electrical load requirement is higher for electrodialysis, the self-sufficiency of the plant in producing its own heat and power negates the higher energy requirements. For adsorption and precipitation, the modeled product yields were 20 and 25 percent lower than that of electrodialysis; for chemical precipitation a significant amount of ancillary chemicals (strong acid, ammonia, and methanol solvent) are required, and additional waste is generated (through precipitation), leading to substantially
higher operating costs, high costs were incurred periodically to replace the adsorptive membrane (higher maintenance capital requirement).

### 3.4.4 Energy Analysis

For energy analysis, literature-derived energy inputs were used. The gross energy balance for the 20 year time horizon is tabulated in Table 3-17.

<table>
<thead>
<tr>
<th>Value Chain Operation</th>
<th>Energy Input (1)</th>
<th>Units</th>
<th>Optimal Value (2) ×10³</th>
<th>Units</th>
<th>Input Energy Value (1) × (2) GJ</th>
<th>Output Energy Value (1) × (2) GJ</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Switchgrass Production</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Establishment</td>
<td>15.57</td>
<td>KJ/kg DMIB</td>
<td>4671,226</td>
<td>Tons</td>
<td>3,825,944</td>
<td></td>
</tr>
<tr>
<td>Growth</td>
<td>25.49</td>
<td>KJ/kg DMIB</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Harvest</td>
<td>200.31</td>
<td>KJ/kg DMIB</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Transport</td>
<td>233.80</td>
<td>KJ/kg DMIB</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fertilizer</td>
<td>471.40</td>
<td>KJ/kg DMIB</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>TOTAL</strong></td>
<td>946.57</td>
<td>KJ/kg DMIB</td>
<td>4,671,226</td>
<td>Tons</td>
<td>3,825,944</td>
<td></td>
</tr>
<tr>
<td><strong>Energy Case Production</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Establishment</td>
<td>158.83</td>
<td>KJ/kg DMIB</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Growth</td>
<td>0.00</td>
<td>KJ/kg DMIB</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Harvest</td>
<td>2.20</td>
<td>KJ/kg DMIB</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Transport (Southwest Land)</td>
<td>233.80</td>
<td>KJ/kg DMIB</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Transport (South-central Land)</td>
<td>526.06</td>
<td>KJ/kg DMIB</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fertilizer</td>
<td>1126.56</td>
<td>KJ/kg DMIB</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>TOTAL (Southwest)</strong></td>
<td>1521.40</td>
<td>KJ/kg DMIB</td>
<td>2,253,409</td>
<td>Tons</td>
<td>1,293,162</td>
<td></td>
</tr>
<tr>
<td><strong>TOTAL (South-central)</strong></td>
<td>1813.65</td>
<td>KJ/kg DMIB</td>
<td>847,026</td>
<td>Tons</td>
<td>1,293,162</td>
<td></td>
</tr>
<tr>
<td><strong>Process Chemicals</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ammonia</td>
<td>47.08</td>
<td>KJ/kg DMIB</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>CTX</td>
<td>12.75</td>
<td>KJ/kg DMIB</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>DsP</td>
<td>7.61</td>
<td>KJ/kg DMIB</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Enzyme</td>
<td>223.34</td>
<td>KJ/kg DMIB</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>TOTAL</strong></td>
<td>290.78</td>
<td>KJ/kg DMIB</td>
<td>7,771,661</td>
<td>Tons</td>
<td>2,259,833</td>
<td></td>
</tr>
<tr>
<td><strong>Product Transport</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ethanol to NO</td>
<td>11.04</td>
<td>KJ/gal</td>
<td>341,315</td>
<td>1000gal</td>
<td>3,767</td>
<td></td>
</tr>
<tr>
<td>Ethanol to JR</td>
<td>26.49</td>
<td>KJ/gal</td>
<td>15,453</td>
<td>1000gal</td>
<td>409</td>
<td></td>
</tr>
<tr>
<td>Ethanol to TX</td>
<td>11.04</td>
<td>KJ/gal</td>
<td>119,977</td>
<td>1000gal</td>
<td>1,324</td>
<td></td>
</tr>
<tr>
<td>Succinic Acid to NO</td>
<td>3.64</td>
<td>KJ/kg</td>
<td>109,938</td>
<td>Tons</td>
<td>400</td>
<td></td>
</tr>
<tr>
<td>Succinic Acid to TX</td>
<td>3.64</td>
<td>KJ/kg</td>
<td>128,432</td>
<td>Tons</td>
<td>468</td>
<td></td>
</tr>
<tr>
<td><strong>Output Energy</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ethanol</td>
<td>80.20</td>
<td>KJ/gal</td>
<td>476,745</td>
<td>1000gal</td>
<td>38,234,921</td>
<td></td>
</tr>
<tr>
<td>Succinic Acid (combustion)¹</td>
<td>12.900</td>
<td>KJ/kg</td>
<td>238,371</td>
<td>Tons</td>
<td>3,074,982</td>
<td></td>
</tr>
<tr>
<td>Succinic Acid (displacement)²</td>
<td>70,000</td>
<td>KJ/kg</td>
<td>238,371</td>
<td>Tons</td>
<td>16,685,951</td>
<td></td>
</tr>
<tr>
<td>Electricity</td>
<td>3,412</td>
<td>KJ</td>
<td>1,061,418</td>
<td>1000kwh</td>
<td>3,621,769</td>
<td></td>
</tr>
<tr>
<td><strong>TOTAL</strong></td>
<td>10,526.257</td>
<td></td>
<td></td>
<td></td>
<td>44,931,613²</td>
<td>58,542,582²</td>
</tr>
</tbody>
</table>

The input values that are used in table 20 were derived using certain yield and energy efficiency assumptions that are listed below along with their references (Table 21).
Following the table a methodology is discussed to establish how the reference values from table 3-18 were used to calculate the unit input energy values in table 3-16.

**Table 3-18: Energy inputs used to derive the value chain energy balance for optimal design**

<table>
<thead>
<tr>
<th>Input Parameter for Energy Calculation (units)</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diesel Energy Content (KJ/gal)</td>
<td>135,500</td>
</tr>
<tr>
<td>Distance (southwest fields to facility, miles)</td>
<td>80</td>
</tr>
<tr>
<td>Distance (southwest fields to facility, miles)</td>
<td>180</td>
</tr>
<tr>
<td>Truck Diesel Efficiency (mpg)</td>
<td>6</td>
</tr>
<tr>
<td>Biomass Load per Truck (kg)</td>
<td>17,000</td>
</tr>
<tr>
<td>Switchgrass Yield (kg per acre)</td>
<td>6,000</td>
</tr>
<tr>
<td>Cane Yield</td>
<td>10,000</td>
</tr>
<tr>
<td>Cane Nitrogen Required (kg/ac)</td>
<td>120</td>
</tr>
<tr>
<td>Cane Phosphorus Required (kg/ac)</td>
<td>60</td>
</tr>
<tr>
<td>Cane Potassium Required (kg/ac)</td>
<td>60</td>
</tr>
<tr>
<td>Energy Input, Ammonia (KJ/kg)</td>
<td>29,000</td>
</tr>
<tr>
<td>Process Ammonia Required for AFEX (kg / kg DMB-year)</td>
<td>0.0016</td>
</tr>
<tr>
<td>Energy Input, CSL (KJ/kg)</td>
<td>6,800</td>
</tr>
<tr>
<td>Process CSL Required (kg / kg DMB)</td>
<td>0.0019</td>
</tr>
<tr>
<td>Energy Input, DAP (KJ/kg)</td>
<td>29,000</td>
</tr>
<tr>
<td>Process DAP Required (kg / kg DMB)</td>
<td>0.00026</td>
</tr>
<tr>
<td>Energy Input, Enzyme (KJ/kg)</td>
<td>2,850</td>
</tr>
<tr>
<td>Process Enzyme Required (kg / kg DBM)</td>
<td>0.078</td>
</tr>
<tr>
<td>Rail (gal diesel per ton-mile)</td>
<td>0.000054</td>
</tr>
<tr>
<td>Distance from site to NO</td>
<td>500</td>
</tr>
<tr>
<td>Distance from site to AR</td>
<td>1,200</td>
</tr>
<tr>
<td>Distance from site to TX</td>
<td>500</td>
</tr>
<tr>
<td>Total Land Used (1000 acres)</td>
<td>663</td>
</tr>
</tbody>
</table>

The diesel energy inputs for biomass production, harvesting, and storage were calculated using the following equation (given the amount of diesel required from references):
The diesel energy required to transport dry biomass from field to plant was calculated as follows:

\[
\frac{KJ}{\text{Kg DBM Purchased}} = \left(\frac{KJ}{\text{gal Diesel}}\right) \times (\text{Diesel Input}) \times \left(\frac{\text{Kg DBM}}{\text{Acre Land Harvested}}\right) \tag{3.3.113}
\]

For process chemicals, the inputs required per unit biomass and the energy inputs for the production of each process chemical were derived from literature; the energy input was then derived as follows:

\[
\frac{KJ}{\text{Kg DBM Processed}} = \left(\frac{KJ}{\text{Kg Process Chemical}}\right) \times \left(\frac{\text{Kg Chemical}}{\text{Kg DBM Processed}}\right) \tag{3.3.114}
\]

It should be noted that I assumed 100% ammonia recovery while CSL, DAP, and enzymes were assumed to be perishable; consequently, ammonia energy inputs were annualized on a per year basis for the entire planning horizon. In real life there will be some loss of ammonia through the AFEX process requiring replenishment through additional chemical purchases, consequently changing (marginally) the energy balance of the value chain.

The energy input for product transportation to markets (via rail) was calculated as follows:

\[
\frac{KJ}{\text{product transported}} = \left(\frac{KJ}{\text{ton-mile product}}\right) \times \left(\frac{\text{tons unit product}}{\text{product transported}}\right) \times 2 \times Distance_{\text{plant,market}} \tag{3.3.115}
\]

It should be noted that the second term on the right hand side of the above equation is used to convert tons of product into the measurement units of product output; this convert
tons of ethanol to gallons of ethanol sold (specific volume = 0.33 gal per kilogram), while leaving succinic acid in the same unit (1 ton per unit product).

Additionally, while ethanol energy analysis is straightforward as it is a fuel source, for succinic acid 2 different types of analyses can be conducted – based on its heat of combustion or based on an energy displacement criteria; (5) both results are shown in the table and a discussion about how we arrived at the energy displaced value for succinic acid follows in the next paragraph.

The energy value of succinic acid usage had to be estimated using the following methodology:

1. Assume that biomass-derived succinic acid will displace crude-oil derived succinic acid;
   a. Crude oil-derived succinic acid is primarily derived using the following production chain:
      
      \[ \text{Crude Oil} \rightarrow \text{Butane} \rightarrow \text{Maleic Acid} \rightarrow \text{Succinic Acid} \]
      
      i. The yield assumptions were:
      
      \[ 42 \text{ gallons} \rightarrow 4 \text{ kg} \rightarrow 4 \text{ kg} \rightarrow 3 \text{ kg} \]

2. Therefore 1/42 gallons of crude oil is actually used for succinic acid production;

3. The crude oil energy content was assumed to be 6000 MJ per barrel (42 gallons);

4. The energy allocation towards succinic acid production:

   \[ E A^{SA} = 6000 \times \left( \frac{4\times4\times3}{42} \right) = 70 \frac{GJ}{\text{ton S.Acid}} \quad (3.3.117) \]

5. Assume that there is no net additional energy expended on converting butane to succinic acid;
a. This is a simplifying assumption but in its absence, the results would be even more positive for the case of bio-based succinic acid;

6. We assumed that the rest of the crude oil is used for its usual purposes (fuels and chemicals) without impacting the butane to succinic acid conversion chain;

7. Therefore, the Energy displaced ($ED^{out}$) by bio-based succinic acid was estimated as follows:

$$ED^{out} = EA^{SA} = 70 \frac{GJ}{\text{ton } SA\text{cid}}$$

There are many simplifying assumptions in the above estimation, but we do think that this is a solid baseline to build better, more detailed comparative models for energy analyses.

To compare the energy metrics investigated in this dissertation, we use reference cases for corn ethanol, crude oil, and sugarcane ethanol. The next table uses the energy metrics described previously (GER, NER, ERFOEI) along with the data from tables 3-17 and 3-18 to estimate the energy metrics for the optimal design case.

### Table 3-19: Energy performance metrics for multiple fuel production chains

<table>
<thead>
<tr>
<th>Metrics</th>
<th>Optimal Design Value¹</th>
<th>Optimal Design Value²</th>
<th>Cellulosic Ethanol Only</th>
<th>Fuel Oil from Crude</th>
<th>Corn Ethanol</th>
<th>Sugarcane Ethanol (2020 Scenario)</th>
</tr>
</thead>
<tbody>
<tr>
<td>NER</td>
<td>4.27</td>
<td>5.56</td>
<td>5.00</td>
<td>5.60</td>
<td>2.67</td>
<td>11.00</td>
</tr>
<tr>
<td>NEV (Mj / gal)</td>
<td>72.17</td>
<td>100.72</td>
<td>73.35</td>
<td>97.52</td>
<td>39.04</td>
<td>114</td>
</tr>
<tr>
<td>Land Efficiency (Mj / ac)</td>
<td>46,840</td>
<td>65,370</td>
<td>55,576</td>
<td>N/A</td>
<td>23,280</td>
<td>106,109</td>
</tr>
<tr>
<td>EROFEI</td>
<td>3.27</td>
<td>4.56</td>
<td>4.00</td>
<td>4.60</td>
<td>1.67</td>
<td>10.57</td>
</tr>
<tr>
<td>GER</td>
<td>3.89</td>
<td>5.07</td>
<td>3.67</td>
<td>3.68</td>
<td>1.67</td>
<td>10+</td>
</tr>
</tbody>
</table>

For cellulosic ethanol and electricity only, we fixed the succinic acid product variables to zero and ran the optimization model to obtain results. For the optimal design, the GER values are obtained by dividing the gross totals for energy outputs by the gross totals
for energy inputs (Table 3-17), while the NEV and EROFEI considers the net energy outputs (ethanol, succinic acid, and excess energy) and the net fossil energy inputs; the net fossil energy inputs are considered assuming that all biomass production and transportation, and product transportation will require fossil energy while all process operations utilize energy that is generated using renewable fuels (lignin, biogas, sludge).

From Table 3-18, there are a few observations that require explanation:

1. For fuel oil production from crude oil, the NEV, GER, and EROFEI metrics all show a great deal of efficiency when compared to corn-based ethanol, primarily because of the mature nature of the technology and process efficiencies attained through heat integration and recycle in the extraction and refining processes;

2. Sugarcane ethanol provides a significant energy benefit exemplified by all energy efficiency metrics, again buoyed by the mature nature of Brazil ethanol technology (high ethanol yield per unit of feedstock), significantly higher feedstock yields (cane sucrose) per acre of land, and electricity credits from bagasse combustion;

3. Corn ethanol seems to be the least efficient in terms of energy utilization as significant amounts of energies are used in corn production (diesel and natural gas) and biorefining (natural gas). Additionally, very little co-product credits are obtained as there is a net usage of fossil-derived electricity as opposed to renewable electricity credits;

4. The design cases with only cellulosic ethanol and electricity and where succinic acid energy allocation is based on amount of crude oil displaced provide very comparable results to the fuel oil value chain energy efficiency metrics;
5. The case where the heating value of succinic acid is employed as opposed to the fossil energy displaced, there is about a 28 percent reduction in energy efficiency primarily driven by the methodology used to allocate energy output to succinic acid;

The above analysis shows that while the design cases obtained as a result of spatial and process optimization provides very reasonable energy efficiency metrics, although the allocation methodology employed to allocate succinic acid energy yield has a significant impact on the overall energy efficiency of the optimal design cases. The next section utilizes the energy efficiency results obtained here to analyze and compare the carbon efficiency of the optimal design cases.

3.4.5 Carbon Analysis

Carbon efficiency metrics were introduced in the model description section of this dissertation; these include Net Carbon Ratio (NCR) which represent the ratio carbon savings that are achieved from fossil product displacement and the fossil carbon that is emitted while operating the renewable product value chain; Net Carbon Savings per gallon of biofuel which represents the carbon savings that are achieved by displacing fossil fuels with biofuels; Land efficiency of carbon which represents the net carbon savings per acre of land that is planted with energy crops. It should be noted that we have neglected soil carbon sequestration levels (for CRP Land ~ 750 kg CO$_2$-e per acre) for the current comparison in order to maintain consistency while comparing the metrics with other value chains. I will discuss the impact of including soil carbon sequestration into the analysis after stating and discussing the base case results (without soil carbon considerations). Finally, the last carbon metric compared is Carbon Savings on Fossil Carbon Emitted which represents the net carbon savings that are
achieved per unit of fossil carbon that is emitted to operate the optimal value chain. In all cases, carbon emissions during construction of processing facility and of biomass production and logistical equipment is neglected; although this leaves the analysis incomplete, it is my belief that the lifetime of the equipment will deem the carbon impact of construction negligible in terms of the overall results. Table 3-20 enlists the carbon analytics for the optimal design case (with ethanol, succinic acid, and electricity and displacement method for succinic acid), and compares the results with other similar fossil and biofuel value chains.

Table 3-20: Carbon efficiency metrics for multiple fuel production chains

<table>
<thead>
<tr>
<th>Metrics</th>
<th>Optimal Design Value</th>
<th>Cellulosic Ethanol Only</th>
<th>Fuel Oil from Crude</th>
<th>Corn Ethanol</th>
<th>Sugarcane Ethanol (2020 Scenario)</th>
</tr>
</thead>
<tbody>
<tr>
<td>NCR</td>
<td>3.13</td>
<td>4.21</td>
<td>-4.26</td>
<td>1.55</td>
<td>7.50</td>
</tr>
<tr>
<td>Net Carbon Savings (kg CO2-e/gal)</td>
<td>5.00</td>
<td>6.10</td>
<td>-3.18</td>
<td>2.11</td>
<td>9</td>
</tr>
<tr>
<td>Land Efficiency (Kg CO2-e Saved/ac)</td>
<td>3.243</td>
<td>4.621</td>
<td>N/A</td>
<td>926</td>
<td>8.288</td>
</tr>
<tr>
<td>CSOFCE</td>
<td>2.13</td>
<td>3.21</td>
<td>-5.26</td>
<td>0.55</td>
<td>6.50</td>
</tr>
</tbody>
</table>

As can be noticed from the table, the carbon performance of a sugarcane ethanol value chain is the best. The carbon impact of fuel oil production is understandably negative as there is no carbon sequestration that takes place during the value chain operation. For the optimal design case, approximately 8 Kg CO2-e improvement is achieved for every gallon of gasoline equivalent that is used as a transportation fuel. On a per acre basis a 4-fold improvement in carbon efficiency is noticed for the optimal design case, compared to corn ethanol, as is the case for carbon savings achieved per unit of fossil carbon that is emitted. Interestingly, when the production of succinic acid is suppressed in the optimization model (cellulosic ethanol and electricity production only), a marked improvement is noticed; this
can be attributed to the re-allocation of biomass resources towards more bio-electricity production which consequently improves the carbon efficiency of the entire value chain.

With the inclusion of soil carbon sequestration impacts in the analysis, the optimal design case and cellulosic ethanol only case results are stated in table 3-21. It should be noted that soil carbon sequestration will only impact the carbon efficiency results for switchgrass production on CRP land, as energy cane production is assumed to simply replace sugarcane production on currently productive agriculture land.

### Table 3-21: Carbon efficiency metrics when soil carbon sequestration is taken into account

<table>
<thead>
<tr>
<th>Metrics</th>
<th>Optimal Design Value</th>
<th>Cellulosic Ethanol Only</th>
</tr>
</thead>
<tbody>
<tr>
<td>NCR</td>
<td>2.39</td>
<td>3.36</td>
</tr>
<tr>
<td>Net Carbon Savings (kg C / gal)</td>
<td>4.12</td>
<td>5.48</td>
</tr>
<tr>
<td>Land Efficiency (Kg Saved/ac)</td>
<td>2,730</td>
<td>4,615</td>
</tr>
<tr>
<td>C$\text{SO}_{\text{FCE}}$</td>
<td>1.39</td>
<td>2.36</td>
</tr>
</tbody>
</table>

We notice from the table above that for the optimal design case that there is a 20 percent reduction in all carbon efficiency metrics, while there is about a 15 percent reduction for the cellulosic ethanol case study. It can be inferred that soil carbon sequestration, for the optimal design case and in general, for energy crop-based biofuel and biobased chemical production, has a major impact (15-20 percent) on the entire carbon balance of the value chain.

Before moving on to other aspects of evaluating the optimal design case and the sensitivity of the design to variation in input parameters we want to make one final point; the
input values that are used to calculate the carbon efficiency metrics are inherently uncertain with large standard deviations possible in the values used here and the true value (which may not be known). It is essential that a nationwide (even worldwide) measurement system be developed associating “generally accepted carbon accounting values” for various supply, production, and demand chains. It is essential before the implementation of any carbon cap and trading scheme that a uniform measurement scheme be established that can be applied across multiple industry verticals.

3.4.6 Sales and Financial Analysis

Figure 3-19 depicts the sales trends along with the price trends and average market share for each product over the time horizon. The prices shown in the figure are adjusted for transportation and selling costs. The average market share is estimated by following formula:

\[ Mkt\ Share_{m,p} = \frac{\sum_t Demand\ Filled_{p,m,t}}{\sum_t Total\ Demand_{p,m,t}} \times 100\% \]  

(3.3.119)

The market share basically predicts what percentage of the total market demand for product p will be optimal for the processor to meet over the planning horizon. The demand and prices for each product are modeled using an S-curve based forecasting methodology with a positive elasticity between price and demand; this implies that as market demand increases the price (spot) asked per unit of product will also increase. This is a rather simplifying assumption as factors such as product supply, costs of production (impacting supply), macro-economic factors (inflation, interest rates, GDP growth), and cross-price elasticities with fossil-derived products (gasoline, succinic acid) are not considered. We will try to incorporate such a model in later sections when the impact of uncertainty of capacity design for the optimal technology and spatial design is analyzed. For now, we assume that
the demands and prices follow an S-curve based increase for ethanol and niche markets for succinic acid, qualitatively implying that as markets accept the use of these biobased counterparts for fossil-based fuels and chemicals the demands and prices of the products will rise (exponentially) initially. As product supply then catches up with market demand and the market itself gets saturated, the demand and prices will approach a ceiling asymptotically, reaching equilibrium. For butanediol (BDO) applications of succinic acid, it is assumed that prices will fall initially as large supplies will initially hit the market, with the prices reaching a floor (at equilibrium) as demand catches up with supply. These are trends that I model under qualitative assumptions about the markets for each product; in the next section (sensitivity analysis), we will analyze the impact of different qualitative trends on the optimal design and enterprise NPV.
Figure 3-19: Sales trends along with the evolution of market share for each product

From the sales figures, it is apparent that niche markets for succinic acid provide the greatest opportunity for profitability; achieving higher sales levels in this market can significantly appreciate the strategic value of the biorefiner. Additionally, ethanol demand is primarily met in local Louisiana markets and Texas driven by higher sales margins (price less transportation and sales costs) associated with selling. The Shreveport market’s (blending station) demand for ethanol is initially met (up to year 8) following which sales are withdrawn; this can be attributed to more feedstock being diverted towards succinic acid (niche and BDO) production which may be optimal mathematically, but may not work in real life as customer service will be greatly impacted if product supply is suddenly withdrawn from a market. It should be noted that price appreciation modeled for the base case can easily
be supplemented for margin expansion over the planning horizon; margin expansion can occur through operating cost reduction (through more efficient plant operation), yield improvement (learning by doing), and also through signing discounted raw material procurement contracts as better supplier relationships are established. In all cases the monetary impact will be felt on the enterprise bottom-line which is aptly modeled using price appreciation. The projected margins for the optimal design case are presented in figure 3-20.

**Figure 3-20: Margin analysis for the optimal value chain configuration**

As predicted the impact of price appreciation is noticed in the overall margins of the biorefiner; all costs indicated in the figure are presented per dollar of revenue collected. Therefore, if revenue increases without a proportional increase in the direct costs (cost of goods or COGS), a margin expansion is noticed. Nevertheless, the impact of direct cost reduction is exactly the same as revenue growth as both impact the enterprise bottom-line identically. We also notice that depreciation, amortization and tax costs increase over time; this is primarily driven by the depreciation schedule that is adopted and the fact that enterprise profitability increases (leading to higher taxes). Additionally, succinic acid
capacity is incremented leading to higher depreciation costs. Also noticeable is the decrease in the fixed operating costs over time (indirect costs); this can be attributed to achievement of higher economies of scale as production revenues are scaled up while fixed operating costs do not increase leading to an expansion in operating margins. The formulae used for calculation of margins along with their average values over the time horizon are provided in table 3-22.

Table 3-22: Enterprise margin performance metrics

<table>
<thead>
<tr>
<th>Margin Category</th>
<th>Formula</th>
<th>Years =4-9</th>
<th>Years = 10-15</th>
<th>Years = 16-20</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gross Margin</td>
<td>( \frac{R - COGS}{R} )</td>
<td>31%</td>
<td>57%</td>
<td>59%</td>
</tr>
<tr>
<td>EBITDA Margin</td>
<td>( \frac{R - COGS - IDC}{R} )</td>
<td>17%</td>
<td>49%</td>
<td>51%</td>
</tr>
<tr>
<td>Operating Margin</td>
<td>( \frac{R - COGS - IDC - D&amp;A - Tax^{net}}{R} )</td>
<td>10%</td>
<td>28%</td>
<td>28%</td>
</tr>
<tr>
<td>Net Margin</td>
<td>( \frac{R - COGS - IDC - D&amp;A - Tax^{net} - I}{R} )</td>
<td>6%</td>
<td>25%</td>
<td>25%</td>
</tr>
</tbody>
</table>

From table 3-22, it is clear that significant margin expansion is achieved after the 9th year. This is directly attributable to 2 modeling inputs; (1) the S-curve based forecasts for prices had prices increasing significantly around year 8-9 of the planning horizon (see figure 3-19), and (2) succinic acid capacity is incremented (see figure 3-17) leading to greater economies of scale as fixed costs remain constant while gross profits increase. Again, this is purely a modeling assumption, and further numerical experiments should be carried out in order to investigate the impact of different price trends on enterprise margins. We again want to re-iterate that price trends not only represents price increases, but can easily be thought of as process yield improvements or input cost reductions, all of which have the same impact on margins. The next figure represents the free cash flows (and its components) that are
generated from the operation of the optimal design and the evolution of the cumulative NPV of the portfolio of enterprise projects.

![Free cash flow components and the evolution of the optimal project NPV](image)

**Figure 3-21: Free cash flow components and the evolution of the optimal project NPV**

We notice that the project payback period is 16 years; by any measure this is an extremely long payback period. In real life scenarios, such long payback periods are not looked upon favorably by equity investors and consequently, strategies are required shorten payback periods of biofuel project investments and provide an active source of monetary returns to equity investors throughout the project. One financial strategy that can be adopted is re-directing the investment and production tax credits, and/or depreciation and amortization benefits obtained by the enterprise to equity investors (tax equity) during the initial period of investment; there would be a negative impact on the portfolio NPV and the
enterprise value for the biorefiner though. A more profitable product portfolio comprising of higher margin, lower volume specialty products like pharma- and neutraceuticals is another avenue that can be investigated from a product and techno-economic perspective; incorporation of these high value co-products can improve the NPV of the project significantly (through margin expansion), while producing higher volume products such as ethanol and succinic acid can help the biorefiner take full advantage of the economies of scale from operating a commercial scale facility (bottom-line control).

Apparent from figure 3-21 is that the portfolio NPV evolves dynamically with investments made on a continuous basis. The NPV can be broken up into 2 major components; (1) the discounted value of operating cash flows, that describe the value of plant operations, and (2) the discounted value of capital investments made in the plant over the time horizon. It should be noted that the optimization model was formulated so as to allow investments over the entire time horizon (dynamic) as opposed to a static formulation where investment is made only in the current time period. Over a strategic time horizon, it is important to model and value this decision-making flexibility, especially for product markets like biofuels and biochemicals that are in their nascent stages of development. The final NPV is derived as the difference between the discounted operating and investment cash flows; this is the true NPV of the portfolio of ethanol and succinic acid projects which was calculated to be $57 million. In traditional discounted cash flow analyses, the project NPV is usually the only metric that is investigated based upon which investment decisions are made, but in an enterprise context there are broader metrics that can provide a better, more complete description of the value of the project for multiple enterprise stakeholders. Some of these
metrics were discussed earlier and their formulae along with their numerical values are stated in table 3-23, for the optimal design case.

Table 3-23: Key overall financial performance metrics

<table>
<thead>
<tr>
<th>Metrics</th>
<th>Description</th>
<th>Value ($ \times 10^5)</th>
</tr>
</thead>
<tbody>
<tr>
<td>NPV</td>
<td>Discounted value of operating assets</td>
<td>$57,064</td>
</tr>
<tr>
<td>TV</td>
<td>Continuing value of operating assets beyond planning horizon</td>
<td>$821,173</td>
</tr>
<tr>
<td>FV</td>
<td>Gross value of firm = NPV + TV</td>
<td>$878,237</td>
</tr>
<tr>
<td>DV</td>
<td>Total debt held by enterprise at the end of planning horizon</td>
<td>$192,322</td>
</tr>
<tr>
<td>CV</td>
<td>Total cash held by enterprise at the end of planning horizon</td>
<td>$550,258</td>
</tr>
<tr>
<td>SKE</td>
<td>Cumulative enterprise earnings that are payable to the stockholders of the enterprise</td>
<td>$550,258</td>
</tr>
<tr>
<td>SHV</td>
<td>The net value of the firm's operating, cash and debt assets attributable to shareholders</td>
<td>$1,236,174</td>
</tr>
<tr>
<td>CRBV</td>
<td>Value of carbon taxes and credits generated and sequestered through operations</td>
<td>$11,177</td>
</tr>
<tr>
<td>SKV</td>
<td>Total value of enterprise to all stakeholders = SHV + CRBV</td>
<td>$1,247,351</td>
</tr>
</tbody>
</table>

For the optimal design the terminal value of the project was estimated to be $821 million. The total firm value can then be estimated as the sum of the discounted project NPV and the discounted terminal value of the project ($878 million). The enterprise holds a total of $192 million in debt at the end of the planning horizon with $550 million cash holdings yielding a net cash balance of $348 million. Project profits, equity capital raises, and debt borrowings all add to the total cash balance of an enterprise, while operating losses, equity payments and loan repayments all reduce the total cash balance. The net cash that an enterprise possesses at any given time can be estimated as the difference between all cash inflows and outflows during a time period. At the end of the planning horizon, the enterprise holds a cash balance (or deficit) that should be valued appropriately and preferably separately from the operating assets (plant). For the optimal design case the net cash on the balance sheet is $348 million at the end of the planning horizon; this is important as not having cash on the balance sheet in real life can severely reduce decision-making flexibility for an
Having liquid cash on the balance sheet enables an enterprise to modulate operating and investment decisions with evolving markets, and provides the biorefiner with liquid assets that can be used to better manage their operational working capital. If the debt held by the enterprise is greater than their liquid cash holdings, the impact on the cost of capital for the enterprise can be negative, restricting the growth-related capital expenditures that they can partake. While the ending cash balance for the optimal design case is indeed positive, the cash balance evolution goes through periods where the net cash approached zero (figure 3-22). Imposing minimum cash balance constraints during optimization can mitigate such scenarios. Additionally, a better capital structure optimization model is also suggested as an extension to this work to more accurately model the impact of capital management decisions on the strategic value of the biorefining value chain.

A total of $210 million was raised as equity capital for investment in plant equipment while a total of $180 million was paid out as dividends sourced from free cash flows. The
shareholder value generated from the optimal design, calculated as the sum of the firm value and the net cash on the balance sheet was estimated to be $1.2 billion; this implies that the optimal design case, given the input market and process scenarios, has the potential to generate value of greater than $1 billion over the planning horizon, if implemented. Again this is just a point estimate based on one set of input conditions and ideally multiple scenarios should be tested to investigate their impact on the strategic value of the enterprise (Sensitivity Analysis & Numerical Experiments). Qualitatively, the following are some of the major takeaways from the financial valuation metrics:

1. The project value, calculated as discounted difference of the operating cash flow and the capital investment levels, was $57 million, indicating a profitable project investment;

2. The enterprise value generated by the project was calculated to $878 million of which approximately 7 percent is generated by operating the biorefinery over the time horizon, while 93 percent is the assumed future value (terminal) that can be generated from operations beyond the planning horizon. This is a direct consequence of the longer payback period (16 years) as most value of the optimal design is pushed into the future (terminal value) while invested capital is recovered.

3. The enterprise holds $192 million in debt and a liquid cash value of $550 billion, which can be used to reinvest in the business beyond the planning horizon;

4. Of the total shareholder value that is generated by the project over the time horizon ($1.2 billion), $250 million is generated through government-derived cash flow, with producer and investment tax credits at $150 million and government cash grants (BCAP and plant investment grants) making up the balance at $100 million.
a. This value is rather high (about 20 percent) exemplifying why investment and production tax credits, cash grants are essential in the current environment for cellulosic biofuels and biochemical industries to grow;

Now that the optimal design case has been stated and discussed at length, the next section will discuss how sensitivity analyses and numerical experiments will be utilized to further lend some character to the design case and provide more insight into how design and operational parameters impact the strategic objective of the prospective biomass-to-bioproducts value chain.

3.5 Sensitivity Analysis

Sensitivity Analysis was conducted in order to determine what parameters have a profound impact on important decision variables and the NPV. Traditionally, sensitivity analyses are conducted on spreadsheet-type models where important decision variables such as operating capacities, utilization rates, and sales levels are fixed a priori; input parameters such as prices and yields are then varied and their impact on enterprise objectives such as costs and profits are analyzed. We propose a little different an approach in order to lend some more perspective to the optimal design case. In the first part of this analysis, we posit that the input parameters can effectively impact 2 separate sets of decisions – design decisions and operational decisions. Additionally, certain input parameters such as yields and prices can only become apparent once design decisions are made and the spatial and technological network is established with optimal capacities; consequently production, sales and raw material sourcing decisions (to some extent) are the only decisions that can realistically be altered if price and/or yield scenarios change. On the other hand, there are certain parameters
that impact even the design decisions; these can include resource availability, cost of capital, and equipment capital costs (although engineering and construction capital costs will only become apparent after capacities are established). Consequently, with variability in these parameters one should expect that technology, spatial, and capacity design decisions may be impacted. The summary of parameters that are varied and the category of decisions (design or operational) that they impact is provided in table 3-24.

**Table 3-24: Operating and design parameters that are tested during sensitivity analysis**

<table>
<thead>
<tr>
<th>Operating Parameters</th>
<th>Design Parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>Biomass Yield</td>
<td>Biomass Resource Availability</td>
</tr>
<tr>
<td>Sugar Yield</td>
<td></td>
</tr>
<tr>
<td>Fermentation Yield</td>
<td></td>
</tr>
<tr>
<td><strong>Ethanol</strong></td>
<td></td>
</tr>
<tr>
<td><strong>Succinic Acid</strong></td>
<td></td>
</tr>
<tr>
<td>Recovery Yield</td>
<td></td>
</tr>
<tr>
<td><strong>Succinic Acid</strong></td>
<td></td>
</tr>
<tr>
<td><strong>Ethanol</strong></td>
<td></td>
</tr>
<tr>
<td>Fuel Yield</td>
<td>BCAP program</td>
</tr>
<tr>
<td>Total Energy Load</td>
<td>Government Cash Grant</td>
</tr>
<tr>
<td>Product Prices and Demand</td>
<td></td>
</tr>
<tr>
<td><strong>Ethanol</strong></td>
<td></td>
</tr>
<tr>
<td><strong>Succinic Acid, Niche</strong></td>
<td></td>
</tr>
<tr>
<td><strong>Succinic Acid, BDO</strong></td>
<td></td>
</tr>
<tr>
<td>Cost of Goods (Overall)</td>
<td></td>
</tr>
<tr>
<td>Indirect Costs (Overall)</td>
<td></td>
</tr>
<tr>
<td>Ethanol Tax Credits</td>
<td></td>
</tr>
<tr>
<td>Cost of Capital</td>
<td>Total Equipment Costs</td>
</tr>
<tr>
<td>Capital Cost for Engineering and Construction</td>
<td>Cost of Capital</td>
</tr>
<tr>
<td></td>
<td>Capital Availability</td>
</tr>
</tbody>
</table>

In both sets of parameters though, optimization as opposed to simulation can be utilized to quantify not only their impact on strategic objectives of the bioproducts enterprise, but also to investigate how operating (or design) decisions change (optimally) as parameter scenarios are varied. This of course, implicitly implies that the biorefiner, given changes in real life scenarios, will choose to make decisions in an optimal manner, which maximizes
their strategic and tactical objectives. In order to quantify the impacts of these input parameters we will use the following methodology:

1. For parameters that impact design decisions, the binary variables for spatial and technological node selections will be allowed to vary during optimization and we will focus on how the spatial and technological superstructure design changes along with their impact on portfolio NPV and shareholder value;

2. For parameters impacting operating decisions, we will fix the spatial and technological configuration to the optimal design case and study how the operating decisions changes with variation in the inputs along with their impact on the portfolio NPV and shareholder value.

3.5.1 Operational Sensitivity to Process Parameters

The first set of parameters that were investigated for their impact on the portfolio NPV included system yield and energy parameters. Output yields were comprised of land yield (biomass) fractionation yield (total fermentable sugar), and fermentation yield (final recoverable product). Energy parameters that were investigated included the total thermal and electrical energy demand of the processing facility. In all cases the initial capacity design was fixed but decisions regarding production and sales were allowed to vary optimally. The results along with the percentage of variation for each input are shown in a tornado diagram below (figure 3-23).
Figure 3-23: Tornado chart for process parameter sensitivity analysis

The tornado chart shows that the fermentation yield of ethanol has the largest impact on the portfolio NPV. While a shortfall in biomass yields has the largest downside impact, an improvement in total ethanol yield (post-fermentation) provides the largest upside. An improvement in energy efficiency of the facility while environmentally more beneficial, does not provide a large economic upside as the additional electricity (excess) that can be sold to the grid is essentially a very low margin product. On the other hand, a shortfall in the total energy output (low residual solids yield or poor energy management) has a significant impact the portfolio NPV as additional biomass is purchased and co-fired in the CHP generation plant in order to satisfy plant energy loads. From this analysis we can safely assume that for a real operating facility to operate sustainably over the long term, yield outputs are an essential parameter to monitor and control. Biomass yields, although subject to large weather-related variability, can be control to an extent through judicious crop management practices and larger investments in R&D to develop better, more robust qualities of energy crops. Additionally harvesting and storage logistics can be improved to minimize losses before the feedstock is processed including baling of the harvested crop or some other densification method such as pelletization; the major objective here would be to minimize exposed area to nature while controlling operating costs of logistics. Additionally, chemical preprocessing
that preserves the structural and compositional integrity of biomass should also be considered. Major questions to answer then from a design perspective will include:

1. **What technologies should be used for preprocessing?**

2. Spatially, where to locate these facilities (crop harvest sites, intermediate facilities, or at plant sites);

3. What capacities should be established in order to achieve reasonable feed protection while minimizing financial impact (optimization problem).

The problem of choosing appropriate preprocessing technologies at the harvest site was addressed mathematically in the optimization model proposed earlier; different harvesting and baling configurations, whose data was derived from Chen (2011), were included as binary decision variables. A mixture of square and round bales (2/3 square and 1/3 round) was yielded as the optimal choice. Despite the results, a deeper tactical analysis for preprocessing technology choice, wherein, the time steps for modeling are more granular is deemed necessary; the time steps should ideally be of the scale of a few weeks so as to represent time-varying changes in feedstock quality and composition while in storage. In our case study, the design objectives were mostly strategic, and consequently the results are more oriented towards investment appraisal (strategic objective) as opposed to tactical decisions regarding supply chain operations. Ideally, a tactical model should optimize biomass compositions over a time horizon over one harvesting season and feed the aggregate results into the proposed strategic optimization model in order to choose the optimal preprocessing technology that minimizes product losses while maintaining low investment risks for the biorefining enterprise.
The total sugar (fermentable) yield from pretreatment and saccharification is another process parameter that has significant downside risks; the upside is capped to an extent, as in the base case (optimal) scenario, we assumed a sugar yield of 80 percent of the total hemicellulosic (xylose yielding) and cellulosic (glucose yielding) fraction in the biomass. If the base case scenario assumed a lower sugar yield, we may indeed notice a greater upside to improving yield. Additionally, fermentation yields were assumed to be 70 and 60 percent (of total sugar post fractionation) for ethanol and succinic acid, respectively. Consequently, the upside shown by the tornado charts is also greater. Sugar yield improvements can theoretically be achieved through better process design for the ammonia reactor (AFEX), and better enzyme loading and input management (process control) for the saccharification process. Additionally, schemes where glucose inhibition (of the enzyme hydrolytic process) can be minimized, such as simultaneous saccharification and co-fermentation (SSCF), also provide valuable opportunities. From a design perspective, designing more robust enzymes that can act even in severe operating conditions can also be investigated.

No matter what the case, it is easy to infer from the tornado charts that process yields are one of the most important components towards determining the long-term sustainability and profitability of a biomass-to-bioproducts value chain. Using the proposed framework, a stakeholder can determine not only the impact of process parameter variability, but also examine the tradeoffs between higher investments in new technologies and improvement in overall value chain yields; in a lot of cases it may prove that the marginal cost of yield improvement is too high for investment in a new technology. Using the optimization and sensitivity analysis based decision framework it is easy to establish benchmark targets for technology-based yield improvement in conjunction with cost parameters that are necessary
to implement the technology on a commercially sustainable scale and time frame. As a part of the efforts at the PSE group at LSU, we are actively working on establishing industrial and academic partnerships where technological impact assessment and cost and yield benchmarking are deemed important for emergent biobased process technologies still in the RD&D stage (research, development and demonstration).

3.5.2 Margin Parameters

Next, we evaluated the impact of cost parameters on the portfolio NPV; cost parameters that were deemed to have the largest (predicted) variability from the values that were used as input to the base case model include raw material costs (Cost of Goods Sold, COGS), capital expenses related to construction and engineering, and indirect costs of operations.

Raw material costs are direct costs that scale (almost) proportionally with increasing revenues; for the case study COGS includes (a) feedstock production costs such as seeds, fertilizer and chemicals, and direct energy costs for farm equipment (diesel and natural gas), and (b) costs related to purchase of process chemicals, enzymes, and micro-organisms. Usually, the best way to counteract rising COGS is either through increasing output prices of products or achieving process efficiencies through better value chain yield management. Since the products that are produced in this case study are commodities (cannot differentiate between different sources of the same product, such as gasoline and ethanol), price increases are usually constrained by demand elasticity for consumers, although some input cost inflation will be reflected in market prices. Nevertheless, better yield management and additionally, optimal capacity utilization rates are the most plausible ways of managing direct input cost inflation (especially in case of rising prices). To investigate the impact of COGS
inflation on the portfolio NPV, the S-curve based cost model was utilized; COGS were assumed to increase (or decrease) with time reaching the ceiling (or floor) which was arbitrarily set as a percentage of base case COGS (equation 120). In the equation below, \( \delta \) is the rate of cost inflation while \( \bar{t} \) is the average time of the planning horizon.

\[
COGS_t = COGS^{base} + \left( \frac{COGS^{max} - COGS^{base}}{1 + e^{\delta x (t - \bar{t})}} \right)
\]  
(3.3.120)

Engineering and Construction expenses are assumed to be unpredictable due to material costs inflation and cost overruns due to a lack of standard operating procedures for constructing a biorefinery. According to NREL’s nth plant cost analysis (Kazi et al, 2010), as there is a lack of experience with constructing commercial scale biorefineries, cost overruns during construction are entirely possible for newer plants; to counteract such happenstances, a contingency fund can be setup to fund increases in construction costs. For the base case 20 percent of total direct and indirect costs was assumed to be set aside (and used) during the initial construction of the biorefinery. These costs were assumed to be 10 percent for any subsequent capacity expansion projects. Additionally, general material cost inflation, especially in steel, copper, and cement prices can also lead to cost overruns. For sensitivity analysis, the percent set aside for project contingency was varied in order to investigate the impact of higher or lower capital costs on the portfolio NPV.

Indirect operating costs are assumed to comprise of (a) transportation costs for movement of feedstock to plants and final products to markets, (b) selling and marketing costs related to contractual expenses with product marketers, and (c) labor and administrative expenses. These costs are usually fixed (for different capacity ranges) and decrease with larger network capacities (economies of scale). As initial capacities were fixed as inputs, the only way for the optimization model to counter an increase in indirect operating costs is
through expansion of capacity, while a reduction in costs is directly reflected in value chain operating margins. The cost inflation is modeled in a similar way to COGS inflation, except a larger range of cost variability is modeled to reflect uncertainty in transportation costs (fuel-related) and labor costs (related to economic growth). The results for each margin parameter are shown in the tornado chart (figure 3-24) below along with the table showing the variability modeled in each cost.

![Tornado chart for input and capital cost parameter sensitivity analysis](image)

**Figure 3-24: Tornado chart for input and capital cost parameter sensitivity analysis**

It is apparent from the figure above that variability in COGS has a marked impact on portfolio profits and NPV; this is expected as inflation in COGS can only be countered by price increases or improvement in resource utilization and plant yields. Since neither of these two circumstances were modeled (understandable so in order to understand the true impact of COGS on NPV), the variability in NPV is significant. One suggestion, from a modeling perspective, would be to model product price as a function of feedstock costs and model product demand as a function of product prices. In this way inflation in feedstock production costs can be studied on product prices and eventually the quantity demanded at a given price (setting sales levels). It should also be mentioned that feedstock costs comprised 40 percent
of total COGS while enzyme costs were 30 percent of COGS. Consequently controlling these two costs becomes an essential part of cost management for a real operational plant.

Increase in indirect operating costs has a much greater downside risk as opposed to upside potential; this is primarily because operating capacities were fixed implying higher indirect costs impacted the value chain bottom line directly. Decreasing costs on the other hand do not impact the portfolio NPV in any significant way as they are a very small percentage of overall plant margins.

3.5.3 Market Parameters

The next set of parameters that were tested included product prices, namely, market prices for ethanol, succinic acid serving niche markets and succinic acid for downstream processors as feedstock for BDO. From a modeling perspective, market parameters are an important consideration as all other parameters that are discussed previously are, to an extent controllable, although gross margins and consequently input cost is another exogenous parameter that are hard to control; yield, although uncertain, can be controlled by better operating practices and investment in technological innovation. Market parameters, on the other hand, are by their very nature set in the open markets based on aggregate macro-economic conditions, supply-demand fundamentals for the commodity, and the regulatory framework that govern the supply and demand. Consequently, studying the impact of exogenous variables such as market prices and demands becomes an important exercise for biomass processors and value chain actors, in order to develop a cogent and implementable strategy for profitable and sustainable operations for the biorefining value chain.

With regards to the products being studied in the base case, we assumed that ethanol production will serve the gasoline additive markets while succinic acid produced can be sold
into either specialty niche markets such as coatings and additives or into more mass markets as a feedstock for BDO, which is used in polymer production. For sensitivity analysis and deterministic optimization, we have focused less on developing a fundamental model for these price processes, but more on getting the general long term trends right; the price and demand trends for each product (for the base case) were provided in figure 3-19. These trends were used under the following assumptions:

1. Cellulosic ethanol prices and demand will follow gasoline prices (and demand) which, for the base case, are assumed to increase with time at a compounded annual growth rate (CAGR) of 2-3.5 percent (different for different markets) reaching a ceiling (price-elastic demand) for a total increase of 50-100 percent over the time horizon;

2. Specialty markets for succinic acid were assumed to be mature markets with most demand increases coming from displacement of petroleum-derived succinic acid and prices increase at a CAGR of 2 percent;

3. BDO markets for succinic acid were assumed to grow rapidly initially (CAGR = 10 percent) as rapid displacement of petroleum-derived maleic anhydride occurs, which then slows down to a CAGR of 2 percent as markets mature. Additionally, we assume that the price process decreases (inverse proportionality to demand) over time as market supplies increase rapidly for BDO applications (high volume commodity) reaching equilibrium over time (a price floor).

Again, these are general assumptions that are made in the base case for market dynamics which are difficult to determine over a long term as these markets are relatively under-developed (cellulosic biofuels and biochemicals) and not well understood.
Nevertheless certain qualitative assumptions can be made about each market, but one needs to test how the model decisions are impacted under different trend scenarios. We study the impact of different trends and different CAGR’s under each trend during sensitivity analysis (figure 3-25).

![Figure 3-25: Tornado chart for market parameter sensitivity analysis](image)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Best Case</th>
<th>Worst Case</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ethanol Markets (base case)</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>Succinic Acid, Niche Markets (base case)</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>Succinic Acid, BDO Markets (base case)</td>
<td>1</td>
<td>1</td>
</tr>
</tbody>
</table>

The best case NPVs are observed under a directly proportional price-demand relationship with CAGR ranges from 3-5 percent for each product while the worst cases are observed under inverse proportionality between demand and prices, with the prices decreasing rapidly over time (3-5 percent annually), while demand remains flat, or increases (different scenario trends tested). The tornado diagram above displays the best and worst case values observed all scenarios tested for each product market. We notice that ethanol market variability has the largest impact on portfolio NPV with high upside if prices and demand increase over time and significant downside if prices decrease over time. A similar trend is observed for specialty succinic acid markets although the impact is not nearly as high as ethanol, primarily because the base case demand is assumed to be a lot lower (specialty versus commodity ethanol) that ethanol. Interestingly, the impact of lower prices in the BDO
markets has a much lower downside (from the base case) but appreciable upside if prices go higher over time; succinic acid derived production of BDO almost seems like an option on the biorefinery, implying that the upside potential is significant with disproportionately lower downside risk. One possible reason is that the majority of the profits in the base case are derived from the other two markets (ethanol, specialty succinic acid).

The impact of different market trends are discussed in much greater depth later when we investigate the impact of exogenous uncertainty on strategic design decisions of the studied value chain.

3.5.4 Tax and Financial Parameters

The final set of parameters investigated include government subsidies and cash assistance programs and the cost of capital; specifically, we investigate the impact of no ethanol subsidy for producers and a constant ethanol subsidy (of $1.01 per gallon), the impact of a perpetual and no BCAP program, and the impact of higher interest rate and investor risk premium demanded, on the portfolio NPV. For the base case, ethanol subsidies and BCAP programs are assumed to expire after 5 years.

![Tornado chart for tax and federal subsidy parameter sensitivity analysis](image-url)

**Figure 3-26: Tornado chart for tax and federal subsidy parameter sensitivity analysis**
From the figure, we notice that ethanol credits have a significant impact on portfolio NPV; as was the case with product prices, tax credits have a direct impact on enterprise bottom-line by reducing the payable taxes directly. It should be noted that the tax credits are assumed to be non-refundable, that is, the number of credits applied to the profits can only reduce the tax burden to zero; this is opposed to a refundable tax credit where the enterprise can actually receive payments from the government.

On the other hand, the BCAP program are direct payments to crop producers (biorefiner in our case study), but is constrained by total crop establishment and operating expenses and a hard cap based on congressional funding. For the base case, we assumed that the cap on BCAP is set at $55 million spread over 5 years (~12 percent of total budget, USDA Biomass Crop Assistance Program), with $40 million available in the first 2 years for crop establishment, and $3 million available annually for crop growth, collection, and transportation. Nevertheless, if the biorefiner is able to extend operating cost payments for the entire planning horizon (75 percent of total cost), the upside is significant as it directly reduces the cost of feedstock production.

Finally, variability in the cost of capital was simulated using higher input interest rates on debt and higher investment risk premiums demand by the investors; these parameters are not only used to calculate the cost of capital, but also determine interest payments to debt holders, which impacts the income and cash flow statement of the biorefiner. The impact of the cost of capital to the upside and downside with the upside being catalyzed by lower interest payments and a higher weight given to future cash flows (discount rate), while the opposite scenario (higher interest rates and lower weight for future cash flows) is felt for the downside scenario. From a quantitative perspective, it is hard to model long term values for
cost of capital, as a multitude of factors including future profits for the enterprise, will impact the actual cost of capital. Qualitatively though, we assumed that as the market matures for bioproducts, risk premia and debt lending rates will decrease over time (for optimistic scenarios), while conversely, if the markets do not mature and plant failures exist over time in the aggregate economy, the cost of capital will increase.

3.5.5 Design Parameters

In this section, we provide a summary of varying input parameters such as yields, costs, and prices on design variable selection during optimization; specifically, we will focus on how technologies and spatial configurations change with changing input parameters. Additionally, we will analyze the parameter impact on average annual biomass throughput capacity design and the gross annual sales levels for each product. This exercise is carried out in order to determine what kind of technological investments can be made in each technology configuration in order drive higher value extraction from the respective configuration. We next provide a matrix representation of parameters that were tested and their impact, the coefficients of variations for each parameter, their impact on decision variables, and the selection of technological and spatial parameters that result from each variation.
Table 3-25: Impact of design parameters on portfolio NPV, technology selection and optimal biomass throughput capacity design

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Variance (%)</th>
<th>Optimistic Scenario</th>
<th>Pessimistic Scenario</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>NPV</td>
<td>Average Annual Capacity (tons)</td>
</tr>
<tr>
<td>Energy Cane Availability</td>
<td>+50</td>
<td>+++</td>
<td>+++</td>
</tr>
<tr>
<td>Switchgrass Availability</td>
<td>+50</td>
<td>+</td>
<td>+</td>
</tr>
<tr>
<td>Expected Process Yield</td>
<td>+15</td>
<td>++</td>
<td>+</td>
</tr>
<tr>
<td>Expected Margin</td>
<td>+25</td>
<td>++</td>
<td>+</td>
</tr>
</tbody>
</table>

From the matrix above a couple of observations are important to mention:

1. Increased energy cane availability (or reduced switchgrass availability), along with improvements in expected margins (net after-tax profit as a percentage of total revenue) or reduction in capital costs shifts the choice of processing facility location to the south-central region;

2. Improvement in overall process yield (total product as a percentage of biomass input) or reduction in total capital costs shifts the choice of optimal fractionation-
fermentation technology configuration to dilute acid pretreatment followed by saccharification and separate sugar fermentation.

The first point implies increased energy cane availability can have a significant impact on portfolio NPV, total processing capacity establishment, and spatial design of optimal network. Studying the base case parameters, we included a much larger availability of switchgrass land (CRP land) as opposed to energy cane resource base (sugarcane producing land) consequently creating a bottleneck with respect to energy cane as the major feedstock being processed. If larger quantities of energy cane can be acquired, the impact on value chain profitability and total product output (or biomass throughput capacity) can be significant. This leads us to believe that under no resource constraints, energy cane may be the optimal feedstock choice with switchgrass used as make up.

The second point mentioned above implies that total process yield and equipment capital costs are major bottlenecks for the dilute acid-SSSF technology selection; if higher process yields can be achieved and/or lower capital costs can be guaranteed, the choice of optimal technology can shift towards the acid-SSSF configuration. If we delve deeper into the analysis of yields from each technological system in the configuration, we notice that total fermentable sugar yield from pretreatment is the major difference between AFEX and dilute acid pretreatment. More specifically, we modeled loss of hemicellulosic fraction (solubilization) using dilute acid pretreatment while assuming that the structural integrity of the hemicellulosic fraction is maintained during AFEX. If this situation can be avoided the overall process economics may favor dilute acid more so than AFEX.
The next section summarizes qualitative takeaways from the sensitivity analyses and suggests modeling initiatives that will be undertaken in order to incorporate these results in the development of strategic analytics for the value chain design.

3.6 Conclusions and Takeaways

This section provides a summary of qualitative takeaways from the deterministic process and network design exercise along with sensitivity analyses for process and cost parameters impact the operation and design of the value chain. We first discuss the takeaways from the optimization process:

1. An AFEX-SSCF technology configuration was selected as the optimal fractionation-fermentation technology combination driven by higher sugar (total fermentable) and product yields;
2. The south-central region is selected as the optimal location for processing facility siting driven by access to a large resource base (CRP land for switchgrass), lower permitting costs, and proximity to major product markets (Texas and Louisiana gulf coast) for ethanol and succinic acid;
3. While portfolio NPV is positive, the payback period for investment is estimated to be 16 years necessitating the need for higher margin products in the portfolio (pull forward the payback period) and/or innovative methodologies to provide intermediate cash flow to investors;
4. The energy and carbon performance of the optimal configuration is much better than corn ethanol and (depending on the allocation method employed for succinic acid) standalone facilities for cellulosic ethanol. Additionally, the energy efficiency of the optimal design is comparable to that of crude oil, although the
literature value for sugarcane ethanol are still markedly better than the optimal
design cases;

5. Value chain profitability is derived in part from process yields, and more
specifically fermentation yield for ethanol and total land yield of usable biomass
feedstock;

6. Additionally, higher gross margins for operation, achieved through lower
feedstock and enzyme costs or higher product prices is an important value driver;

7. The existence of tax credits and transfer payment programs through government
agencies is important in providing initial support for value chain design, while
extension of credits and transfer payments beyond the capacity establishment
period can drive much higher product outputs and strategic value;

8. While switchgrass is selected as the major feedstock source for the optimal design
(base case), greater availability of an energy cane resource base can switch the
optimal feedstock, spatial location of processing facility (closer to energy cane
resource base) and have a significant impact on value chain profitability;

9. Achievement of higher fermentable sugar yield using dilute acid pretreatment can
switch the optimal technology configuration from AFEX-SSCF to Dilute acid-
SSSF with only a minor impact on portfolio NPV.

Finally we provide a summary of results from sensitivity analyses and suggest a
strategy for deeper analytics and modeling endeavors in order to model future uncertainty in
parameter evolution and mitigate risks that arise from these uncertainties.
Table 3-26: Qualitative results summary from sensitivity analyses

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Category</th>
<th>Impact**</th>
</tr>
</thead>
<tbody>
<tr>
<td>Process Yield</td>
<td>Product per acre land</td>
<td>Exogenous/Endogenous</td>
<td>High</td>
</tr>
<tr>
<td>Construction Costs</td>
<td>$ per unit capacity</td>
<td>Exogenous</td>
<td>Low</td>
</tr>
<tr>
<td>Energy Load</td>
<td>KJ</td>
<td>Endogenous</td>
<td>Low</td>
</tr>
<tr>
<td>Cost of Goods</td>
<td>$ per unit feedstock</td>
<td>Exogenous</td>
<td>Medium</td>
</tr>
<tr>
<td>Ethanol Prices</td>
<td>$ per unit Product</td>
<td>Exogenous</td>
<td>High</td>
</tr>
<tr>
<td>Credits and Subsidies</td>
<td>$ per unit Product</td>
<td>Exogenous</td>
<td>High</td>
</tr>
</tbody>
</table>

**Low = [0, 50%)**  
**Medium = [50%, 100%)**  
**High = [≥ 100%)**

Based on the above table it can be concluded that product prices and availability of subsidies are the highest impact exogenous parameters, while overall value chain yields (biomass, sugar and fermentation) are the highest impact process parameters. Consequently, it should be imperative to control these parameters for an operating biorefinery; the process yields can be controlled by developing good operating practices and driven higher through investment in research and development. Exogenous parameters are harder to control, and strategies to mitigate their impact should be developed. In the next chapter I will delve into a model-based strategic decision support strategy in order to mitigate the impact of exogenous price and margin risk on a biorefinery’s design and operation.
4. CAPACITY DESIGN UNDER EXOGENOUS UNCERTAINTY USING DECISION OPTIONS MODELING AND OPTIMIZATION

4.1 Introduction and Problem Re-statement

Following the deterministic technology and spatial design problem introduced and analyzed in the previous chapter, this chapter will focus on modeling and optimizing strategic design decisions under endogenous and/or exogenous uncertainty. As a demonstration of the decision analysis framework, we will pick parameters that will be modeled considering uncertainty in their dynamic evolution. Our choice of uncertain parameters will be based on the analyses that were carried out in the previous chapter and certain qualitative assumptions regarding the value chain and market dynamics. We will suggest a methodology to incorporate stochastic optimization techniques into the decision-making framework and moreover study the impact of uncertainty on the optimized design using Monte Carlo simulations. We begin by re-stating the case study results obtained from the previous section and describing how we will proceed with the decision analysis in order to add additional value and granularity to the analytical framework.

Problem Restatement

From the previous optimization and analyses endeavors the optimal spatial configuration established one processing site in the southwest region of Louisiana that utilized both switchgrass and energy cane (66 and 33 percent) sourced from within a 100 mile radius of the processing site, with majority of sources located within a 50 mile radius. A technology configuration comprising of AFEX-SSCF was found to be optimal with distillation and molecular sieves used for ethanol recovery and purification while electrodialysis followed by evaporative crystallization is used for succinic acid recovery
operations. An optimal capacity of 25 million annual gallons for ethanol is found to be optimal while optimal succinic acid capacity is found to be 17,000 annual tons. Texas and Louisiana Gulf coast are chosen as optimal markets to serve for both products with a railroad-based transportation mode for product movement. The portfolio NPV that is obtained using the optimal design comes in at approximately $58 million with a payback period of approximately 16 years.

Following sensitivity analyses it was determined that ethanol prices have a significant impact on portfolio profitability along with direct raw material costs (COGS) and process yields. While process yields are much easier to control for the biorefiner through better operating practices and technological innovation (RD&D), ethanol prices and input costs are exogenous parameters that are set in the open market, making it harder for the biorefiner to control the evolution of these parameters.

For the demonstration of modeling and optimizing design under uncertainty the following assumptions are made to setup the case study:

1. We assume that the optimal spatial and technological configuration obtained from deterministic optimization will be enacted in real life by the enterprise;
2. Equipment costs for various sizes, permitting, engineering and construction costs can be estimated within a reasonable margin of error prior to construction through vendor and contractor quotes;
3. We assume that a mix of energy cane and switchgrass can be obtained from land owners and farmers within a 50 mile radius; in order to reduce model complexity, we will not model each source for each feedstock type individually. Rather, we
will assume a total acreage available and an average yield (tons per acre) for all biomass types combined. Addition of an index to select the type of feedstock is straightforward (as was done for deterministic optimization) but given the goal of this model is to derive optimal capacity design plans under market uncertainties we choose to ignore the biomass selection aspect for the current case study;

4. It is assumed that the biorefiner will provide funding for crop establishment and pay rent on land that is contracted based on opportunity costs for each type of biomass;

5. The landowner will be responsible for funding operating costs for crop growth and harvesting but will be compensated by the biorefiner (for costs and additional profit margin) based upon the quantity of biomass delivered; the structure on the supply contract and the pricing for the feedstock is discussed in more detail later on in this chapter.

Given this setup the biorefiner wishes to use the decision analysis framework in order to design and choose multiple strategic pathways in order to build network capacity over time horizon of approximately 15 years. The biorefiner realizes that the markets for products (supply/demand/prices) are highly uncertain and wishes to develop strategic options detailing how to proceed with capacity establishment and future expansions under different evolutions of market scenarios. Additionally, the biorefiner wants to evaluate if they should enter into long term supply agreements to supply refiners with ethanol for blending, supply chemical processors with succinic acid as a feedstock for value addition. With regards to succinic acid, the niche market demand provides a higher price point for sales but also provides low demand growth as markets are relatively mature with most biobased product demand driven
by displacement of the petroleum-derived succinic acid. Additionally, butanediol provides an attractive high growth market for succinic acid as a feedstock although pricing remains an issue as downstream polymer processors demand lower price points in addition to a long term commitment by the biorefiner to supply biobased succinic acid. Consequently, the biorefiner wants to evaluate which succinic acid markets are best to serve, estimate what quantities of demand should be served in each market, and if long term supply contracts are a viable option to sign (assuming that production quality constraints will be satisfied). Additionally, the biorefiner has the ability to invest in a research, development, and demonstration facility with 3 different levels of investment which are predicted to improve process yields at varying percentages from current plant yield; the enterprise wants to establish what investment levels are the most optimal under the assumption that the investment level will almost certainly lead to the expected yield improvement.

This section will describe the model that is used to describe the capacity design problem using decision options. The model is formulated as a stochastic mixed integer based linear program (MILP) with a 14-year planning horizon and bi-annual time steps, yielding a total of 7 time steps. The choice of the time horizon is arbitrary and is based off the payback period that was derived in the previous section (16 years). Special emphasis is laid on the strategic aspects of capacity design leading to a long-term planning horizon. Bi-annual time steps were chosen to represent a full business cycle so that shorter term fluctuations in market conditions are averaged out. The market prices and demands for bioproducts were selected as the uncertain parameters (exogenous uncertainties) that affect the capacity plan going forward; we want to reiterate that there are multiple sources of uncertainty that are endogenous in nature such as biomass supplies and production yields. The current modeling
endeavor is meant to introduce a capacity design problem for prospective biorefineries using decision options and further literature will be submitted by our research group describing the incorporation of endogenous uncertainties into the design decisions of the enterprise.

For the current setup, we assume that prices and demands for bioproducts are impacted primarily by crude oil prices as oil is the primary determinant of alternative transportation fuel markets. We assume that average, bi-annual crude oil prices can move up or down with a given probability from the current time period to the next, yielding a Markov chain based decision tree. Each node in the decision tree is represented as a price scenario for crude oil (and consequently for bioproduct markets) and over the 7 time periods this yields a total of 64 oil price scenarios. The decision tree is designed as a non-recombinant decision tree (Wang et al, 2005), where the trajectory followed by the price is as important as the point estimate of the price at any given point. The decision tree is further illustrated and populated with numbers in the Market Parameters subsection.

The overall model is broken into several sub-models for ease of description, which include biomass production model, a biomass conversion and product recovery model, a market model, a financing and tax model, a cash flow model, and a decision options model. The process systems’ model is derived from the previously stated model (deterministic optimization) with technology and spatial binary variables fixed as the optimal solution obtained from model optimization discussed in the previous chapter. The financing and tax model and the cash flow optimization model, on the other hand, are reformulated along with a market model to forecast product supply/demand/prices. The novelty in the proposed framework is the modeling and valuation of decision options which describe managerial flexibility in making future decisions based on evolution of market scenarios. The process
models for capacity design of biomass production and conversion, as described previously, are integrated with the financing and cash flow models using capital and operating costs to describe the processing and logistical activities; the market model describes the price and demand evolution of the uncertain parameters and are integrated with (1) the process models using a sales variable in a mass balance on the final products, and (2) with the cash flow and financing models using demand and capacity constraints; the decision options model is formulated using binary integer constraints to represent actions taken by the enterprise (regarding RD&D investments, capacity investments, and signing of feedstock supply and product sales contracts) to execute a particular option. The next few subsections are dedicated to a brief description of the modeling equations and corresponding parameters that impact the model. We choose to restate the process systems’ models in order to include scenario based equations, which are different from the deterministic For equations described henceforth, table 4-1 provides subscript descriptions.

<table>
<thead>
<tr>
<th>Subscript</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>plt</td>
<td>Type of production platform</td>
</tr>
<tr>
<td>p</td>
<td>Type of product</td>
</tr>
<tr>
<td>t</td>
<td>Time</td>
</tr>
<tr>
<td>s</td>
<td>Scenario</td>
</tr>
</tbody>
</table>

4.2 Design of Decision Options

There are an infinite number of decision options that can be embedded in a long-term capacity design problem such as the present case study. A prospective biorefinery is particularly amenable to design using decision options for the following reasons:

1. A lignocellulosic biorefinery is based on a new, emergent technology platform (biochemical) whose commercial viability is still not proven;
2. A large, upfront capital investment is required to establish infrastructure for producing and converting biomass to value-added biofuels and biochemicals thus elevating the capital risks in investment;

3. The cash flow power of prospective biorefineries is still unclear, with exogenous market uncertainties, endogenous yield uncertainties, and competitive uncertainties from rival products such as fossil-derived fuels and chemicals.

In such a scenario, it is advisable and even prudent, to move with caution in building out the infrastructure for commercial production of biofuels and biochemicals. From an investor perspective, valuation of such emergent technologies is still in its early stages of development and multiple methods have been proposed to incorporate their risk characteristics into valuation. A commonly used method is discounted cash flow analysis where projected cash flows from commercial investments are discounted with a large discount factor to reflect a riskier investment. From a theoretical perspective this may work, but in reality, the future value of project investment is not correctly represented in modeling results with very little insight into how project profitability can be improved. Due to the high levels of uncertainty in project investment, decision making flexibility in future periods holds very high intrinsic value, and the valuation of this flexibility can provide a better, more realistic estimate of the future worth of investing in a renewable energy technology that is still in its nascent stages of development.

Decision options provide a very convenient means of building decision making flexibility into project design, while also providing a robust methodology to value a project where flexible decision making is of prime importance. In the current formulation we utilize a combination of parameter restrictions, and binary and continuous variable constraints, to
design decision making flexibility in our capacity design problem. Each variable represents an option “on” or “in” the project investment while parameter values such as process yields are restricted if options are not exercised. An option “on” the project represents a flexible decision on the implementation of the entire project, where the project is treated as a black box (Wang and Neufville, 2005). An option “in” the project represents flexibility that is engineered into the system where the project treatment is more granular and requires a deeper understanding of the system itself (Wang and Neufville, 2005). We will model decision options both “on” and “in” the prospective biorefinery. The options modeled here are a first attempt to represent and value flexibility in future biorefinery designs; we believe that this lays out a substantial basis to build more modeling capabilities and greater granularity in representing macro- and micro-level options for process design of biorefineries.

1. Deferral Option:
   a. Decision option “on” the project;
   b. Can be thought of as a management’s decision to hold off investing in new capacity given poor market conditions on process uncertainties that need resolution;
   c. A binary variable is used to represent investment in processing capacity;
   d. Investment in project can be delayed given market uncertainties;
   e. The deferral option is counter-balanced by a rise in capital costs assuming that demand for technologies and general cost inflation will increase investment costs for land and equipment purchase;
   f. Additionally, we modeled market share losses (lost demand) as a function of time, if market demands are not served;
g. This setup will enable us to compare the decision to invest now under greater market uncertainty, against the decision to wait and let market uncertainties reveal themselves with a reduction in addressable market demand;

h. Option expiration time is set arbitrarily, for the current study, at 6 years (3 time steps) from the start of the planning horizon.

2. Research, Development and Demonstration Option:

i. Decision Option “on” the project;

ii. Can be thought of as management’s decision to invest in research and development to improve product yields before investing in commercial production capacity;

iii. Research here can be targeted towards any process system in order to improve overall process yields for the production process;

iv. A binary integer variable is used to represent investment in RD&D;

v. Model is given a choice between investing in RD&D or establishing commercial capacity without and RD&D;

vi. Without RD&D investment, a 33 percent yield improvement is realized over the time horizon as a consequence of operating efficiencies (assumption);

vii. The investment in RD&D is modeled as a learning option where an additional 33 percent improvement in overall process yield is achieved over the time horizon as compared to the yields without RD&D;

viii. Option expiration time is set arbitrarily, for the current study, at 4 years (2 time steps) from the start of the planning horizon, that is, no investment is RD&D is allowed after the 2\text{ND} time step.
3. Flexibility Option
   i. Decision Option “in” the project;
   ii. Can be thought of as management’s decision to optimize capacity levels based on expected market scenarios;
   iii. As opposed to stochastic programming where capacity decisions are made deterministically and utilization rates are then varied based on market evolution, a flexibility option models management’s ability to invest in optimal capacity levels based on current and expected market scenarios;
   iv. This implies that given current values of a stochastic parameter, design decisions can be made flexibly based on the current values of stochastic parameter(s). For capacity design, this means that the level of capacity that is installed will be different for different price levels (stochastic parameter) of ethanol and succinic acid;
   v. A continuous capacity establishment variable is used to represent the flexibility option wherein, the optimal value for the design variable can be different for different price levels of crude oil (correlated with ethanol and succinic acid prices and demand).

4. Sequential Growth Option:
   a. Decision option “in” project;
   b. Can be thought of as management’s decision to invest in additional, innovative plant designs that enable incremental addition of production capacity with improving market conditions;
   c. This is juxtaposed to investing in commercial capacity right away instead of ramping up utilization rates as market conditions evolve;
d. Model given a choice between a growth-oriented and inflexible platform using a binary selection variable;

e. Continuous capacity design and investment level variables are used to distinguish capacity establishment and expansion decisions for each platform;

f. Growth-oriented platform allows production of multiple products with no charges for switching biomass allocation amounts towards different products;

g. Growth-oriented platform has a 25 percent larger upfront capital cost than the inflexible platform, in terms of additional land purchase and construction and engineering expenses;

5. Contract Option

a. Decision option “on” project

b. Can be thought of as management’s decision to sign a long term sales agreements with downstream processors to supply finished products;

c. This is juxtaposed to selling products in spot markets at spot prices which are inherently uncertain and show a great deal of variability depending on spot supply and demand for the product;

d. On the other hand, signing long term agreements can lock the enterprise into price and quantity agreements that may prove to be unfavorable if future scenarios do not evolve as expected. For example, product sales agreements in a certain price range enable an enterprise to mitigate spot price volatility in a commodity market but an appreciation in spot prices can hamper an enterprise from taking advantage of higher spot prices as they are locked into a supply agreement which gives the counter-party the first right on plant output. Conversely, setting a price floor through a contractual
agreement can shield the enterprise from depressed price scenarios in the spot markets during unfavorable supply/demand and macro-economic conditions;

The next sections describe each sub-model that comprises the decision options optimization model, with each decision variable and/or parameter tabulated and their input values provided.

4.3 Biomass Production Model

The biomass production model assumes that our startup enterprise can contract land from local farmers and landowners for the dedicated production of biomass using energy crops. The capital costs for land development and crop establishment are also assumed by the enterprise. The enterprise pays a price for purchasing biomass from the farmer to compensate the operator for overhead and fertilizer/nutrient/herbicide costs (operating expenses). The amount of biomass that is available for purchase is based on an expected yield from the land modeled in tons per acre of land. It is assumed that biomass yields increase over the time horizon, following an experience curve, due to learning effects from commercial operation. The establishment costs for the energy crop are capitalized and depreciated using a 6-year accelerated depreciation schedule, while the operating cost payments are made to the land operator on a variable payment schedule based on the total amount biomass delivered, and transportation expenses based on a $20 per dry ton base rate plus any adjustments for crude oil price scenario realizations.

\[ BMP_{t,s} \leq Land_{t,s}^{util} \times YLD_{t}^{BM} \]  \hspace{1cm} (4.1)

\[ Land_{t,s}^{util} \leq TotLand_{t,s}^{Constr} \]  \hspace{1cm} (4.2)
\[ \text{TotLand}_{t, s}^{\text{Contr}} = \text{TotLand}_{t-1, s}^{\text{Contr}} + \omega_1 \times \text{NewLand}_{t, s} + \omega_2 \times \text{NewLand}_{t-1, s} \]  

(4.3)

\[ \text{Capex}_{t, s}^{BM} = E\text{Cost}_t \times \text{Land}_{t, s}^{\text{Contr}} \]  

(4.4)

\[ \text{Ope}_{t, s}^{BM} = C_{\text{Var}, t, s}^{BM} \times \text{BMP}_{t, s} + C_{\text{Fixed}, t, s}^{BM} \times \text{TotLand}_{t, s}^{\text{Contr}} + C_{t, s}^{\text{Export}} \]  

(4.5)

<table>
<thead>
<tr>
<th>Parameter/Variable</th>
<th>Description</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( B\text{MP}_{t, s} )</td>
<td>Total Biomass Purchased in tons</td>
<td>Variable</td>
</tr>
<tr>
<td>( \text{Land}_{t, s}^{\text{Util}} )</td>
<td>Land utilized</td>
<td>Variable</td>
</tr>
<tr>
<td>( YLD_{t, s}^{BM} )</td>
<td>Net biomass yield from land</td>
<td>6 tons per acre at ( t=1 )</td>
</tr>
<tr>
<td>( \text{TotLand}<em>{t, s}^{\text{Contr}}, \text{NewLand}</em>{t, s}^{\text{Contr}} )</td>
<td>Cumulative (total) and new land contracted</td>
<td>Decision Variable</td>
</tr>
<tr>
<td>( \omega_1, \omega_2 )</td>
<td>Fraction of contracted land available for harvesting</td>
<td>10%, 90%</td>
</tr>
<tr>
<td>( E\text{Cost}_t )</td>
<td>Unitary establishment costs for contracting land</td>
<td>$275 per ac at ( t=1 )</td>
</tr>
<tr>
<td>( \text{Capex}_{t, s}^{BM} )</td>
<td>Total cost of establishing a crop on contracted land</td>
<td>Decision Variable</td>
</tr>
<tr>
<td>( C_{\text{Var}, t, s}^{BM}, C_{\text{Fixed}, t, s}^{BM}, C_{t, s}^{\text{Export}} )</td>
<td>Unitary costs of biomass (variable, fixed, transport)</td>
<td>Calculated $60 per acre $20 per ton</td>
</tr>
<tr>
<td>( \text{Ope}_{t, s}^{BM} )</td>
<td>Total operating costs payable to land operator</td>
<td>Variable</td>
</tr>
</tbody>
</table>

### 4.4 Process Systems Model

The biomass conversion and product recovery model is comprised of a capacity design formulation, and conversion formulation, and a product recovery formulation. The capacity design model proposed in the previous chapter (deterministic optimization) is used here to design production capacities under different price-demand trajectories. A 2 year construction delay (from the time of investment) is assumed for any new capacity to come online; in order to model investment in research, development and demonstration (RD&D), we indexed capacity investments (index plt) with respect to the level of investment in RD&D, which in turn determined the maximum expected yield that can be achieved.
following the RD&D investment. This point is demonstrated using the following equation set:

\[ CPBVE_{plt,t,s} \times Cap^{LB}_{p,t,s} \leq CapExp^{Biomass}_{plt,t,s} \leq CPBVE_{plt,t,s} \times Cap^{UB}_{p,t,s} \]  
(4.6)

\[ CPBVE_{plt,t,s} \leq \sum_{t \leq t} RDDBV_{plt,t,s} \]  
(4.7)

\[ CSBV_{p,t,s} \times Cap^{LB}_{p} \leq CapExp^{Recovery}_{p,t,s} \leq CSBV_{p,t,s} \times Cap^{UB}_{p} \]  
(4.8)

\[ CSBV_{p,t,s} \leq \sum_{plt,t < t} CPBVE_{plt,t,s} \]  
(4.9)

In the equation set above, \( RDDBV_{plt,t,s} \) is the RD&D investment variable (binary) while \( CPBVE_{plt,t,s} \) is the biomass capacity establishment variable (binary); we match the investment level in RD&D using the index plt, wherein, choice of plt will determine the investment and the subsequent yield improvement (units product per unit biomass) that can be achieved through the investment. Equation 6 is used to constrain the capacity establishment variable by the RD&D binary variable stating that “An investment in RD&D is necessary before any capacity can be established”. Equation 8 is used to design recovery capacity for each product while equation 9 constrains recovery capacity establishment stating that “biomass capacity has to be established before recovery capacity can be established”. In order to match the yield with the RD&D investment level, the yield parameter was indexed to plt with maximum achievable yield improvement being unique to each plt (equation 10 below).

\[ BMP_{t,s} \times YLD_{p,plt,t}^{prod} = Product_{p,t,s}^{eff} \]  
(4.10)

\[ Product_{p,t,s}^{rec} = \phi_{p} \times Product_{p,t,s}^{eff} \]  
(4.11)
Equations 10 and 11 represent the conversion and recovery efficiencies for each product processed using the optimal technology configuration; the yield is a time varying parameter with improvements over time determined by the investment level in RD&D (represented by the index plt). Equation 12 is a storage loss adjusted mass balance on each product produced. We assume that each product can be sold into the spot markets or long term contract for supplying bioproducts to downstream processors can be signed (equation 13); downstream processors for ethanol include blenders who blend ethanol with gasoline, while those for biosuccinic acid are represented by biopolymer or specialty chemical manufacturers. We assume that spot markets can be tapped by the biorefinery at any time with any scale of sales (equation 15), but for contractual agreements, the biorefinery has to supply a minimum amount of product to downstream processors every time period after the supply contract is signed (equation 14). The contract option is represented by a binary variable ($PSBV_{p,t,s}$) in equation 14. The exercise of this option is juxtaposed to deferring the exercise of the option; from a modeling perspective we model a declining market share ($MktShr_{p,t} \in [0,1]$) in equation 14 implying that the more the option exercise is delayed, the lower the addressable contractual market will be for the biorefiner. Such a formulation balances the upside of deferring signing a long term sales agreement against a loss of serviceable demand (lost revenue).
The capital investment in equipment was divided into three categories; (1) fixed investment in purchase and preparation of land, (2) direct equipment costs that are derived from Kazi et al (2010) describing purchase prices of processing equipment, and (3) construction, engineering, and permitting costs as a percentage of direct equipment costs. The operating expenses were sub-divided into two categories; (1) variable operating costs related to purchase of enzymes, nutrients, microbes, and other ancillary raw materials like ammonia, waste disposal costs (digestion enzymes), and utility generation costs, and (2) fixed costs related to marketing, selling, general and administrative costs, labor costs, and equipment and instrument maintenance costs. Additionally, it was assumed that 15 percent of net asset investment was used as re-invested capital to replace/maintain operational units.

\[
Capex_{p,t,s}^{RDD} = CapCost_{p,t}^{RDD} \times RDDBV_{p,t,s} \tag{4.16}
\]

\[
Capex_{t,s}^{Land} = LANDBVE_{t,s} \times FC_{t}^{Land} \tag{4.17}
\]

\[
Capex_{p,t,s}^{eqp} = \sum_{p} (BV_{p,t,s}^{Eqp} \times FC_{p,t}^{Eqp} + Capacity_{p,t,s}^{Exp} \times VC_{p,t}) \tag{4.18}
\]

\[
Capex_{t,s}^{TIDC} = \sum_{p,t} Capex_{p,t,s}^{RDD} + Capex_{t,s}^{Land} + Capex_{t,s}^{LP} + Capex_{t,s}^{eqp} + Capex_{t,s}^{C&E} \tag{4.19}
\]

\[
FCI_{t,s} = Capex_{t,s}^{Cont} + Capex_{t,s}^{TIDC} \tag{4.20}
\]

\[
Capex_{t,s}^{WC} = 0.15 \times FCI_{t,s} \tag{4.21}
\]

\[
TCI_{t,s}^{growth} = FCI_{t,s} + Capex_{t,s}^{WC} \tag{4.22}
\]

\[
VarOpex_{p,t,s}^{process} = \left\{c_{t,s}^{eq} + c_{t,s}^{nt} + c_{t,s}^{other} \right\} \times Product_{p,t,s}^{eff} + \left\{c_{t,s}^{utility} + c_{t,s}^{waste} \right\} \times Product_{p,t,s}^{rec} \tag{4.23}
\]
\[ FxOpex_{t,s}^{\text{process}} = \{C_{t,s}^{SGA} + C_{t,s}^{\text{labor}} + C_{t,s}^{\text{mtn}}\} \]  
\[ \text{Capex}_{t,s}^{\text{reinvest}} = 0.10 \times (\text{Capex}_{t,s}^{\text{Eqp}}) \]

### Table 4-3: Parameters and variables capital investment model

<table>
<thead>
<tr>
<th>Parameter/Variable</th>
<th>Description</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \text{Capex}<em>{t,s}^{\text{process}}, \text{Depr}</em>{t,s}^{\text{process}} )</td>
<td>Capital and depreciation costs</td>
<td>Decision Variable</td>
</tr>
<tr>
<td>( \text{CapCost}_{t,s}^{\text{Eqp}} )</td>
<td>Equipment costs</td>
<td>Kazi et al., 2010, Lynd et al. 2005 (adjusted to $2010 using CPI)</td>
</tr>
<tr>
<td>( \text{CapCost}_{t,s}^{\text{Engr}} )</td>
<td>Engineering, Construction, and permitting costs</td>
<td>50% (single product, inflexible), 75% (multiple, inflexible), 100% (multiple, flexible)</td>
</tr>
<tr>
<td>( \text{CapCost}_{t,s}^{\text{Fixed}} )</td>
<td>Fixed investment in land acquisition and preparation</td>
<td>$10 million (single, inflexible), $20 million (multiple, inflexible), $30 million (multiple, flexible)</td>
</tr>
<tr>
<td>( \text{CapIncr}_{t,s} )</td>
<td>Increment in capacity</td>
<td>Decision Variable</td>
</tr>
<tr>
<td>( \text{VarOpex}<em>{t,s}^{\text{process}}, \text{FxOpex}</em>{t,s}^{\text{process}} )</td>
<td>Variable and Fixed operating costs</td>
<td>Decision Variable</td>
</tr>
<tr>
<td>( \text{Capex}_{t,s}^{\text{reinvest}} )</td>
<td>Reinvestment of capital to maintain operations</td>
<td>Decision Variable</td>
</tr>
<tr>
<td>( C_{t,s}^{\text{Eq}}, C_{t,s}^{\text{mtn}}, C_{t,s}^{\text{labor}}, C_{t,s}^{\text{other}} )</td>
<td>Cost of enzymes, nutrients, and other raw materials</td>
<td>Kazi et al., 2010, Lynd et al. 2005 (adjusted to $2010 using CPI)</td>
</tr>
<tr>
<td>( C_{t,s}^{\text{utility}}, C_{t,s}^{\text{waste}} )</td>
<td>Cost of utilities and waste processing</td>
<td>Kazi et al., 2010, Lynd et al. 2005 (adjusted to $2010 using CPI)</td>
</tr>
<tr>
<td>( C_{t,s}^{\text{SGA}}, C_{t,s}^{\text{labor}}, C_{t,s}^{\text{mtn}} )</td>
<td>Fixed selling and administrative costs, direct labor costs, cost of daily maintenance</td>
<td>Kazi et al., 2010, Lynd et al. 2005 (adjusted to $2010 using CPI)</td>
</tr>
</tbody>
</table>

#### 4.5 Financial Model

The Financing cash flow statement was used as a model to represent the capital structure of the biorefinery. A cash balance was used as the governing equation. Debt and equity capital along with government grants were assumed to be the possible sources of capital for capacity investment. Debt capital is controlled by an upper bound on total availability and a debt to total capital ratio which are set arbitrarily here, but are usually a function of enterprise’s appetite for risk and their cash flows. Govern grants are controlled by a cost sharing constraint, where total grant has to matched by total capital that is raised, at the very least. As a part of the capital structure, we assumed that equity investors are enticed by
providing a tax credit based securitization on equity capital (Wiser and Pickle, 1997); in such a formulation, the local and federal tax credits for investment and production are passed onto the equity investors instead to enhancing enterprise cash flows. The purpose of such a formulation is 3-fold; (1) “sweetens the deal” for equity investors by providing guaranteed cash flows, (2) reduces required rate of return (discount rate for cash flows), and (3) imparts much realism to the model as this kind of capital structure has been utilized in solar and wind energy project investments (DeVillar, 2010; Delony, 2007).

\[ CFF_{t,s} = Debt_{t,s}^{new} + Grant_{t,s} + \sum_{eq} Equity_{t,s}^{new} - Debt_{t,s}^{repay} \]  
(4.26)

\[ Debt_{t,s}^{tot} = Debt_{t-1,s}^{tot} + Interest_{t,s} + Debt_{t,s}^{new} - Debt_{t,s}^{repay} \]  
(4.27)

\[ Equity_{eq,t,s}^{tot} = Equity_{eq,t-1,s}^{tot} + Equity_{eq,t,s}^{new} - Equity_{eq,t,s}^{buyback} \]  
(4.28)

\[ Grant_{t,s}^{tot} \leq \min[Grant_{ts}^{max}, Debt_{t,s}^{tot} + \sum_{eq} Equity_{eq,t,s}^{tot}] \]  
(4.29)

Additionally, a minimum cash balance constraint was employed and set at 2 times the debt interest due at the end of every period (Interest Coverage Ratio), and interest payments are mandated every time period as the minimum debt service bound. A balance sheet constraint was imposed to assure that the biorefinery assets were funded through debt, equity, and retained earnings, where retained earnings is calculated as the net income adjusted for dividend payments to equity investors (tax benefits). The tax-related cash flow were divided into 3 groups (equation 30); (1) investment related tax credits modeled as a cash inflow, (2) production tax credits modeled as an inflow, and income tax expenses modeled as an outflow. Investment credits were further divided into R&D and renewable energy investment credits (federal) and green jobs credits (state), while production credits were divided into
biofuel producer tax credits and emission mitigation credits. Additionally, the investment tax credits were realized based upon the depreciation schedule for capital investments in research and development and processing equipment. The overall tax cash flow formulation is shown below where tax assets are created through tax deductions, tax deferrals for operating losses, and tax credits; it is assumed that tax deferrals can be carried forward and used to reduce tax gross taxable income (Equation 34) for that period as is the case for depreciation-based deduction (equation 31). Additionally, we assume that the tax credits can be carried forward and be used optimally to reduce the payable tax burden for the enterprise (equation 35); we assume that all credits earned are non-refundable in nature, that is, they can only reduce the tax burden of the enterprise to zero (the enterprise can’t get money back from the government in the form of refundable credits). Equation 31 is the familiar earnings equation (before interest and taxes but after depreciation related deductions, $EBIT_{t,s}$); equation 32 Calculate the earnings before taxes (EBT) while equation 33 imposes that taxable earnings cannot be negative (implying an operating loss leading to the creation of a tax deferral asset ($tax_{t,s}^{def,er}$); equations 36-38 are recursive equations to track the amount of tax assets (net amount) held by the enterprise at the end of each period, adjusted for any new tax assets and any previous assets that are utilized. Finally, equation 39 keeps a track of the total tax assets that the enterprise possesses; these assets can be used at any time for payment to investors in order to provide them with a stable cash flow stream while they wait for the production facility to generate a return on their investment (tax equity investors).

$$tax_{t,s}^{cred} = T_{C,t,s}^{mit} E_{M,t,s}^{recyl} + \sum_p T_{C,p,t,s}^{prod} Product_{p,t,s}^{rec} + T_{C,t,s}^{inv} Depr_{t,s}^{Eqp} + T_{C,t,s}^{RND} Depr_{t,s}^{RND}$$

(4.30)
\[ EBIT_{t,s} = Rev_{t,s}^{\text{tot}} - Cost_{t,s}^{\text{tot}} - tax_{t,s}^{\text{deduct,release}} \] (4.31)

\[ EBIT_{t,s} = EBIT_{t,s} - Interest_{t,s} \] (4.32)

\[ EBIT_{t,s}^{\text{taxable}} = EBIT_{t,s} + tax_{t,s}^{\text{defer}} \] (4.33)

\[ tax_{t,s}^{\text{payable}} = (EBIT_{t,s}^{\text{taxable}} - tax_{t,s}^{\text{defer,release}}) \times (1 - tax^{\text{rate}}) \] (4.34)

\[ tax_{t,s}^{\text{net}} = tax_{t,s}^{\text{payable}} - tax_{t,s}^{\text{cred,release}} \] (4.35)

\[ tax_{t,s}^{\text{deduct,balance}} = tax_{t-1,s}^{\text{deduct,balance}} + Dep_{t,s}^{\text{tot}} - tax_{t,s}^{\text{deduct,release}} \] (4.36)

\[ tax_{t,s}^{\text{cred,balance}} = tax_{t-1,s}^{\text{cred,balance}} + tax_{t,s}^{\text{cred}} - tax_{t,s}^{\text{cred,release}} \] (4.37)

\[ tax_{t,s}^{\text{def,release}} = tax_{t-1,s}^{\text{def,release}} + tax_{t,s}^{\text{def}} - tax_{t,s}^{\text{def,release}} \] (4.38)

\[ tax_{t,s}^{\text{assets,tot}} = tax_{t,s}^{\text{deduct,balance}} + tax_{t,s}^{\text{cred,balance}} + tax_{t,s}^{\text{def,release}} \] (4.39)

**Table 4-4: Parameters and variables in financial and tax model**

<table>
<thead>
<tr>
<th>Parameter/Variable</th>
<th>Description</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( CFF_{t,s} )</td>
<td>Financing cash flows</td>
<td>Decision Variable</td>
</tr>
<tr>
<td>( Debt_{t,s}^{\text{tot}}, Interest_{t,s}^{\text{tot}}, Debt_{t,s}^{\text{new}}, Debt_{t,s}^{\text{repay}} )</td>
<td>Debt, interest, new borrowings, repayments</td>
<td>Decision Variable</td>
</tr>
<tr>
<td>( Equity_{t,s}^{\text{tot}}, Equity_{t,s}^{\text{new}}, Equity_{t,s}^{\text{buyback}} )</td>
<td>Total equity, new equity raise, equity repurchases</td>
<td>Decision Variable</td>
</tr>
<tr>
<td>( Grant_{t,s}^{\text{tot}} )</td>
<td>Total government grants</td>
<td>Decision Variable</td>
</tr>
<tr>
<td>( Grant_{t,s}^{\text{max}} )</td>
<td>Maximum grants available</td>
<td>$40 million (t=1,2); $20 million (t=3,4); None Thereafter;</td>
</tr>
<tr>
<td>( TC_{t,s}^{\text{mit}}, TC_{t,s}^{\text{prod}}, TC_{t,s}^{\text{inv,GI}}, TC_{t,s}^{\text{BND}} )</td>
<td>Credits for mitigation, production, green jobs investment, and R&amp;D</td>
<td>$20 per ton CO(_2) at t=1; $1.01 (t=1,2); $0.56 (t=3,4); $0 thereafter; 10 percent of total investment; 40 percent of total R&amp;D cost;</td>
</tr>
<tr>
<td>( tax^{\text{rate}} )</td>
<td>Tax rate (state and federal combined)</td>
<td>40 percent</td>
</tr>
</tbody>
</table>
The carbon credit was assumed to be a function of stochastic crude prices (an assumption) at 2.5 percent indicating that higher crude prices will drive traded carbon prices higher. The green jobs and renewable energy investment credits were assumed to expire after the third period (years 5-6) under the assumption that the bio-industry will reach an inflection point where specific tax breaks for investment will be withdrawn, while the R&D credit was assumed to remain over the planning horizon.

4.6 Objective Function

The objective function chosen here was the discounted value of the biorefinery to all equity investors (equation 41); this was done in recognition of the fact that for feasibility of the project, equity capital will be necessary for the build out. Maximization of the prospective equity value of the project can then used as a good metric to determine the value of the biorefinery to equity investors. The equity value was determined using the projected free cash flows to equity (equation 40) that would result for the optimal capacity design of the biorefinery. Additionally, recognizing that equity investors may elect to hold onto their investment in the project beyond the planning horizon, we also calculated a terminal value of the project beyond the horizon (equation 43), based on an expected growth rate in free cash flows (equation 42). Finally, a salvage value (equation 44) was determined using the total capital investment (over the planning horizon) less the depreciation costs. The terminal and salvage values were weighted by a probability of successful operation and failure (bankruptcy) beyond the planning horizon, respectively, and added to the discounted equity value (equation 45); the probability weighted sum of the terminal and salvage values denotes the expected value of the biorefinery to all stakeholders beyond the planning horizon (equation 46).
\[ FCFE_{t,s} = Rev_{t,s}^{\text{contr}} + Rev_{t,s}^{\text{cspot}} - Opex_{t,s}^{\text{tot}} - Tax_{t,s}^{\text{net}} - Debt_{t,s}^{\text{net}} + Dividend_{t,s} \]

(4.40)

\[ EQV_{s} = \text{prob}_{T,s} \times \sum_{t} \frac{FCFE_{t,s}}{(1+\text{E}[\text{ROE}]_{T})^{t}} \]

(4.41)

\[ EarningPower_{s} = \frac{1}{T} \sum_{t} (Rev_{t,s}^{\text{tot}} - Opex_{t,s}^{\text{tot}} - Interest_{t,s}) \times (1 - \text{tax}^{\text{rate}}) \]

(4.42)

\[ TV_{s} = \frac{\text{prob}_{T,s} \times EarningPower_{s} \times (1+GR)}{E[\text{ROE}]_{T}-GR} \]

(4.43)

\[ SV_{s} = \frac{\text{prob}_{T,s} \times EarningPower_{s} \times (1+GR)}{E[\text{ROE}]_{T}-GR} \times \sum_{t} (\text{Capex}_{t,s}^{\text{tot}} - \text{Depr}_{t,s}^{\text{tot}}) \times (1 - \text{tax}^{\text{capgain}}) + Tax_{t,s}^{\text{assets,tot}} \]

(4.44)

\[ E[EQV, TV, SV] = \sum_{s} [EQV_{s}, TV_{s}, SV_{s}] \]

(4.45)

\[ SKV = E[EQV] + \text{prob}^{\text{success}} \times E[TV] + (1 - \text{prob}^{\text{success}}) \times E[SV] \]

(4.46)

**Table 4.5: Parameters and variables in objective function model**

<table>
<thead>
<tr>
<th>Parameter/Variable</th>
<th>Description</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>(FCFE_{t,s})</td>
<td>Free Cash flow to equity</td>
<td>Variable</td>
</tr>
<tr>
<td>(Rev_{t,s}^{\text{tot}}, Opex_{t,s}^{\text{tot}})</td>
<td>Total revenue and operating costs</td>
<td>Variable</td>
</tr>
<tr>
<td>Dividend_{t,s}</td>
<td>Tax credits to equity providers</td>
<td>Variable</td>
</tr>
<tr>
<td>(EQV_{s}, TV_{s}, SV_{s})</td>
<td>Equity, terminal, and salvage values</td>
<td>Variable</td>
</tr>
<tr>
<td>(E[EQV, TV, SV])</td>
<td>Expected values</td>
<td></td>
</tr>
<tr>
<td>(\text{E}[\text{ROE}]_{t})</td>
<td>Expected return on equity</td>
<td>20% at (t=1); declining at 2% CAGR</td>
</tr>
<tr>
<td>(\text{tax}^{\text{capgain}})</td>
<td>Capital gains tax</td>
<td>15%</td>
</tr>
<tr>
<td>(EarningPower_{s})</td>
<td>Predicted earnings power</td>
<td>Variable</td>
</tr>
<tr>
<td>(GR)</td>
<td>FCFE growth rate</td>
<td>4 percent p.a.</td>
</tr>
<tr>
<td>(T)</td>
<td>Time horizon</td>
<td>7 periods, or 14 years</td>
</tr>
<tr>
<td>(\text{prob}<em>{t,s}, \text{prob}</em>{T,s})</td>
<td>Probabilities of price-demand scenario at (t)</td>
<td>Calculated using Eq. 2.4.10</td>
</tr>
<tr>
<td>(\text{prob}^{\text{success}})</td>
<td>Probability of successful capacity design at the end of time horizon</td>
<td>80%</td>
</tr>
<tr>
<td>(SKV)</td>
<td>Total Stakeholder Value</td>
<td>Variable</td>
</tr>
</tbody>
</table>
4.7 Macro-Economic Model

A macro-economic model is suggested to derive interest rates, GDP growth rates, risk free interest rates, and inflation rates. All rates are derived using crude oil prices as a proxy for the state of the economy; figure 4-1 details a process that we utilized to derive macro-economic parameters based on trailing crude oil prices. We do not claim that this model is completely representative of how these parameters are set in the economy, but rather for the case demonstrating the utility of the decision analysis framework it appropriately represents the broader correlations amongst macro-economic parameters. Additionally, it has been suggested that oil prices are an excellent proxy to determine the state of an economy (King et all, 2011); for a net importer like United States, rising (or falling) oil prices will undoubtedly have an impact on the aggregate economy. Crude oil is used as a stochastic input based on which these macro-economic parameters are derived. Consequently, we emerge with different sets of economic parameters based on the stochastic projections of crude oil prices. The price process for crude oil is described mathematically later in this chapter, but here we focus our attention on the correlations used to derive these macro-economic parameters based on crude oil inputs.
We start with trailing values for oil prices, per capital GDP and growth rate, risk free interest rate (10-year treasury bond yield), and inflation rate. Based on crude price movements in the future the following correlations are used to derive other macro-economic parameters:

\[
GDP_{t+1,s}^{growth} = GDP_{t,s}^{growth} - 0.4\% \times \frac{\text{Crude}_{t+1,s}^{price} - \text{Crude}_{t,s}^{price}}{\text{Crude}_{t,s}^{price}}
\] (4.47)

\[
GDP_{t+1,s}^{capita} = GDP_{t,s}^{capita} \times (1 + GDP_{t+1,s}^{growth})
\] (4.48)

\[
Inflation_{t+1,s} = Inflation_{t,s} + 0.55\% \times \frac{\text{Crude}_{t+1,s}^{price} - \text{Crude}_{t,s}^{price}}{\text{Crude}_{t,s}^{price}}
\] (4.49)

\[
RFR_{t+1,s} = RFR_{t,s} + 0.5 \times (Inflation_{t+1,s} - Inflation^{gt}) + 0.5 \times (GDP_{t+1,s}^{growth} - GDP^{gt})
\] (4.50)

Equation 47 assumes that the economic GDP growth rate is crude price-elastic with an elasticity of -0.4 percent (IEA, 2004), equation 48 then calculates the nominal GDP.
estimate based on the predicted growth rate. Inflation is estimated (equation 49) using another elasticity relationship assuming that for every percent change in crude price there will be a one percent increase in expected inflation rate (IEA, 2004). Finally the risk free interest rates are calculated using Taylor Rule (Taylor, 1993) where the risk free rates are set using the central bank’s target for long term inflation and GDP growth rate (equation 50). Following the determination of these macro-economic parameters, real interest rates on debt, expected return on equity, and weighted average cost of calculations are determined using the cost of capital model provided below.

\[
ir_{t,s}^{\text{debt}} = RFR_{t,s} + \beta_{t,s}^{\text{debt}} \times (MR_{t,s} - RFR_{t,s}) \quad (4.51)
\]

\[
E[ROE]_{t,s} = RFR_{t,s} + \beta_{t,s}^{\text{equity}} \times (MR_{t,s} - RFR_{t,s}) \quad (4.52)
\]

\[
\lambda_t = \frac{Equity_{t,s}^{\text{tot}}}{Equity_{t,s}^{\text{tot}} + Debt_{t,s}^{\text{tot}}} \quad (4.53)
\]

\[
Equity_{t,s}^{\text{tot}} = \sum_{eq} Equity_{eq,t,s}^{\text{investor}} \quad (4.54)
\]

\[
\beta_{t,s}^{\text{equity}} = \beta_{UL,t,s}^{\text{equity}} \times \left(1 + (1 - \text{taxrate}) \times \frac{1 - \lambda_{t,s}}{\lambda_{t,s}}\right) \quad (4.55)
\]

\[
WAC_{t,s} = \lambda_{t,s} \times E[ROE]_{t,s} + (1 - \lambda_{t,s}) \times ir_{t,s}^{\text{debt}} \times (1 - \text{taxrate}) \quad (4.56)
\]

4.8 Product Market Model

Liquid ethanol commodity markets exist, where pricing is determined by different market forces; these market forces are discussed briefly below.

**Corn prices:** a majority of the ethanol, especially in the US markets, is derived from corn as the feedstock. Additionally, a major portion of the input cost for corn ethanol is related directly to the feedstock cost. The market supply and demand balance for corn-based ethanol is a function of the cost incurred by the marginal cost producer, which in large part are a
function of their cost of acquisition of corn feedstock. As a general comment, the competitive market for corn as a food crop and as a feedstock for fuel production makes it susceptible to supply and demand imbalances (Tenenbaum, 2008). Despite technological and biotechnology advancements, corn yields annually are determined by multiple exogenous factors such as prevailing weather conditions thus impacting the crop’s market dynamics.

**Gasoline (crude oil) prices:** Since ethanol, in its current form, is used primarily as an additive to gasoline (Cynthia et al, 2009) in E5-15 blends, ethanol pricing is also a function of gasoline pricing as blenders’ (energy marketers) and refiners’ margins are impacted by their cost of acquisition of ethanol. There is actually a complicated link between blenders’ acquisition costs and the price they have to pay to purchase waivers (called renewable identification number, RIN) through the EPA or on the open market if biofuel is not blended, as per the regulatory requirements of Renewable Fuel Standard 2 (RFS2), in minimum quantities annually (Schnepf and Yacobucci, 2010). For each gallon of biofuel blended the refiner or blender can gain RIN credits; each fossil fuel processor has to satisfy minimum blending requirements annually and if they blend more than the regulatory requirement they gain additional RINs that can essentially be sold in the open market to refiners/blenders who have not met the regulatory requirement. These regulatory constraints essentially guarantee a market for biofuel producers no matter what the market prices for biofuels are (Schnepf and Yacobucci, 2010). On the other hand, this creates market distortions in the biofuels markets as prices are not driven simply by supply-demand fundamentals of the commodity. The fact that refiners and blenders can purchase credits without actually blending the mandated levels of biofuels makes the price of RINs an important determinant of demand, and consequently prices, for biofuels. Furthermore, wholesale prices for gasoline, in addition to biofuel
acquisition costs and RIN prices, determines what type of prices a biofuel producer can get on the spot market. To conclude, with regards to the impact of fossil fuel markets on biofuels, biofuel prices (cellulosic ethanol) are a function of wholesale fossil fuel (gasoline) prices, refiner/blender acquisition costs for the biofuel (blending costs and transportation), and the purchase price of RFS2 waivers (RINs) on the open market. Qualitatively, higher gasoline prices can stimulate demand for biofuels, provided the margin on blending is higher than the RIN purchase prices; to this end a biofuel producer can stimulate demand for the biofuel if pricing is low enough for refiners and blenders to not only satisfy RFS2 standards, but also generate additional revenue through the sale of RIN credits. The pricing for biofuel is also driven higher by increasing petroleum prices with a price ceiling equivalent to the petroleum fuel price, although the true price for a gallon of cellulosic biofuel will be derived from a confluence of factors including petroleum prices, blending margins, marginal cost of biofuel production, and price and availability of RIN credits.

**Marginal cost of production:** While a major component of corn ethanol cost (and consequently pricing) is the feedstock itself, the cost of production for cellulosic ethanol are driven by a different set of forces; these include the annualized capital cost of facility construction (5-6 times that of corn ethanol), cost of enzyme for saccharification, and to a lesser extent the cost of feedstock acquisition. Additionally, given that the distribution infrastructure for ethanol is at best under-developed the freight rates for transporting ethanol to end markets also plays a significant role, with higher petroleum prices driving the freight costs higher. In its current state, the marginal cost of cellulosic ethanol production used in our formulation to be ~$3 per gallon (direct operating costs); add to this the capital cost of an annual gallon ($8 per annual gallon used), it seems obvious why cellulosic ethanol is not a
profitable value proposition with the current state of technology. Even if all capital costs are funded through a mix of debt and equity, the interest charges when incorporated into the product pricing equation elevates the cost of cellulosic ethanol production to ~$3.10 per gallon. Transportation expenses are approximated at about 25 cents per gallon while annual labor and maintenance charges are estimated at about 50 cents per annual gallon of capacity. All said, the total cost of producing one gallon of cellulosic ethanol is approximated to be about $4 less any electricity credits (~0.10 per gallon of ethanol at $0.04 per Kwh). Fortunately, producer and investment tax subsidies can offset the cost by about $1.10 per annual gallon yield a net minimum pricing of approximately $2.90 per annual gallon. It should be noted that these costs are not adjusted for inflation and any material cost inflation will undoubtedly have an adverse impact on the producer margins. With higher operating costs, the market supply for cellulosic ethanol will be determined by the cost for the marginal producer in relation to the margin that the producer can expect to make (based on expected market prices for ethanol).

**Macro-economic factors:** In addition to market factors specific to the cellulosic ethanol value chain, macro-economic factors such as interest rates, per capital GDP growth, and inflation rates will also impact the demand (and prices) for the biofuel. Higher growth rates can spur demand for gasoline thus stimulating ethanol demand as a consequence.

For biobased succinic acid, the market forces that will impact the supply/demand fundamentals and the resultant prices are harder to predict. Nevertheless, certain qualitative assumptions can be made regarding market drivers and subsequently a hypothetical model can be proposed to forecast long term trends in biobased succinic acid markets. These assumptions are listed below:
1. Under the assumption that biobased succinic acid will serve markets that are currently served by petroleum derivatives, we can assume that petroleum prices will be a major driver of biobased succinic acid; higher petroleum prices can potentially not only increase demand for the biobased chemical, but also provide upward momentum to spot prices;

2. Additional demand drivers will include cost of production to the marginal producer (dependant of technological advancements) and a secular shift by downstream processors towards more environmentally friendly feedstocks;

3. Supply will also be driven by prevailing petroleum prices, expected spot demands, and marginal cost of production;

4. The spot prices drivers, besides petroleum prices, will include any environmental premium that can be added to the product price (diminishing as supply increases) and more importantly, the supply-demand balance in the spot market.

Besides spot markets for each commodity, it can be conjectured that blenders, refiners, and downstream succinic acid processors will try to establish long term supply contracts will biobased producers in order to secure a consistent supply for their feedstocks (ethanol or succinic acid), while also eliminating price uncertainties that may arise if all purchases are made in the spot markets. Consequently, contractual pricing for cellulosic ethanol and biobased succinic acid may also become more prevalent, with a component of pricing derived from spot prices, but levers such as price floors and ceiling set in the contractual terms in order to lend more certainty to refiner/blender/processor feedstock costs.

Given the aforementioned qualitative assumptions for bioproduct markets, we suggest a hypothetical market model to predict long term evolution of supply/demand/price
fundamentals in the bioproduct markets. Since the prediction horizon will be long, we need to ensure that multiple scenarios and dynamic trajectories are included in the prediction results. The impact of each parameter on bioproduct markets is also hard to predict with relatively little amounts of historical data available for cellulosic ethanol and succinic acid (at least in the public domain); consequently hypothetical elasticity parameters will be utilized primarily to demonstrate the impact of market evolution and related probabilities of each evolutionary scenario on the enterprise decisions regarding strategic capacity design and investment planning. Over time as bioproduct markets take shape, one should update the market model and related elasticity parameters with the availability of more data.

The market model is used to forecast the procurement costs for purchasing biomass feedstock, and supply, demand and prices for each bioproduct. We try to include multiple scenarios for parameter evolutions in order to provide a complete strategic plan based on multiple possibilities of future occurrences in the bioproduct and biomass feedstock markets. For feedstock, we assume that the bioprocessor can contract land for biomass production from land owners and/or farmers; besides providing upfront payments for establishment costs, the bioprocessor also makes annual land rent and overhead payments (inflation adjusted over time) and ongoing variable payments based upon the amount of feedstock delivered (operating expense compensation to farmers). While the establishment and overhead costs are decided through negotiations between the bioprocessor and farmer, the variable payment is indexed off the prevailing spot prices for ethanol, a preset margin on feedstock costs for the bioprocessor, and a predetermined price floor and ceiling (based on minimum operating expenses for the farmer); this contractual formulation allows the farmer to participate in the upside during periods of high ethanol prices and caps the farmers
downside during periods of low ethanol pricing. For the bioprocessor, this provides a maximum cost estimate (based on price ceiling) while protecting margin during periods of low ethanol prices. In the absence of liquid energy crop markets, such pricing agreements between feedstock producers and processors can help alleviate profitability worries for the farmer and secure consistent biomass supplies for the bioprocessor. Other pricing mechanisms can also be formulated including pricing indexed off other commodities that the farmer may produce (for example sugar prices in case of sugarcane land being replaced by energy cane) or any other food crop; such formulations in essence try to compensate the farmer for opportunity costs arising from foregoing food crop production. For switchgrass production on expiring CRP land, the ethanol-indexed pricing can prove especially viable in the future as opportunity costs are harder to determine in the absence of any food crop being produced on the (often nutritionally marginal) land resource.

For product sales, two markets are assumed that the enterprise can sell their products into; (1) the spot markets characterized by high price and demand volatility, and (2) contractual markets where the pricing is based on the biorefinery’s feed and production costs and demand is fixed based on downstream processor (polymer producer, blender or refiner) demand. The contractual markets are characterized by lower price volatility where the downside is limited but the upside is also capped. In a real world scenario, a biofuel or biochemical producer would ideally like to have a mix of contractual and spot sales in order to maximize equipment utilization and still participate in the upside potential for price appreciation through the spot markets.

The spot supply for cellulosic ethanol is determined using the following inputs as independent variables:
1. Previous period’s supply-demand balance;

2. Petroleum prices;

3. Marginal cost of production;

The spot supply for biosuccinic acid is determined using the following inputs as independent variables:

1. Previous period’s supply-demand balance;

2. Petroleum prices;

3. Marginal cost of production.

The spot demand for cellulosic ethanol is determined using the following inputs as independent variables:

1. Petroleum prices;

2. Secular growth component to indicate a fundamental shift in the economy towards more sustainable fuels.

3. GDP growth;

The spot demand for biosuccinic acid is determined using the following inputs as independent variables:

1. Petroleum prices;

2. Secular growth component to indicate a fundamental shift in the economy towards more sustainable chemicals.

3. GDP growth;

4. Previous period’s pricing.
The spot prices are determined using the following independent variables as inputs:

1. Supply-demand balance;
2. Petroleum prices;
3. Blend Margins (for biofuels only);
4. RIN pricing (waiver credit);
5. Government subsidy;

![Diagram](image)

**Figure 4-2: Hypothetical spot market model indexed off crude prices**

For contractual pricing of bioproducts, I assume that the consensus bioproduct pricing mechanism is based on the following inputs:

1. Feedstock prices (with price ceiling and floor);
2. Estimated cost of production for one unit of bioproduct (with price ceiling and floor);

3. Freight and storage costs;

The contractual demand for bioproducts is assumed to be limited by the downstream processor’s requirements, which in our case is chosen arbitrarily to a reasonable estimate based on current contractual supply agreements in the economy.

**Figure 4-3: Hypothetical contract market model indexed off feedstock prices**

It should be noted that the use of petroleum prices as a common input in all calculations for feedstock costs and product market parameters may be an oversimplification of the actual long-run dynamics of biofuel and biobased chemical markets. In real life bioproduct markets will undoubtedly be impacted by a multitude of other factors including the regulatory state in the economy, competition from imported bioproducts (and any import
tariffs), and advent of any new bioproducts that may replace the ones being studied in this dissertation. The model proposed here is purely with demonstrative motives; it is used here as a part of a complete decision support framework, in order to provide a fundamentally derived predictive system to estimate parameter values that are exogenous in nature. A reasonable conclusion that can be derived from this exercise is the necessity of a robust predictive system that is capable of including multiple exogenous forces in order to predict market parameters that will impact a bioproduct value chain at all levels of decision making. This dissertation does not claim that the value of the parameters used here are correct, but rather the model structure adequately represents the major forces that will impact future demand of biofuels and biochemicals. Furthermore, the price/demand trajectories represent a wide range of stochastic parameter realizations, thus providing a sufficiently large range of future values within which the capacity design can be optimized. We will move ahead with the implementation of the stochastic capacity design problem under the assumption that the model used to predict the supply/demand/price behavior of biofuel and biochemical markets is a satisfactory representation of how future cellulosic biofuel and biochemical markets may evolve.

The price of crude oil is represented as a stochastic input following Geometric Brownian Motion (GBM), based upon which the bioproduct market parameters are derived, yielding stochastic price-demand sets. The GBM assumption implies that crude oil prices follow a continuous lognormal distribution characterized by the expected value and standard deviation at any time. The entire process of modeling bioproduct markets is shown in Figures 4-2 and 4-3. Also shown are the models used for crude oil and bioproduct pricing and bioproduct demands, and Table 34 shows the parameters used to solve these models. The
inflation-adjusted oil prices (equation 57) will be generated using the binomial methodology discussed previously and the gas prices will be calculated using a long-term regression formula (Tyner and Taheripour, 2007, equation 58 where A, B are in table 44).

\[ p_{oil}^{it} = e^{((\ln(p_{oil}^{it-1}) - 0.5 \times \sigma^2) \pm \sigma \sqrt{\Delta t} + in_t^{avg})} \]  

(4.57)

\[ p_{gas}^{t} = A + B \times p_{oil}^{t} \]  

(4.58)

Feedstock pricing contract model proposed here is calculated as a mix of a fixed up-front payment made to the farmer and a variable payment made based on the delivered amount of biomass and the prevalent crude prices. Additionally, we set a floor and a ceiling to feedstock pricing in order to incentivize producer participation in feedstock production (price floor) and mitigate input cost risks for the biorefinery (price ceiling).

\[ C_{t,s}^{ValBM} = \min(0.200, \max(0.06, PCT \times P_{t,s}^{EtOH} \times YLD_{t,s}^{EtOH} \times GM)) \]  

(4.59)

Product demand for ethanol is modeled using a log-log model based on an assumed elasticity of the demand to independent parameters as shown in equation 60; the independent parameters include the percent change in annual crude prices and annual GDP per capita. Additionally, a secular growth component is used to simulate a fundamental shift in fuel usage from fossil fuels to biofuels. Ethanol supplies are also modeled as a function of crude price and per capital GDP changes; in addition, changes marginal cost of production are included and related to changes in biofuel supply quantities using an elasticity parameter (of supply). The spot ethanol prices are modeled as a function of gasoline prices (energy equivalent basis), refiner/blender margins on blending (includes any transportation costs), the supply-demand balance in the spot market, and the price of a RIN (RFS waiver); the price of
a RIN is assumed deterministically and a price floor and ceiling is set in order to better control the price process of ethanol.

\[
D_{t,s}^{Eth} = D_{t-1,s}^{Eth} \times \left( 1 + \alpha_t^{Eth} + \gamma^{Oil} \times \left( \frac{\Delta p_{t,s}^{oil}}{p_{t-1,s}^{oil}} \right) + \gamma^{GDP} \times \left( \frac{\Delta GDP_{t,s}}{GDP_{t-1,s}} \right) \right)
\]

(4.60)

\[
S_{t,s}^{Eth} = S_{t-1,s}^{Eth} \times \left( 1 + \gamma_t^{Cost} \times \left( \frac{\Delta c_{t,s}^{prod}}{c_{t-1,s}^{prod}} \right) + \gamma_t^{g_{oil}} \times \left( \frac{\Delta p_{t,s}^{oil}}{p_{t-1,s}^{oil}} \right) + \gamma_t^{GDP} \times \left( \frac{\Delta GDP_{t,s}}{GDP_{t-1,s}} \right) \right)
\]

(4.61)

\[
p_{t,s}^{Spot,Eth} = 0.67 \times p_{t,s}^{gas} - BM_{t,s} + \beta^{Eth} \times \ln \left( \frac{S_{t,s}^{Eth}}{B_{t,s}} \right) + \min \{ 1, \max \{ 0, 0.25, p_{t,s}^{gas} - c_{t,s}^{Eth} \} \}
\]

(4.62)

For biosuccinic acid market, we priced biosuccinic acid based of certain assumption about rival fossil-based production whose production chain is shown below:

\[ CRUDE OIL (CO) \rightarrow LPG (Butane) \rightarrow Maleic Anhydride (MA) \rightarrow Succinic Acid (SA) \]

The yield (YLD) assumptions for this production chain are as follows (in the same order as above):

\[ 1 \text{ barrel CO} \rightarrow 8 \text{ kg LPG (50% Butane)} \rightarrow 4 \text{ Kg MA} \rightarrow 3 \text{ Kg SA} \]

We assumed that butane is priced based on prevailing gasoline prices using the following correlation (Lidderdale, 2001):

\[ \text{Butane} \left( \frac{\$}{kg} \right) = \left( \frac{1 \text{ gal Butane}}{9.40 \text{ Kg Butane}} \right) \times \left\{ -0.001324 + 0.564 \times \text{Gasoline} \left( \frac{\$}{gal} \right) \right\} \]

(4.63)
It should be noted that a large percentage of world butane supplies are derived from natural gas liquids, and consequently butane prices are more realistically related to the ratio of crude oil to natural gas prices (energy equivalent basis); for the sake of simplicity, we ignore the natural gas correlation here and focus on butane pricing indexed off crude oil prices. Qualitatively, we can assume that higher crude oil prices will increase butane prices in the world markets. Based on market prices for butane, a 40 percent feedstock margin (feed cost as a percentage of total production cost) for Maleic Anhydride production, and a 15 percent net margin (NM) on Maleic Anhydride sales, the market price for Maleic Anhydride can be calculated as follows:

\[
Price^{MA} \left( \frac{\text{S}}{\text{Kg}} \right) = \left(\frac{Price^{Butane \times YLD^{Butane \rightarrow MA}}}{40\% \ \text{feedstock margin}}\right) \times (1 + NM^{Butane \rightarrow MA}) \tag{4.64}
\]

Following a similar logic for the Maleic Anhydride to Succinic Acid production chain, one can estimate the market price for fossil-derived succinic acid, based on a 40 percent feedstock margin and 15 percent net margin (NM):

\[
Price^{SA\_fossil} \left( \frac{\text{S}}{\text{Kg}} \right) = \left(\frac{Price^{MA \times YLD^{MA \rightarrow SA}}}{40\% \ \text{feedstock margin}}\right) \times (1 + NM^{MA \rightarrow SA}) \tag{4.65}
\]

This is the competitive price for biobased succinic acid on which we assume a 10 percent “ecological premium or EPR” to value the improved sustainability characteristics of biobased succinic acid. Since price-competitiveness is guaranteed in the proposed pricing scheme, the demand for biobased succinic acid will follow the demand from broader markets for succinic acid which we assume grows (compounded annual growth rate or CAGR) in a price elastic manner:

\[
Price \ \text{Range} \in \{(0,3), [3,4), [4,5), [5,6), [\geq 6]) \rightarrow CAGR \in \{25\%, 20\%, 15\%, 10\%, 5\%, 2\%}\}
\]

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Finally, we assume that biobased succinic acid supplies are dependent on the marginal cost of production with decreasing costs (increasing prices) leading to higher supplies; based on the supply-demand balance the forward price (period ahead) for biobased succinic acid is adjusted according to the following equation:

\[
Price_{SA, Bio\text{based}}^{\text{\$}} = Price_{SA, fossil}^{\text{\$}} \times (1 + EPR) + \beta_{S/D, BioSA}^{SA} \times \ln \left( \frac{S_{BioSA}}{D_{BioSA}} \right)
\]

(4.67)

It should be noted that shift in feedstock or net margins for the fossil-based production chain operators can have a significant impact on biobased succinic acid prices in the proposed pricing scheme. Additionally, dry gas and natural gas liquid markets (ethane, propane, butane) are not taken into account here, but they undoubtedly will have a significant impact on the supply of fossil-based succinic acid (through butane).

For the contractual pricing scheme, we assumed a pre-determined product yield per ton of biomass and a production and transportation cost; in real life these costs have to be negotiated between the bioprocessor and downstream customer. Once the cost structure is fixed, the bioprocessor can reduce actual production costs through operating efficiencies; as contractual production costs remain fixed, such a contractual structure gives the bioprocessor an opportunity to improve their margin on every unit of bioproduct sold to the downstream customer. For the customer, such a contract fixes their cost basis for processing (or blending) the bioproducts supplied.
\[ p_{t,s}^{ Contr, EtOH } = \eta_1^{ET} \times \left( c_{Var,BM}^{Avg} + c_{Production}^{Prod} + c_{Xport}^{Xport} \right) \]  
\[ p_{t,s}^{ Contr, BChem } = \eta_1^{BChem} \times \left( c_{Var,BM}^{Avg} + c_{Prod,avg}^{BChem} + c_{Xport,avg}^{BChem} \right) \]  

The parameters are described below.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( p_{oil}^{oil} )</td>
<td>Current, bi-annual, average oil price</td>
<td>$100</td>
</tr>
<tr>
<td>( \sigma_{oil}^{oil} )</td>
<td>Standard Deviation of average oil price</td>
<td>$15</td>
</tr>
<tr>
<td>( \pm )</td>
<td>The direction of movement of oil price</td>
<td>+ ( \rightarrow ) up; - ( \rightarrow ) down</td>
</tr>
<tr>
<td>( \Delta T )</td>
<td>Time step length</td>
<td>2 years</td>
</tr>
<tr>
<td>( i_{P_{oil}}^{avg} )</td>
<td>Average bi-annual inflation adjustment</td>
<td>Calculated</td>
</tr>
<tr>
<td>( p_{oil}^{gas} )</td>
<td>Current, bi-annual, average gasoline price</td>
<td>Calculated</td>
</tr>
<tr>
<td>( \Lambda, \beta )</td>
<td>Regressed parameters for oil-gas price correlation</td>
<td>0.3, 0.0256</td>
</tr>
<tr>
<td>( p_{oil}^{EtOH} )</td>
<td>Price of ethanol</td>
<td>Calculated</td>
</tr>
<tr>
<td>( BM )</td>
<td>Blend Margin</td>
<td>3 percent of ( P_{oil}^{etoh} )</td>
</tr>
<tr>
<td>( D^{EtOH}<em>{t} ), ( D^{BChem}</em>{t} )</td>
<td>Demands for ethanol and Biochemicals</td>
<td>Calculated</td>
</tr>
<tr>
<td>( \alpha_t )</td>
<td>Secular demand growth component</td>
<td>30 percent</td>
</tr>
<tr>
<td>( \beta_t )</td>
<td>GDP growth rate</td>
<td>2 percent</td>
</tr>
<tr>
<td>( \gamma_{Price,EtOH} )</td>
<td>Self Price elasticity of ethanol demand</td>
<td>-10 percent</td>
</tr>
<tr>
<td>( \gamma_{Price^{oil}} )</td>
<td>Elasticity of product demand to oil price</td>
<td>-20% (EtOH), 60% (biochemicals)</td>
</tr>
<tr>
<td>( \gamma_{GDP} )</td>
<td>Elasticity of bioproduct demand to GDP growth</td>
<td>10 percent</td>
</tr>
<tr>
<td>( c_{Var^{BM}}^{oil} )</td>
<td>Variable Biomass Costs</td>
<td>Calculated</td>
</tr>
<tr>
<td>( \gamma_{PCT} )</td>
<td>Percent of total Biomass Costs paid at variable rate</td>
<td>100 percent</td>
</tr>
<tr>
<td>( YLD_{t}^{EtOH} )</td>
<td>Assumed ethanol yield for biomass contract on a per acre basis</td>
<td>900 gal per acre</td>
</tr>
<tr>
<td>( GM )</td>
<td>Assumed contribution of biomass to ethanol production cost</td>
<td>50 percent</td>
</tr>
<tr>
<td>( S_{ts} )</td>
<td>Predicted Bioproduct supply</td>
<td>Calculated</td>
</tr>
<tr>
<td>( \alpha_1^{Cost} ), ( \alpha_2^{Price} ), ( \alpha_3^{GDP} )</td>
<td>Supply Elasticity parameters to processing cost, oil prices, and GDP</td>
<td>7,500</td>
</tr>
<tr>
<td>( EPR )</td>
<td>Ecological premium added on biochemical market prices</td>
<td>10 percent</td>
</tr>
<tr>
<td>( \eta_1^{ET}, \eta_1^{BCHEM} )</td>
<td>Margin demanded contractually on ethanol and succinic acid supplied</td>
<td>1.20, 1.40</td>
</tr>
<tr>
<td>( \beta^{S/D} )</td>
<td>Price adjustment factor for supply-demand balance</td>
<td>-1 (ETOH), -2 (S. Acid)</td>
</tr>
<tr>
<td>( c_{Export}^{Xport} )</td>
<td>Freight Costs</td>
<td>$0.25</td>
</tr>
<tr>
<td>( c_{Prod,Tot}^{Prod} )</td>
<td>Expected Production Costs</td>
<td>Variable</td>
</tr>
<tr>
<td>( p_{t,s}^{Spot} )</td>
<td>Predicted spot price</td>
<td>Calculated</td>
</tr>
<tr>
<td>( p_{t,s}^{contr} )</td>
<td>Predicted contract price</td>
<td>Calculated</td>
</tr>
</tbody>
</table>
4.9 Results

The model presented above was solved in GAMS using a CPLEX linear solver. The results are presented below.

4.9.1 Option Sets Tested

In order to compare the value of decision options, the aforementioned model was optimized with and without the embedded options. We built the options incrementally and sequentially into the model, that is, each decision option was embedded one at a time in the modeling framework following which the model was optimized. We wanted to distinguish, specifically for the readers, between (1) capacity establishment and (2) incremental capacity design; capacity establishment is the process of establishing the first production capacity, while incremental capacity design is the addition of new capacity to the initial capacity that is established. That said, the following were the different optimization runs:

1. Base Case: The binary variable for capacity establishment was forced to one in the first time period. **Only ethanol capacity (25 MM annual gallons) was assumed**, implying that the biorefinery design was based on a single-product. **No research, development and demonstration investment** was included and **all capacity was assumed to be established in the first time period**. This amounts to a static, discounted cash flow analysis, where decision making flexibility is not present. This formed the base case against which all options results will be compared.

2. Multi-product facility: The model was **forced to establish all capacity in the first time period**, as was the case for the base case. But, in this case **succinic acid was**
allowed into the product mix (5,000 annual tons), giving the biorefinery the option to switch feedstock allocation between two products (ethanol and succinic acid).

3. Research, Development and Demonstration Option: Two different process yield trajectories were simulated. For capacity design without RD&D option, the process yields were assumed to improve 33 percent over the planning horizon. For capacity design with an embedded RD&D option, the overall process yields were assumed to improve 66 and 100 percent over the planning horizon, with different levels of RD&D investment ($25 and $52 million respectively). The model was given the option to invest or not invest in RD&D; in case of RD&D investment, capacity establishment (25 MM gallons Ethanol and 5,000 tons succinic acid) was assumed in the second time period (years 3-4), while the option to not investment in RD&D implied capacity establishment was allowed in period 1 (years 1-2). No capacity expansions were allowed.

4. Growth Option: The model was forced to invest in RD&D in the first time period and establish commercial capacity (25 MM gallons Ethanol and 5,000 tons succinic acid) in the second time period but, capacity design was assumed to be incremental, that is, additional capacity was allowed to come online after the second time period. This result was compared to the base case to determine the option value.

5. Deferral Option: To value this option, it was assumed that RD&D investment was mandated in the first time period but the decision to invest in capacity establishment can be delayed up to three time periods (6 years); this is what we termed as the option expiration date previously. No capacity establishment is required
at any time as the decision is left to the optimizer. However, after the option expiration dates, capacity establishment option cannot be executed, while the incremental capacity design (Flexibility option) remains active throughout the time horizon. A penalty function of $10 million is assumed against the final portfolio NPV for every period of investment deferral (in capacity). The results were compared to the results from:

a. Base case (**no deferral, no multi-product, no flexibility, no RD&D**),

b. The Multi-product option (**no deferral, no flexibility, no RD&D**),

c. The Multi-product + RD&D options (**no deferral, no flexibility**),

d. The Multi-product + RD&D + Flexibility options (**no deferral**),

e. The combined Multi-product + RD&D + Flexibility + Deferral Options.

Table 4-7 lists the different cost structures, design possibilities, and yield expectations for each option set described above.

<table>
<thead>
<tr>
<th>Decision option Type</th>
<th>Products &amp; Yields (product/ton biomass)</th>
<th>Capacity Increment Periods</th>
<th>Fixed Capital Costs, $MM</th>
<th>E&amp;C Costs, %</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base Case</td>
<td>ET (60 to 80 gal)</td>
<td>1 (t=1)</td>
<td>3 (Land)</td>
<td>50</td>
</tr>
<tr>
<td>Flexible Multi-product (MP)</td>
<td>ET (60 to 80 gal)</td>
<td>1 (t=1)</td>
<td>5 (Land)</td>
<td>75</td>
</tr>
<tr>
<td>MP + RD&amp;D</td>
<td>ET (60 to 120 gal) SA (100 to 400 kg)</td>
<td>1 (t=2)</td>
<td>5 (Land) + 50 (RD&amp;D)</td>
<td>75</td>
</tr>
<tr>
<td>MP + RD&amp;D + Growth</td>
<td>ET (60 to 120 gal) SA (100 to 400 kg)</td>
<td>1 (t=2) + 3 (t=3-5)</td>
<td>7 (Land) + 50 (RD&amp;D)</td>
<td>100</td>
</tr>
<tr>
<td>MP + RD&amp;D + Growth + Deferral</td>
<td>ET (60 to 120 gal)</td>
<td>4 (t=2-5)</td>
<td>7 (Land) + 50 (RD&amp;D)</td>
<td>100</td>
</tr>
</tbody>
</table>

4.9.2 Results Summary

Table 4-8 displays, for each decision option set, the expected stakeholder value, the incremental decision option value, and the total decision option value of each option set that
was modeled. The incremental option value refers to the value of the new option that is added to the design problem, while the total option value is the total value that is generated from the combination of all options modeled in the decision problem. The calculations for the incremental and total decision option value are as follows:

\[ ROV^{\text{incr}} = E[SKV]^{\text{option}} - E[SKV]^{\text{previous}} \]  
\[ (4.70) \]

\[ ROV^{\text{tot}} = \sum_{\text{options}} ROV_{\text{options}} \]  
\[ (4.71) \]

<table>
<thead>
<tr>
<th>Number</th>
<th>Decision option Type</th>
<th>E[NPV], $MM</th>
<th>Incremental Decision option Value, $MM</th>
<th>Total Decision option Value, $MM</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Base Case</td>
<td>-54</td>
<td>--</td>
<td>--</td>
</tr>
<tr>
<td>2</td>
<td>Base Multi-product (MP)</td>
<td>-72</td>
<td>--</td>
<td>--</td>
</tr>
<tr>
<td>3</td>
<td>MP + R&amp;D</td>
<td>-20</td>
<td>+52</td>
<td>52</td>
</tr>
<tr>
<td>4</td>
<td>MP + R&amp;D + Growth</td>
<td>-13</td>
<td>+6</td>
<td>58</td>
</tr>
<tr>
<td>5</td>
<td>MP + R&amp;D + Growth + Deferral</td>
<td>+10</td>
<td>+23</td>
<td>81</td>
</tr>
</tbody>
</table>

Table 4-8: Portfolio NPV and options values for each option set

Figure 4-4 shows graphically how the total SKV evolves with the addition of each decision option to the decision process. As can be seen from the figure, the multi-product option does not generate any additional value over the planning horizon, while investment in RD&D has the potential to create a large upside in total portfolio value, although the aggregate NPV at this point is still negative. Capacity growth generates some additional value without making the portfolio NPV positive. The NPV becomes positive, when the option to defer capacity investment and incrementally design processing capacity are combined with the multi-product and RD&D options. We can safely assume that upfront RD&D studies are necessary but as consequential is the option to forego capacity investment under different market scenarios and design commercial capacity incrementally over the planning horizon. The total stakeholder value (portfolio NPV and carbon value) along with the total shareholder returns that are generated (shareholder value as a percentage of invested
capital) are shown in figure 4-4 (for each option set) along with the evolution of incremental option values. The total option value of all decision options modeled is shown in column 5 of table 4-8; this value was calculated to be $81 million indicating a large return that can be generated by maintaining decision making (financial and operational) flexibility while planning for biorefining investments. Additionally, valuation of decision options, as can be seen from table 4-8, changes the NPV of the biorefining project from negative to positive.

![Figure 4-4: Option value evolution and corresponding return on invested capital (ROIC)](image)

Table 4-9 shows the expected annual biomass throughput rates, the requisite gross investment over the time horizon, and the expected shareholder return on invested capital that investors can expect from the operation of the optimal design. We note that the all these values provided are expected values which are obtained by averaging the probability-weighted sums of the decision variables over the planning horizon. Additionally, the shareholder returns are calculated based on the total shareholder value of the enterprise, which takes into account the portfolio NPV, the carbon value, and the terminal market value of the enterprise at the end of the planning horizon (terminal value); to this end we note that in calculating the ROIC we intrinsically assumed that at the end of the planning horizon, the
A prospective enterprise can be sold in the public market to global shareholders, at firm value (SKV + terminal value). These metrics are provided here to give readers a feel for the scale of production outputs that can be expected for an optimized biorefinery design along with the funding requirements to implement the design and the optimal capital structure and returns that are possible. By no means are these values “set in stone”, but rather should be used as a guiding force to shape expectations from a multi-product biorefinery. In a real world setting, the actual production and capacity utilization rates are governed more so by the periodic gyrations of product markets and matching long-term goals and targets with medium- and short-term execution is an essential aspect of any profitable process operation. Nevertheless, it is important to discuss what kind of long-term expectations can be sought from investing in a multi-product, state-of-the-art biorefinery and that is precisely the purpose of this paper.

Table 4-9: Key performance indicators for options optimization

<table>
<thead>
<tr>
<th>Decision option Type</th>
<th>Expected Annual Biomass Capacity (tons)</th>
<th>Expected Capacity Allocation (ET / SA)</th>
<th>Expected Funding Requirement, $MM</th>
<th>E[ROIC], %</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base Case</td>
<td>355,000</td>
<td>--</td>
<td>155</td>
<td>-22</td>
</tr>
<tr>
<td>Multi-product (MP)</td>
<td>390,000</td>
<td>8.3</td>
<td>164</td>
<td>-18</td>
</tr>
<tr>
<td>MP + R&amp;D</td>
<td>330,000</td>
<td>15</td>
<td>216</td>
<td>78</td>
</tr>
<tr>
<td>MP + R&amp;D + Growth</td>
<td>390,000</td>
<td>5.1</td>
<td>238</td>
<td>87</td>
</tr>
<tr>
<td>MP + R&amp;D + Growth + Deferral</td>
<td>280,000</td>
<td>3.1</td>
<td>174</td>
<td>90</td>
</tr>
</tbody>
</table>

Table 4-9 summarizes some key investment metrics for the representative options that are modeled in this case study. The expected annual biomass capacity is calculated by taking the average of the probability-weighted sums of biomass capacities during each time period; capacity establishment was mandated in all cases besides the option set including the deferral option. The highest capacity is noticed for the option set that includes the multi-product, the RD&D, and the sequential growth option, where capacity establishment is mandated following RD&D investment, but sequential additions to capacity are allowed during the
planning horizon. The initial capacity establishment can be presumed to be the primary reason for the highest resultant annual expected capacity, as the optimizer tries to maximize the expected SKV under the mandatory capacity establishment constraint. The option set where deferral is allowed, gives the best estimate for the optimal capacity levels over the planning horizon.

The next column shows how capacity is allocated, on an average over the planning horizon, towards the production of cellulosic ethanol and succinic acid. We notice that capacity allocation towards ethanol is highest for the multi-product sets where capacity expansion is not allowed; qualitatively we can infer that, if capacity expansion is allowed, succinic acid capacity will be grown at a much faster rate than ethanol capacity and consequentially more biomass capacity will be allocated towards succinic acid production. It should be noted that ethanol yield is almost 4 times lower than the succinic acid yields (unit product per ton biomass basis), so it makes sense that a larger amount of processing capacity is allocated towards ethanol production. These option sets highlight the importance of decision-making flexibility when designing future biorefineries, as investment deferrals and sequential capacity additions in response to changing market conditions for products and feedstock(s) can enable an enterprise to optimally allocate capital towards projects lowest risk profiles (option to defer) and highest expected returns (succinic acid capacity).

The next two columns, total funding requirement and the expected return on invested capital invested. We notice that returns on invested capital are positive for the case where RD&D investments are made (with and without capacity growth) despite negative portfolio NPV. This can be attributed to the calculation methodology of shareholder return where we use the market value (NPV + terminal value) to determine the shareholder return as opposed
to only the portfolio NPV. If in fact the project can be sold to shareholders at the end of the
planning horizon and at market value (broad assumption), investors can expect at total return
ranging from [-20, 90] percent based on the option set that is executed. Again, it is evident
that RD&D investments and a growth oriented production platform are imperative in
generating positive returns for investors. We will now discuss in some detail the results for
each option set that was mentioned at the beginning of this section.

4.9.3 Results and Discussion

We state the results from different model optimization runs in this section; different
decision options were built in incrementally and each time, the stochastic optimization model
was run with the incremental set of options. Readers should focus on how incorporating and
valuing different sets of managerial options adds strategic value to the enterprise value chain.

4.9.3.1 Base Case Results

For the base case, we assumed that RD&D investment is not required to setup a
commercial scale facility; this is a rather primitive methodology for capacity establishment
and in most real life situations such instances do not occur, especially for new technologies.
Most enterprises nowadays take a more cautious approach to building commercial production
capacity while necessitating investment in a pilot of a demonstration facility. We use the base
case as a means to illustrate the value of such RD&D investments but simulating a baseline
value against which all other optionality (in decision making) will be valued. Two sets of
design strategies are covered in the base cases; a single-product (ethanol only) facility with
an annual (fixed input) production capacity of 25 million gallons and a multi-product
(ethanol and succinic acid) facility with fixed production capacities (25 MM gallons and
The results for model runs are shown in figure 4-5. It should be emphasized that model decisions comprise only of capacity utilization rates and sales levels (with different market scenarios) as capacity design is a fixed input.

As can be seen from the decision tree above (figure 4-5), it is not advisable to establish a commercial scale, single product (cellulosic ethanol) facility, given the current price scenarios and the possibilities of future price evolutions. The lack of investment in RD&D does not allow the biorefinery to achieve higher yields over the time horizon, reducing the project profitability further. The downside risk of lower crude oil prices (and consequently lower ethanol prices) is especially significant with almost 40 percent of the total loss of value being contributed by the low oil price scenarios (≤ $100 per barrel). The fact that we mandated ethanol production through all price evolutions has the biggest
downside impact on the project NPV. The average annual ethanol production capacity was mandated to be 25 million gallons, contingent on the sugar yields that are expected from biomass fractionation. The expected project NPV generated from this facility is -$55 million, primarily driven by the low expected yields and no prospects of incremental capacity addition. The next figure (figure 4-6) shows the valuation results when a multi-product biorefinery is assumed to be established, producing succinic acid in addition to ethanol.

Figure 4-6: Options decision tree for a multi-product facility producing ethanol and biosuccinic acid with fixed capacity design

The establishment of a multi-product facility that produces ethanol and succinic acid was also tested; as was the case earlier, no RD&D investments were made yielding a 25 percent expected yield improvement for each product driven primarily by operating efficiencies and experience. The expected portfolio NPV along with the decision tree is shown in figure 4-6. If management decides to invest in a multi-product production platform that can produce both cellulosic ethanol (25 million annual gallons, fixed as input) and succinic acid (5,000 annual tons, fixed as input), the value of the biorefinery over the 14-year
time horizon is reduced even further to -$74 million. This result indicates that capacity investment without any significant yield improvements (over time) or lacking prospects of capacity growth over the time horizon seems to be an unprofitable venture, even with the presence of higher value co-products. Although bio-based endeavors would be well served to conjure plant designs that have the ability to produce multiple products, doing so without proper evaluation of long term plant yields and an operating strategy to drive higher plant outputs can prove disastrous.

Additionally, we only assumed a succinic acid capacity of 5,000 annual tons, whereby the economies of scale advantage specifically for succinic acid is not present; larger production capacities for succinic acid may have shown improvement over the single product case study (ethanol only) but is not tested here.

4.9.3.2 Research, Development and Demonstration Option

For noticeable improvement in the portfolio NPV, investment in research, development, and demonstration was tested; we modeled a binary option on investment in RD&D assuming that while the initial yield is the same as for the base case, the learning curve is substantially reduced and significant yield improvements are made as the facility operates over the planning horizon. This in itself is a broad assumption, as investment in RD&D may not always provide the desired results. We assume that there is a 70 percent chance that over yields will improve as expected while there is a 30 percent chance that the final achievable yield will equal to that assumed in the base case. The decision options model is run with the RD&D option twice; once with the improved yield and once with the base case yield. The probability weighted sum of the portfolio NPVs in each case is presented
The investment is partially funded (25 percent) through government grants and the rest is capitalized and amortized over the planning horizon. Additionally, R&D tax credits were assumed to be received proportionally to the amortization schedule. Investment in commercial production capacities (2 years construction delay), which is again fixed to 25 million gallons and 5,000 tons for ethanol and succinic acid respectively, is mandated following RDD investment. Additionally, we provide the model with 2 different levels of RD&D investment intensities with the choice of the investment intensity left as a decision variable. With RD&D activities carried out over 2 years and facility construction over 2 more years, the total lag from first investment to first revenue opportunity is 4 years. Additionally, the model no deferral or staged capacity growth options are provided implying that the capacity design is fixed over the planning horizon. This yielded a model with RD&D investment intensity, capacity utilization rates, and sales levels as the only decision variables. The expected portfolio NPV for different price evolutions is shown in figure 4-7.

![Decision Tree](image)

**Figure 4-7**: Options decision tree for a multi-product biorefinery with RD&D option and optimized capacity design
The higher of the 2 investment levels was chosen as the optimal investment option by the model. The expected option value (weighted by the probabilities of success and failure) is $52 million (after capital investment adjustment), providing a 100 percent return on capital invested in RD&D. Qualitatively, we can infer that instead of rushing to establish production capacity, careful investment in RD&D studies is made to validate and improve technical aspects of a proposed design, large returns can be generated for investors over a longer time horizon. Indeed, these investments will delay the prospects of commercialization and may reduce addressable market demand for an enterprise (competition), but despite these forces (which are modeled in our formulation), it is apparent that RD&D investment and consequent yield improvements are essential at driving long-term profitability of a bio-based fuel and chemical production endeavor. The investment amount and resultant yields are arbitrarily chosen here for the sake of demonstrating the model utility and a deeper look into these costs is recommended; real RD&D costs and resultant yields are almost always proprietary and company specific. Nevertheless, the formulation proposed here can help a public or private enterprise in evaluating the value of investing in research and development, given true estimates of RD&D costs and expected yields.

4.9.3.3 Capacity Growth Options

Next we tested the idea of valuing future prospects of capacity growth (on top of the installed base). To determine an upfront cost of the growth option, we assumed that the management invests additional capital in purchasing a larger piece of land to be able to add capacity in later periods and more capital is spent on engineering and construction services for an advanced plant design. From a valuation perspective, this is a rather opaque
assumption as questions such as “what type of plant design” and the meaning of the term “advanced” are not addressed. From an practical viewpoint, detailed engineering and economic analyses should be carried out to estimate the additional capacity growth prospects and the corresponding investment intensities required to have the option to grow capacity; here we focus on the valuation of such an option under the assumption that purchasing 40 percent more acreage and an additional 25 investment in construction and engineering services will allow the enterprise to grow plant capacities incrementally over time. The optimal decision tree obtained is shown in figure 4-8.

![Options decision tree for a multi-product biorefinery with RD&D and capacity growth options](image)

Figure 4-8: Options decision tree for a multi-product biorefinery with RD&D and capacity growth options
From the optimal capacity growth profile attained, we can ascertain that the larger capital outlay upfront for the purchase of additional land and engineering services generated positive total returns. The ROV of incremental capacity design is also stated in Table 4-8 as $8 million wherein, the portfolio NPV is improved to -$12 million from the previous case. Additionally, a 300 percent increase in expected gross succinic acid production capacity is noticed over the planning horizon (from 5,000 to 15,000 average annual tons) when capacity growth options are included indicating that succinic acid capacity growth is a high value-add to the facility design and investment planning. Adopting such an incremental strategy allows the prospective biorefinery to mitigate market risks by controlling the production capacity of the plant dynamically; as market uncertainties are reduced over the planning horizon, capacity addition becomes more favorable. Qualitatively, we can ascertain that a larger capital investment in land and ancillary engineering now, that allows for seamless capacity expansion in the future, is something that is worth considering for a biorefining enterprise, especially knowing that industry dynamics are bound to change over time as industry matures. Our decision-options formulation can help an enterprise considering investment in a commercial biorefinery to value the return on investment of this extra capital outlay and ascertain what the option value of this flexibility is. For the optimal results, the expected upfront investment in the flexible platform was calculated to be $22 million; this allowed the generation of $8 million of additional NPV in value over the planning horizon, yielding a 36 percent incremental ROI.

4.9.3.4 Deferral of Investment and Optimized Capacity Options

This section tries to evaluate the value of a deferral option; deferral implies that a biorefining management team, during feasibility studies can opt to defer the decision to
invest in capacity due to unfavorable market and/or process conditions. In our case we focus on the market conditions as being the stochastic parameter based upon which managers can choose to either move ahead with capacity establishment or wait and see how the market conditions evolve before making the final decision. During the deferral period(s), the management risks losing market share to other competitors, risks input and capital cost inflation and risks foregoing the current tax benefits and government grants for green investments and advanced biofuels production. We have modeled addressable demand losses (assumed to decrease 10 percent every period where capacity establishment is deferred) as a proxy for marginal producers that can move in to a market and establish relationships with refiners (customer) to satisfy their blending requirements in the case of ethanol, or establish long-term contracts with polymer and food manufacturers for succinic acid (assumed end-use applications). The government grants are assumed to be available only in the first 3 time periods and producer’s tax subsidies for ethanol are assumed to be $1.01 for the first 2 periods, $0.56 for periods 3-4, and $0 thereafter. In such a scenario, our model can be utilized to weigh the option to defer investment in capacity against the risk of losing market share and government aid to arrive at an optimal strategy that balances these risks versus the rewards of deferring investment. Figure 4-9 displays the decision tree that resulted from the incorporation of the option to defer capacity investment along with all other options previously described.
Besides incorporating the risks of deferral in our modeling framework, we also modeled an increase in the discount rate used for discounting during the deferral period to reflect increased investor expectations for provisional equity, as the biorefinery defers investment in the plant. Despite all these incentives to establish capacity today, the value of deferring capacity investment in order to wait for more favorable price-demand points is apparent from the optimal results; the expected portfolio NPV for this option set is calculated to be $10.5 million yielding the option value of deferral to be $23 million. Investment is made in RD&D during the current time period (RD&D option exercised), but capacity investment is deferred if oil prices move lower; the cost of capital impact is estimated to be $10 million, which is assumed as a capital outlay for the bio-enterprise (see figure 4-9).
During period 2 (year 3-4), the expected oil price (high oil scenario) is predicted to average between $100-130 per barrel corresponding to an average annual ethanol price of $2.67-3 per gallon and average annual succinic acid price of $2.7-3.25 per kg. For this case, ethanol capacity of 13 million annual gallons is established while succinic acid capacity investment is deferred owing in large part to the lack of demand. For the low oil scenario, oil prices are predicted to range between $80-100 per barrel yielding ethanol and succinic price ranges of $2-2.50 and 2.35-2.5 respectively; under this scenario, capacity investment is deferred as it seems advisable to forego investment in capacity establishment and risk losing government subsidies and market share, while also incurring a higher cost of capital. Over time (years 5-10) an aggressive growth strategy is adopted if oil prices continue to rise leading to more favorable prices for ethanol and succinic acid in addition to increased consumer demand for alternative fuels and chemicals; under this evolutionary scenario, optimal ethanol capacity is expected to range between 13-33 MM annual gallons while succinic acid capacity is optimized at 17,000 annual tons. On the other hand, if oil prices continue to move lower (leading to unfavorable bioproduct markets and static demand), optimized ethanol and succinic acid capacities are predicted to range between be 0-15 MM annual gallons and 18,000 annual tons, respectively. Adopting this incremental strategy allows the enterprise to mitigate price and demand risk very effectively; the downside (NPV) for the high oil scenario is -$3 million (scenarios 25-32) while that for the low oil scenario is -$0.25 (scenarios 49-64) where no capacity investments are made and RD&D investment is salvaged at 10 percent of initial capital outlay. This is in contrast to the case where all capacity is established at once, where the downsides (in portfolio NPV) are -$5 million -$19 million, for the high and low oil cases respectively.
When comparing figure 4-6 with figure 4-9, it becomes apparent why optimizing capacities given current and expected market conditions is important; optimal capacity level for the higher oil price scenarios is 13 million annual gallons of ethanol capacity establishment (period 2) and deferral of succinic acid investment, while that for the lower oil price scenarios is complete deferral of investment. This is stark contrast to the 25 million gallon facility established in the base case (5,000 tons of succinic acid) indicating that ethanol profitability is driven in large part by market prices for the commodity (in addition to higher achievable yields). The optimization of capacities under market uncertainty yields different capacity plans for different market scenarios; the expected NPVs for the optimized case are +$9 million and +$1.5 million while those for the base case are -$27 million and -$47 million (high and low oil price scenarios respectively).

4.10 Summary and Conclusions

Qualitatively, we can infer that higher petroleum prices are an essential driver of profitability of biorefineries and basing capacity investment decisions on petroleum markets is something that any prospective biorefiners should consider. The model proposed here, is a first attempt to quantitatively model how capacity planning decisions for the production of biofuels and bio-based chemicals can be designed to in conjunction with the evolution of the petroleum markets. Additionally, yield improvement through technological innovation is a high impact process parameter; with the current state of plant yields, large investments in commercial ethanol and succinic acid production facilities was quantified to be a very risky proposition. A cogent strategy for prospective lignocellulosic enterprises would be to focus on technological innovation in order to improve fundamental process performance. Improvement in fermentation and/or sugar fractionation yields for both products seems to
provide an upsized return on investment over the long run. Additionally, current markets for these products carry with them a large amount of price and demand uncertainty which can lead to large capital losses, if investments are rushed. A wait-and-see decision (deferral), given assumed model parameters, seems to be the most appropriate decision, but in no way should deter prospective enterprises from continuing their endeavors towards developing more efficient processing technologies.

From a modeling perspective, there are indeed several refinements that can be made to impart higher degrees of realism to the modeling results, including incorporation of more market drivers for bioproduct markets, a more detailed modeling of the RD&D investment and outputs, and more granular time steps (≤ 1 year) to study capacity planning. But we believe that the use of decision options as tool for strategic decision planning for bio-based production enterprises is a novel contribution of this framework that we hope can generate an intellectual debate on the merits of incorporating aspects of management science to biosystems design and engineering. The next section will test the performance of different capacity strategies under continuous distributions for ethanol and succinic acid markets using Monte Carlo simulations. In order to gauge capital risks, we will generate probability distributions of returns on invested capital (for different capacity strategies), form cumulative risk curves for portfolio NPVs and suggest Value-at-risk metrics for each capacity design.
5. OPTIMAL DESIGN TESTING USING MONTE CARLO SIMULATIONS AND ANALYSIS

5.1 Model Statement

Given the capacity design trajectories, from the decision options formulation, Monte Carlo simulations were conducted for each option configuration described previously. This was done in order to quantify the risk profiles for each design plan given continuous parameter distributions of stochastic price and demand scenarios. One drawback of the modeling strategy from the previous chapter lies in the aggregation of time steps (2 years per period); with aggregate time steps the granularity that may be desired in capacity planning, in terms of price and demand scenarios is severely restricted as discrete estimates of price-demand points only represent single values. In order to generate continuous risk profiles for design plans, we simulated each design plan from decision options using continuous probability distributions for petroleum prices and the formulated fundamental market models for bioproduct markets. Additionally, feedstock supply was determined deterministically in the previous chapter; here we allow of supply distributions as opposed to point estimates of feedstock supply.

5.2 Model Description

The feedstock supply and petroleum price distributions are assumed to normally distributed with expected values derived from the point estimates used in the previous chapter. Optimal capacity plans obtained from decision options optimization were used as inputs and the expected portfolio NPV and expected ROIC was simulated for each design
plan. The simulation model formulated was derived from the options optimization chapter and is stated below.

\[
P_{Oil_{t,s}} = \exp(\ln(\mu_{t,oil}^s) + \sigma_{t,oil}^s) \times N^s(0,1) \quad (5.1)
\]

\[
BM_{t,r}^{avail} = Land_{t,contr}^{s} \times \exp(\ln(\mu_{t,BYLD}^r) + \sigma_{t,BYLD}^r) \times N^r(0,1) \quad (5.2)
\]

\[
P_{t,s}^{ETOH}, P_{t,s}^{SA} = f(P_{Oil_{t,s}}) \quad \text{see Eq} \ 4.59 - 4.67 \quad (5.3)
\]

\[
C_{t,s}^{feed} = \min(\$0.200, \max(\$0.06, PCT \times P_{t,s}^{ETOH} \times YLD_{t,EtOH} \times GM)) \quad (5.4)
\]

\[
prob_{t,s}^{sampled} = 1 - 0.5 \times \left\{1 + \text{erf}\left(\frac{\ln(p_{oil_{t,s}}^s) - \ln(\mu_{oil,typ}^s)}{\sigma \times \sqrt{2}}\right)\right\} \quad (5.5)
\]

\[
prob_{t,s}^{normalized} = \frac{prob_{t,s}^{sampled}}{\sum_s prob_{t,s}^{sampled}} \quad (5.6)
\]

\[
prob_{t,r}^{sampled} = 1 - 0.5 \times \left\{1 + \text{erf}\left(\frac{\ln(BYLD_{t,s}^r) - \ln(\mu_{BYLD,typ}^r)}{\sigma \times \sqrt{2}}\right)\right\} \quad (5.7)
\]

\[
prob_{t,r}^{normalized} = \frac{prob_{t,r}^{sampled}}{\sum_r prob_{t,r}^{sampled}} \quad (5.8)
\]

A total of 250 samples were utilized each from lognormal oil price (scenario index s) and biomass yield (scenario index r) distributions yielding a total of 2500 samples; the lognormal assumption implies the natural log of the stochastic parameter follows a normal distribution (Eq. 1-2). The lognormal assumption also implies that the stochastic parameters cannot be negative. This is a relatively common price distribution for commodity prices and process yields, characterized by a fat right tail and skewed towards the right. The product price and feedstock cost models mentioned previously (Eq. 4-57-4.69) were used to generate the prices for cellulosic ethanol and succinic acid and the feedstock costs respectively (Eq. 3-
4). We utilized an error function approximation (Eq. 5-6) to estimate the lognormal probabilities of a scenario; since the samples were independently generated for each simulation run, all sampled probabilities were normalized to sum to one for each time horizon (Eq. 7-8).

\[
BM_{t,r}^{purch} = \min(BM_{t,r}^{avail}, BM_{t,r}^{purch,ET} + BM_{t,r}^{purch,SA})
\]  
(5.9)

\[
BM_{t,r}^{purch,ET} = \min(\frac{\text{CapSep}_{t}^{ET}}{\text{PYLD}_{t}^{ET}}, BM_{t,r}^{avail})
\]  
(5.10)

\[
BM_{t,r}^{purch,SA} = \max(0, BM_{t,r}^{avail} - BM_{t,r}^{purch,ET})
\]  
(5.11)

\[
Production_{p,t,r} = BM_{p,t,r}^{purch} \times PYLD_{p,t}
\]  
(5.12)

\[
Sales_{p,t,r}^{contr} = \min(Production_{p,t,r}, Sales_{t,r}^{contr,INPUT})
\]  
(5.13)

\[
Sales_{p,t,r,s}^{spot} = \max(0, \min(Dem_{p,t,s}^{spot}, Production_{p,t,r} - Sales_{p,t,r}^{contr}))
\]  
(5.14)

The feedstock purchase decisions were constrained by the total feedstock available (Eq. 9) assuming stochastic availability. It was assumed that, in case of feedstock shortages (stochastic supply) the available feedstock will be diverted first towards ethanol production (Eq. 10) while the remaining feedstock will be used for succinic acid production (Eq. 11). The production for each product was then calculated (Eq. 12) using the allocated biomass quantities and a dynamically evolving product yield (S-curve evolution based on assumed RD&D investment). The contractually obligated sales levels were derived from the optimized results from decision options optimization (Sales_{t,r}^{contr,INPUT}); it was assumed that the contractual sales obligations are to be satisfied first before any spot sales are made (Eq. 13). The spot sales are then calculated based on the production output that remains after meeting
all contractual sales obligations (Eq. 14). It should be noted that if the total production output for either product is lower that the contractual sales obligation (input value) then the entire output is sold to the contracted customer. Alternatively, a penalty cost function can also be used in order to penalize the biorefiner for not meeting its contractual sales obligations.

\[ C^{feed}_{t,r,s} = BM^{Purch}_{t,r} \times P^{feed}_{t,s} \]  \hspace{1cm} (5.15)

\[ COGS_{t,r,s} = C^{feed}_{t,r,s} + C^{Prod}_{t,r,s} \]  \hspace{1cm} (5.16)

\[ C^{Prod}_{t,r,s} = C^{plant}_{t} + C^{Xport,Prod}_{t,s} + C^{Xport,BM}_{t,s} \]  \hspace{1cm} (5.17)

\[ C^{Xport,ETOH}_{t,s} = D^{site,MKT}_{t} \times (8.37 \times 10^{-5} + 8.28 \times 10^{-7} \cdot POil_{t,s}) \]  \hspace{1cm} (5.18)

\[ C^{Xport,SA}_{t,s} = D^{site,MKT}_{t} \times (2.79 \times 10^{-5} + 2.76 \times 10^{-7} \cdot POil_{t,s}) \]  \hspace{1cm} (5.19)

\[ C^{Xport,BM}_{t,s} = D^{site,MKT}_{t} \times (6 \times 10^{-5} + 9 \times 10^{-7} \cdot POil_{t,s}) \]  \hspace{1cm} (5.20)

\[ Cost^{fixed}_{t} = C^{lbr}_{t} + C^{LAND}_{t} + C^{SGA}_{t} \]  \hspace{1cm} (5.21)

\[ C^{Tot}_{t,r,s} = COGS_{t,r,s} + Cost^{fixed}_{t} \]  \hspace{1cm} (5.22)

\[ Capex^{reinvest}_{t} = RIR \times Capex^{eq}_{t} \]  \hspace{1cm} (5.23)

Feed costs are calculated (Eq. 15) as a function of the total biomass purchased under supply scenario \( r \) and feed price scenario \( s \). The total cost of goods is calculated as a function of feed costs, plant operating costs, and transportation costs for biomass and product movement between nodes (Eq. 17); it should be noted that transportation for biomass was assumed using truck transportation while product was assumed to be distributed using railcars (Optimal results from chapter 3). Both costs of transportation were assumed to
depend on petroleum prices (Eq. 18-21; TEMS 2008). Fixed costs including operating labor, land rent and SG&A expenses were fixed based on optimal design parameters obtained from decision options optimization (Eq. 21). Finally Eq. 22 was used to calculate the total cost of production and operation while Eq. 23 was used to determine the maintenance capital that is re-invested into the business in order to maintain current levels of operations at 7 percent of total equipment costs (Kazi et al, 2010).

\[
OCF_{t,r,s} = Rev_{t,r,s} - C_{t,r,s}^{Tot} - \max(0, Taxes_{t,r,s} - TaxCredits_{t,r,s}) \quad (5.24)
\]

\[
FCF_{t,r,s} = OCF_{t,r,s} - Capex_{t}^{\text{reinvest}} \quad (5.25)
\]

\[
NPV_{t,r,s} = \sum_{t} \frac{FCF_{t,r,s}}{(1+WACC)^t} \quad (5.26)
\]

\[
TV_{t,r,s} = \frac{FCF_{t,r,s} \times (1+GR)}{WACC - GR} \times \frac{1}{(1+WACC)^T} \quad (5.27)
\]

\[
ROIC_{t,r,s} = \frac{NPV_{t,r,s} + TV_{t,r,s}}{NPV_{\text{investment}}} \quad (5.28)
\]

\[
E[\text{NPV}] = \sum_{t,r,s} \text{prob}_{T,r}^{\text{normalized}} \times \text{prob}_{T,s}^{\text{normalized}} \times NPV_{t,r,s} \quad (5.29)
\]

\[
E[\text{TV}] = \sum_{t,r,s} \text{prob}_{T,r}^{\text{normalized}} \times \text{prob}_{T,s}^{\text{normalized}} \times TV_{t,r,s} \quad (5.30)
\]

\[
E[\text{ROIC}] = \sum_{t,r,s} \text{prob}_{T,r}^{\text{normalized}} \times \text{prob}_{T,s}^{\text{normalized}} \times ROIC_{t,r,s} \quad (5.31)
\]

The operating cash flows (equation 24) are calculated as the tax adjusted net operating profits, while the free cash flows (equation 25) are calculated as the maintenance capital adjusted operating cash flows. The NPV, terminal value, and return on invested capital (ROIC) for each sampled price and supply scenario and probability are calculated using equations 26, 27, and 28 respectively, while their expected values (probability weighted sum) are calculated using equations 29-31.
The aforementioned model is simulated in GAMS with fixed inputs (optimal design decisions from options optimization) and sampled values from the supply and price distributions (lognormal). The results are presented in the next section.

5.3 Results and Discussion

Model simulations were run for the decision option cases that were mentioned in the previous chapter. Cases that are compared here include the base case (multi-product) versus the cases with RD&D and capacity growth options (no investment deferral) and the case where deferral options are added to the RD&D and growth options. Additionally, design trajectories for cases with capacity growth options and deferral options were different for different oil price trajectories; consequently, 2 design cases were simulated for each option set, one when oil price move higher immediately (scenarios 1-32) and the other when oil prices move lower (scenarios 33-64). Expected values (probability weighted) for design parameters (Contracted land, capacity design, contractual sales, and capital investment intensities) were used for each scenario set as inputs and the operating parameters (feedstock purchase, capacity utilization rates, and spot market sales) were simulated under different supply-price scenarios. The simulated variables that are discussed here focus on portfolio NPV’s and investor return on invested capital (ROIC), which is calculated using invested capital (input) and the sum of the portfolio NPV’s and the resultant terminal enterprise value.
Figure 5-1 indicates that the expected portfolio NPV for the base case is -$60 million; this is in contrast to the value obtained from options optimization (-$54 million). The difference is primarily driven by model granularity wherein 2 year time steps were used with discrete point estimates of price in options optimization, while continuous estimates are used with annual time steps for Monte Carlo simulations. It is important to note that Monte Carlo simulations are a complimentary tool to options optimization, wherein, optimal results should be simulated on a continuous time scale in order to get a complete, more accurate picture of the results. Additionally, supply uncertainties are also simulated here while feedstock yields were assumed fixed (deterministic) in options optimization (to reduce the number of scenario sets). The next figure (figure 5-2) compares the NPV distributions for the cases where capacity growth and investment deferral were included as possible strategies.
Figure 5-2: Simulated NPV distributions and risk curves for capacity growth (right) and deferral option (left) design cases under high oil price evolution.

Figure 5-2 shows simulated NPV’s for the high oil price scenarios (scenarios 1-32); we notice that the capacity growth option perform better than the deferred strategy with an expected NPV of $34 million versus $32 million. This is driven by the fact that for higher product prices (indexed off higher petroleum prices), the downside risk of capacity establishment is removed with minimum achievable NPV of approximately $14 million. For the case without deferral, aggressive capacity growth will generate slightly higher NPV’s as we have not accounted for oil prices moving significantly lower. The picture is more complete when we compare simulated NPV’s for scenarios 33-64 where oil prices move lower (Figure 5-3) resulting in lower bioproduct prices and demands.
In figure 5-3 we notice that when capacity is established today with the option to grow capacity over time, downside risks arise with a maximum downside of approximately $14 million in lost value, while the NPV distribution yielded by the design case where the deferral option was exercised shows good risk characteristics with a maximum possible downside of $4 million in created value. Here in lies the benefit of deferring capacity investment in the face of uncertainty; while figure 5-2 showed that higher product prices do not change the upside potential of either design plan, the downside of lower product prices (tail risk) is mitigated when the deferral option is exercised as compared to the capacity design plan where deferral of investment is not exercised. Further quantification of Value at-Risk is presented for each case in table 5-1 below to quantify different levels of expected NPV at different probabilities.
Table 5-1: Value at-Risk metrics for different capacity strategies

<table>
<thead>
<tr>
<th>Option set</th>
<th>Probabilities</th>
<th>5%</th>
<th>25%</th>
<th>75%</th>
<th>95%</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base Case</td>
<td></td>
<td>≤ 73 MM</td>
<td>≤ 66 MM</td>
<td>≤ 55 MM</td>
<td>≤ 44 MM</td>
</tr>
<tr>
<td>RD&amp;D and Capacity Growth Options, High Price Scenarios</td>
<td>≤ 25 MM</td>
<td>≤ 30 MM</td>
<td>≤ 38 MM</td>
<td>≤ 45 MM</td>
<td></td>
</tr>
<tr>
<td>RD&amp;D and Capacity Growth Options, Low Price Scenarios</td>
<td>≤ -1 MM</td>
<td>≤ 9 MM</td>
<td>≤ 21 MM</td>
<td>≤ 28 MM</td>
<td></td>
</tr>
<tr>
<td>Deferral option, High Price Scenarios</td>
<td>≤ 25 MM</td>
<td>≤ 30 MM</td>
<td>≤ 35 MM</td>
<td>≤ 40 MM</td>
<td></td>
</tr>
<tr>
<td>Deferral option, Low Price Scenarios</td>
<td>≤ 10 MM</td>
<td>≤ 14 MM</td>
<td>≤ 19 MM</td>
<td>≤ 21 MM</td>
<td></td>
</tr>
</tbody>
</table>

Table 5-1 is presented to analyze the NPV at-Risk from the implementation of each design plan. It is evident from the table that the performance of the base case design plan (row 1), where a multi-product facility is established today without any RD&D investment or prospects for capacity growth, is very poor. There is a 95 percent chance that the portfolio NPV will be less than $44 million and with almost no expectation of a positive NPV project. The upside for capacity growth options with RD&D investment is greater than the design case where investment deferral is exercised (row 2 and 4), but so is the downside (row 3 and 5). Given the options optimization results and the simulated NPV and their risk curves, a lignocellulosic enterprise now has the tools to perform a deep analysis of their investment decisions before any actual capital outlay is made. In order to complete our analysis of the design modeling, optimization and analysis of a multiproduct lignocellulosic biorefinery that produces ethanol and succinic acid, we present simulated expectations for returns on invested capital. We re-iterate that these return are calculated assuming that at the end of the planning
horizon, equity investors will have the option to sell their stake to individual investors (possibly by taking the enterprise public); in this case the market value of the biorefining assets will be determined by the sum of portfolio NPV and the terminal value (enterprise value) of the operating assets (less any debt). The expected ROIC is then determined by dividing the net of the enterprise value and the equity investment by the discounted value of the equity investment. We discount the value of the investments because investments are made (or planned to be made) dynamically over the entire planning horizon. Consequently, similar to discounting future cash flows, future investments are also discounted by the cost of capital. The ROIC distributions for the base case, the capacity growth case, and the deferral case are provided in figure 5-4, 5-5, and 5-6, respectively.

Figure 5-4: Simulated ROIC distribution and cumulative probability curve for base case

As can be seen, there is a significant loss of capital return that is predicted, if the base case design is implemented. On the other hand, the expected ROIC is skewed towards the higher end for both capacity growth and deferral option design cases, when bioproduct prices
appreciate over time and the optimal design are implemented (figure 5-5). The expected ROIC for both design cases is approximately 23 percent.

Conversely, for the scenarios when oil prices move lower, the capital risk is much larger for the design case when capacity is established without any deferral of investment, under any market scenario (figure 5-6).

Figure 5-5: Simulated ROIC distribution for the capacity growth (right) and deferral option (left) design cases under high oil price evolution

Figure 5-6: Simulated ROIC distribution for the capacity growth (right) and deferral option (left) design cases under low oil price evolution
The expected ROIC for the design plan where the deferral option was exercised is approximately 15 percent while only a 2 percent return can be expected if the deferral option is not exercised and capacity is established under all price scenarios. The weighted average ROIC for all oil price scenarios for the deferred option design case is approximately 18 percent while that for case with only capacity growth is approximately 12 percent. Furthermore the simulated portfolio NPV for all price scenarios (weighted average) is approximately $25 million for both option design cases, with and without deferral, the biggest difference being the worst case NPV for the design case without deferral is much lower than that for the design plan with an embedded deferral option ($-14 million versus $+4 million).

5.4 Summary and Conclusion

It is left up to specific decision makers to decide what specific capacity design trajectories should be utilized; investment in a facility and research, development, and demonstration project seems essential as the risk curves for base case without this investment show very little upside with significant potential for large losses. The choice of the appropriate design plan to implement strictly depends on the investors’ and management team’s appetite for risk; aggressive management teams can choose to establish processing capacity immediately after the completion of the RD&D program in order to capture tax benefits currently provided by the government. But it is essential that during design planning, enough credence be given to the prospects of capacity growth over time as bioproduct markets mature. Aspects of design like a flexible production platform with levers in the design to expand capacity should be considered seriously. More conservative teams can
utilize the “wait-and-see” approach and invest in capacity on if expectations for bioproduct markets are favorable now and over the long term.

The exercise of Monte Carlo simulations was done to further analyze the risk characteristics of design plan implementation for alternative design strategies that were yielded from decision options optimization. As we have maintained throughout the design of the strategic decision framework, all tools developed here are complimentary to each other and should be utilized as a part of the entire decision support arsenal.

The next section describes, qualitatively and quantitatively, some salient conclusions from the implementation of the decision modeling framework for lignocellulosic biorefinery design and suggests some extensions to the framework.
6. CONCLUSIONS AND RECOMMENDATIONS

6.1 Spatial and Technological Design

The following are the salient features of the results obtained from process superstructure design:

1. Energy crops are an essential resource going forward, that will play an important role in determining the viability of producing cellulosic biofuels from lignocellulosic biomass;

2. According to the results presented here, energy cane is a promising species for energy crops with high yield potential and a reasonable cost structure (higher costs offset by higher yields) while switchgrass grown on CRP land provides a resource base for a stable supply of biomass feedstock without interfering with any food value chains;

3. The CRP land available in Louisiana is more than sufficient to establish and grow commercial scale facilities that can produce a multitude of biofuels and biobased chemicals;

4. For biochemical fuel and chemical production, AFEX combined with simultaneous hydrolysis and co-fermentation of sugars shows the highest promise amongst the configuration sets studied;

5. Additionally, distillation of ethanol is a satisfactory method for ethanol purification, while electrodialysis provides reasonable succinic acid yields, given the high cost of organic acid purification using other operating systems (ionic adsorption and chemical precipitation);
6. Larger scale facilities will require a significant reduction in capital expenses or greater supply of biomass for realization of investor expectations such as reasonable payback periods;

7. Innovative capital structures such as involvement of tax equity investors and securitization of renewable facility investments can provide a satisfactory vehicle to quench investor demand for faster returns;

8. Operationally, ethanol production can be maximized (while optimizing the NPV) if
   a. A reduction in raw material and feed costs (COGS) is accomplished;
   b. Higher product prices are realized;

9. The downside risk of lower process yields is significant; in a real world setting, if commercial facilities are unable to reproduce yields similar to the experimental ones, or feedstock supply shortages, a significant impact will be felt on the long term value, profitability, and customer relations of the biorefinery.

   In lieu of these observations, it makes sense to proceed gradually during capacity establishment and expansion. Strategies to reduce capital costs and improve construction times are something that can be undertaken as an initial endeavor. Post-construction, strategies to mitigate the impact of uncertain process yields and product prices should be devised preemptively. Consequently, an options based decision model can be utilized to analyze design strategies that mitigate the downside impacts of uncertain markets.

   Finally, it should be mentioned that this analysis was done to illustrate a particular utility of the modeling and optimization framework proposed. The framework can be used to study the impact of different input parameters on other decision variables. Either way, given the uncertain future costs, prices, and yields of the value chain, an integrated approach of
modeling, optimization, and sensitivity analysis is deemed necessary to study the true impacts of selecting a particular value chain configuration. The optimal results are contingent on a set of input parameters, which are subject to change as the biorefinery is scaled from bench to commercial scales.

6.2 Decision Options and Monte Carlo Simulations

The strategic design of production capacity for a representative, multi-product biomass refinery under market uncertainties was modeled, optimized, and analyzed:

1. The optimal feedstock mix consisted of complete utilization of energy cane resource base and a large percentage of switchgrass resources;
2. The optimal product portfolio that was obtained included cellulosic ethanol and succinic acid;
3. The optimal technology set utilizes AFEX, SSCF, distillation (ethanol), and electrodialysis (succinic acid) as unit operations for biomass conversion and product purification.
4. The prospective product portfolio provides an attractive mix of low-margin fuels (cellulosic ethanol), high-margin biochemicals (succinic acid), and bio-electricity that are important to hedge risks associated with single product markets.

A stochastic MILP based on the principles of real options analysis was utilized to develop optimal capacity plans under different realizations of the uncertain oil prices. Future oil prices were assumed to be the major uncertain input to the model and prices and demands for cellulosic ethanol and succinic acid were assumed to be functions of the movements in the oil price. A modified version of the theoretically developed real options literature (termed decision options) was utilized to derive a practical framework to design production capacities
over a 14 year time horizon. Multiple sets of decision options were embedded in the modeling framework to determine the optimal design trajectories including a flexible, multi-product production platform option, a research development and demonstration investment option, a sequential capacity growth option, and a deferral to invest option. These option sets were built incrementally into the modeling framework to determine the option sets that yielded the highest quality of results in terms of maximizing the strategic value of a startup biorefining enterprise. All option values were compared to a base case, wherein, a static capacity strategy for the production of cellulosic ethanol only is adopted. The model implementation suggested great value in a flexible production platform where feedstock(s) can be allocated dynamically to the production of different product groups, given the expected profit margins from the production of every unit of final product. Additionally, it was found that investment in RD&D to improve overall process yields is a worthwhile investment that yielded great benefits over a strategic time horizon, although their immediate impact is not realized in terms of profits. It was also found that a larger investment in a growth-oriented production platform that allows for sequential and seamless capacity addition over multiple time periods can markedly impact the future profitability of a biorefinery. Finally, the option to defer investment in a new facility, in order to allow market uncertainties to resolve themselves, was found to have a significant impact at minimizing downside risks of unexpected market scenarios for which, some upside from favorable market scenarios had to be sacrificed.

Monte Carlo simulations were conducted to generate risk curves for 5 different investment strategies that were investigated during options optimization. The risk curves calculated the net present value at risk for each design and investment strategy. It was found
that investment in RD&D and sequential capacity growth are essential components for capital appreciation and the option defer capital investment during unfavorable market conditions has good risk mitigation potential. Additionally, it was noted that an aggressive strategy for capacity expansion can involve an immediate capacity investment following the RD&D, with a growth-oriented production platform for seamless capacity expansion in the future. A more conservative strategy would allow the oil price uncertainties to reduce before any investment in capacity is determined. The correct investment strategy should ideally be based on an enterprise’s risk appetite; the decision modeling framework can be used as a guiding force to systematically and sequentially quantify and analyze investment and design metrics.

6.3 Future Work

While the dissertation emphasizes the case for a biomass to biofuels and biobased chemical superstructure design, several extensions to the framework are suggested. The PSE group at LSU is actively seeking research partnerships to broaden the scope of the proposed decision framework; currently we are working on incorporating a decision tool for energy crop production and supply into the framework architecture. The biomass production tool will utilize a similar methodology to design production capacities for the supply of feedstocks to downstream processors. The tool will focus more so on a farmer’s decision to produce dedicated energy crops based on prevailing markets for traditional food crops and prospective markets for energy crops. A significant contribution of this tool will be the democratization of such a systematic decision making methodology in order to sustainably grow the supply and utilization of biomass resources for the purpose of energy and chemical production in the United States.
Within the framework several improvements can be made including the incorporation of dynamic process simulations and utilization of lab-, bench-, and enterprise scale data to validate the modeling framework. Additionally, we are also working on extending the framework to other renewable industry verticals including thermochemical conversion of biomass to biofuels via gasification and syngas production. Other extensions planned through third-party collaborations include application of this methodology to algae oil value chain design and the production and utilization of geothermal energy.
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