Technology Assessment of Biomass Ethanol:
A multi-objective, life cycle approach under uncertainty

by

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ABSTRACT

A methodology is presented for assessing the current and future utilization of agricultural crops as feedstocks for the production of transportation fuels, specifically, the use of corn grain and stover for ethanol production. The generic methodology integrates chemical process design and decision analysis tools. Four primary concepts are incorporated to address the performance of technologies and policies: 1) expansion of the system boundaries to include the entire process life cycle, 2) incorporation of both economic and environmental metrics for multi-objective optimization with tradeoff analysis using Pareto curves, 3) explicit incorporation of uncertainty analysis using Bayesian updating, and 4) integration of multiple feedstocks, processes, and products, in a network optimization framework, with subsequent decomposition to more refined models, for an improvement assessment of specific research and development goals.

The first step is an assessment of the emerging corn grain ethanol industry in the U.S. Using life cycle assessment with Bayesian uncertainty propagation, the net energy balance of corn grain ethanol production is calculated and shown to be slightly positive. The variability in the system suggests that this variance is dependent primarily on corn production location, distribution requirements, and ethanol conversion and purification efficiency lead to the significant variance. From an economic performance, an optimized facility can produce ethanol competitively with gasoline at $55/barrel, on an unsubsidized and energy equivalent basis. The life cycle greenhouse gas emissions decrease of –5% - 30% between gasoline and ethanol on a miles driven basis.

A potential modification to the process is the use of an alternative feedstock, such as lignocellulosic waste and residues, which have larger resource availability and lower economic cost. Compared to the original case, cellulosic ethanol would have a higher net energy ratio with lower greenhouse gas emissions, but the current projected economic costs are prohibitive. An improvement analysis of potential technology advancements using multiple object network optimization across the entire supply chain suggests that research and development should focus on feedstock logistics and the pretreatment stage.

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Chapter 1 Introduction

Technology innovation is an essential requirement of continual economic development. However, many discoveries or innovations also have critical social and ecological implications. The mapping of the human genome promises the ability to individualize health care, but it also presents the problem of how to insure patients with genetic dispositions to disease. Biotechnology advances allow for the modification of plants with specific traits important for nutrition, but the intellectual property laws may hinder farmers in the developing world. Finally, as is presented in this thesis, the availability of biomass for energy production presents an opportunity to develop renewable, domestic energy sources, but the environmental impacts of a large scale biomass system and the economic impacts of policies and subsidies which promote that system are unknown. Industry leaders and policy makers must have an awareness of these external considerations to effectively make decisions which promote economic, environmental, and social progress. This work presents a framework for technology assessment which moves beyond simply the economics of the product or process to investigate other consequences as well.

Traditional approaches for technology assessment are no longer able to provide sufficient information to policy makers and industry leaders who have to decide between competing alternatives. Modern demands require that economic, environmental, and social objectives be included rather than simply relying on traditional cost-benefit analyses or projected net present values and internal rates of return. The accelerated growth of the process industries over the past century has resulted in unparalleled economic growth. However, this has not come without costs, as many environmental problems have emerged, many of which could have been reasonably anticipated with more comprehensive initial assessments. Because these non-economic metrics can be much more difficult to predictively quantify, modern evaluation methodologies must also be equipped to manage the uncertainty of how well a technology will work and the uncertainty of how it will impact a company's economic bottom line and the external environment. Finally, today's interconnected world mandates that local decisions have to be made while considering global implications. An assessment must consist of more than just an analysis of the product itself, instead, also including the impacts of upstream and downstream processes.

1.1 Thesis statement

A primary objective of this thesis is the systematical integration of the following concepts into the technology assessment decision making framework, enabling decision makers to evaluate the alternatives which have the best economic and environmental performance:

- Incorporating explicit uncertainty analysis
- Expanding the boundaries beyond the process or product
- Optimizing multiple objectives

The first step will be to add to the robustness of environmental assessments. This will be followed by a procedure which combines environmental and economic objectives over a supply chain allowing a decision maker to choose technology options which have the best opportunity for improving both. Finally, each of these tools will be demonstrated using the case study of biomass energy.

1.1.1 Uncertainty in environmental assessment

Life cycle assessment is a recently developed tool which allows users to investigate the overall impacts of a process or product on the environmental. The concept is based on the necessity to expand system boundaries; however, the methodology requires a substantial set of data, most of which is highly uncertain. By utilizing novel mathematical tools for uncertainty analysis, this work will build upon the structure of LCA to minimize the inaccuracies and vagueness to which that uncertainty can lead.

1.1.2 System expansion

The identification of key technology improvement possibilities is critical in the development of new processes and products. However, determining where to focus attention and allocate resources is often difficult. Spending a lot of time and money to improve a process may be the wrong decision when focusing on a different product altogether would be better. This problem is addressed here by presenting a hierarchical approach for energy development. Utilizing a straightforward mathematical programming technique along with subsequent refinements of critical process models will allow for a decision maker to identify which processes and products will have the greatest impact.

1.1.3 Multiple objectives

The system expansion described above will be performed using both economic and environmental objectives informed from the improved life cycle assessments. By visualizing the multiple objectives, the methodology will allow a decision maker to find the optimal path to energy development which has both improved economic and environmental performance.

1.2 Transportation fuels

The development of these tools will be demonstrated by working through an assessment of alternative transportation fuels. The primary focus will be the production of biofuels from agricultural crops. Processes for the production of these alternative fuels have been commercialized, but only in limited capacity, so they can still be considered as emerging. Moreover, potential process modifications which are still in research and development, or even hypothetical will be included.

Decisions on transportation fuel production are growing critical, and will only continue to increase in importance over the next several decades. Energy production in general is vital to consider as its low cost availability is instrumental in continual economic growth. However, transportation fuels present an additional challenge as they require on-demand and storage capabilities. For example, wind and solar are promising energy sources, but because of their intermittency, the power generated from them cannot be counted on for automobiles.

Currently, petroleum is the primary source of transportation fuels and is able to meet demand. However, the continuation of oil use as the only prominent fuel source is unlikely for a number of reasons. First, its ability to meet demand is growing tenuous as world demand continues to increase. While reserves are projected to last throughout the 21st century, the ability to extract the reserves and refine them downstream is becoming more economically challenging. Already in the summer of 2005, the price of a barrel of oil surpassed $70, a record high. While the cost of petroleum is not expected to maintain that level, the expectations of $20 per barrel oil may not be reasonable anymore. Because of this high price, industrial players and government policy makers must seriously consider nontraditional feedstocks for fuel production. Biomass is one such option.

Petroleum based fuels are also significant sources of carbon dioxide emissions, the primary greenhouse gas implicated in global warming. Depending on future carbon restrictions or personal decisions to lower an individual's or group's environmental impact, this consideration will also be imperative in assessing future transportation fuel options. Moreover, not only is the utilization of the fuel important, but also the supply chain for its extraction and production..

Finally, energy security has become an increasingly important issue. Currently, over 60% of the petroleum consumed in the United States is imported (EIA, 2006). While most of the imported oil is from nearby countries such as Canada and Mexico, a large portion comes from more unstable parts of the globe such as the Middle East, North Africa, and Venezuela. Maintaining stability in the accessibility of these oil reserves is becoming increasingly burdensome, both financially and militarily, and many policy makers are calling for a decrease in the dependence on foreign oil by the United States.

1.3 Thesis structure

Chapter 2 presents an introduction to the concept of biomass energy as a fuel source. Within the context of the overall energy sector, the types, availability, processes, and products of biomass are presented. **Chapter 3** outlines the different tools which are typically used for technology assessment within the chemical process sector. Special emphasis is placed on the tools to be utilized in this thesis – traditional chemical engineering process design, environmental assessment, uncertainty propagation using Monte Carlo assessment with Bayesian updating, and multi-objective optimization under a network programming framework. **Chapter 4** presents a detailed description of life cycle assessment along with a presentation of how to incorporate uncertainty analysis into the framework. Additionally, a life cycle assessment of the production of ethanol from corn grain is performed. **Chapter 5** extends the life cycle assessment by comparing the energy balance calculation of this study to a number of other reports. Moreover, the

LCA is performed with an explicit propagation of uncertainty. Utilizing a methodology of Bayesian updating, the importance of system variability is demonstrated. **Chapter 6** involves an economic assessment of the corn grain ethanol process, and integrates that assessment with the environmental performance from the previous chapter for a multiple attribute comparison between corn grain ethanol and gasoline. Additionally, a next generation technology, ethanol production from cellulosic material is presented. **Chapter 7** extends the work on cellulosic ethanol by presenting a network optimization framework for describing an agricultural system with multiple choices for crop production and downstream processing. By comparing the economic and environmental performance of technology advancements, the network program is used to systematically determine a priority ranking for resource allocation between the different options. **Chapter 8 and 9** finish with conclusions and future work.

1.4 Contributions

The following bullet points describe the contributions of the thesis along with some specific conclusions for the biomass ethanol case study.

- Development of a methodology for incorporating explicit uncertainty analysis into life cycle environmental assessment by initial using a Monte Carlo simulation, identifying the parameters contributing most to the variance using a sensitivity analysis, and then updating those critical parameters using a Bayesian framework.
- The demonstration of that methodology to elucidate the importance of system variability in the production of ethanol from corn grain, highlighting the importance of corn production location because of the differences in production practices. This is especially critical when exploring the potential for corn expansion to meet growing ethanol demand as moving into more arid regions with less fertile soil will significantly diminish any environmental benefit of corn ethanol.
- An integration of traditional chemical process design with environmental life cycle analysis and uncertainty propagation to compare corn grain ethanol versus gasoline. Optimized ethanol production is comparable to gasoline at $55/barrel

on an energy equivalent and subsidy and tax free basis. While the ethanol has slight lower greenhouse gas emissions and a net energy production on average, these values are variable within the system. Moreover, ethanol production from corn grain is limited by land space available.

- Incorporation of multiple objective network optimization with Pareto curve analysis to formulate a systematic framework for assessing the improvement potential of technology alternatives.
- Demonstrating how that framework can be used for resource allocation specifically applying it to the Department of Energy's biomass ethanol roadmap to find that feedstock logistics and pretreatment advancements are most important while the DOE's budget diminishes those technologies.

Chapter 2 Bioenergy Case Study

2.1 Introduction

The availability of affordable energy is a critical component for economic development. Currently, the world, and especially industrialized countries are heavily dependent on petroleum, natural gas, and coal. However, concerns have arisen over the depletion of these fossil fuels and the contribution of their combustion to global warming. Moreover, as population continues to grow and countries such as China and India become more industrialized, the demand for these fuels, especially petroleum, has pushed their price to new heights (Foccaci, 2005; Fan, 2005).

While fossil fuels will continue to provide the majority of the world's energy for decades to come, many industrial and government groups have started pursuing alternative energy sources such as nuclear, geothermal, solar, wind, and biomass. These other forms of energy have many environmental advantages over fossil fuels, but most have remained uncommercialized on a large scale due to higher than feasible economic costs. Innovative technologies and integrated uses have enabled the penetration of niche markets by these sources, but further work is needed.

This chapter will begin with overview of the world and U.S. energy situation. This will be followed by a detailed description of biomass energy including a discussion of current and future feedstocks, processes, and products. This will serve as an introduction to the detailed case studies which will follow in later chapters.

2.1.1 World energy overview

The current worldwide consumption of energy is over 450 EJ annually, equivalent to 4 billion SCF natural gas or 70 billion barrels of oil, a 33% increase over consumption in 1990. The International Energy Agency (IEA, 2006) estimates that this value will increase anther three-fold by 2050 with the increase industrialization of the developing world. Current usage is composed of 85% petroleum, natural gas, and coal, almost evenly divided, with the remained 15% consisting of biomass, nuclear, and other renewables. The growth in the next half century will be provided by a slight expansion in petroleum production and significant growth for the natural gas, biomass, nuclear, and other renewables industries. Figure 2.1 shows these global estimates (IEA, 2006). Note that biomass contributes nearly 10% to global consumption, and this percentage is expected in increase. While this growth will most likely come from industrial production, most of the current utilization is from small scale use of biomass for heating and cooking in the developing world.

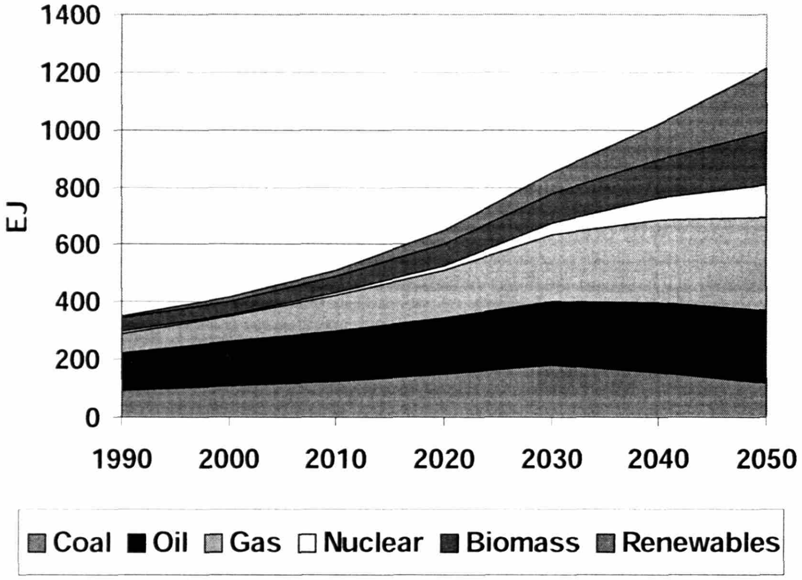

Figure 2.1 Estimates for worldwide energy consumption by source (IEA, 2006)

Simply meeting these potential demands will be difficult. However, the energy industry faces a possibly more challenging concern with the implication that fossil fuels are contributing to global warming through the emissions of greenhouse gases, primarily carbon dioxide, during combustion. To combat this potential environmental impact, government regulatory agencies worldwide are considering greenhouse gas reduction policies, such as what is proposed by the Kyoto Accord (UN, 1997). With average temperatures increasing at current atmospheric concentrations of carbon dioxide, many people are concerned at the impact of continued increases in that concentration, especially with the anticipated energy consumption escalation.

Pacala and Socolow (2004) presented a potential scenario where the increase in energy demand is combined with corresponding "wedges" of 1 Gtonne C each, where seven of these slices will retain a stabilization of current carbon dioxide emissions. Figure 2.2 shows the original figure from their Science article describing these wedges.

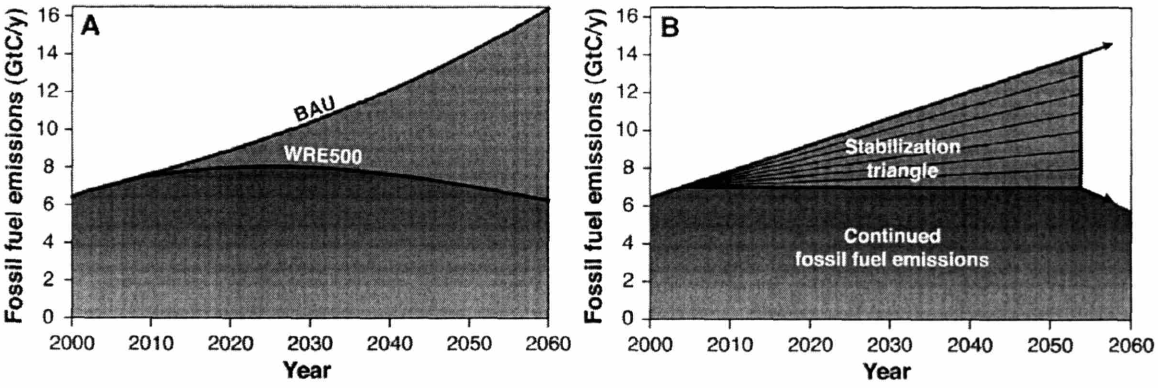

Figure 2.2 Wedge concept for reducing future CO_2 (Pacala, 2004)

2.1.2 U.S. transportation energy

The primary focus of the case studies later in the thesis will be on biofuels produced in the United States. Current U.S. energy consumption is over 100 EJ, nearly 25% of the global consumption. With a population of only 5% of the world's, the U.S. has the highest per capita energy usage by far.

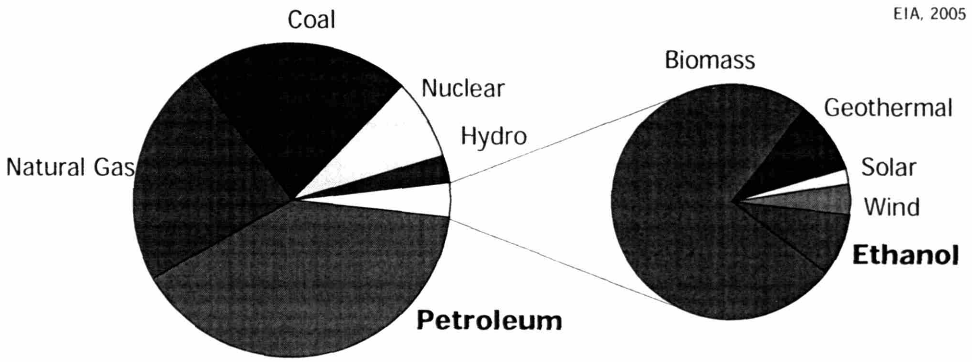

Figure 2.3 Current U.S. energy consumption by sector (EIA, 2006)

Figure 2.3 depicts a pie graph with the current breakdown of energy consumption by primary fuel, with a breakout for renewable energy (EIA, 2006). Currently, large scale biomass energy consumption is concentrated in power generation using residues for the forestry industry and transportation fuel (ethanol) production. The focus of most of this work will be the contribution of biomass to the transportation sector.

The U.S. consumes 21 million barrels of oil per day, over 25% of global production, with this value expected to grow to 26 MMbbl/day by 2025. About 75% of this is used in the transportation sector as gasoline, diesel, jet and marine fuel. The percentage of this total which is imported has been continuously expanding and is currently approximately 60% (EIA, 2006). Because U.S. reserves of petroleum have continued to be depleted, this import fraction will increase over time. This dependence on petroleum, more specifically, imported petroleum, is problematic for a number of reasons.

The U.S. is the largest national consumer of petroleum; however, many developing countries are catching up. For example, China has seen a consumption swell of 100% over the past ten years (EIA, 2006). With this increased worldwide demand, the supply of oil is becoming constrained. While refineries will continue to be built and investment in heavier oils such as tar sands is heating up (Gold, 2006), the continually expanding demand suggests the currently high worldwide petroleum prices may not be a bubble.

The gasoline and diesel composing the majority of transportation sector energy demands are hydrocarbons which emit carbon dioxide during the combustion process from which power is derived. A scientific consensus has concluded that the increasing CO_2 concentrations in the atmosphere are leading to an increase in global temperatures (Pacala, 2004). While the impact of this rising temperature on the economy, the environment, and civilization is highly uncertain and will never be predictable, many are suggesting that technologies and policies be implemented to control this global warming. This concern may eventually lead to additional taxes on petroleum based fuels or additional costs for reducing carbon intensity (Ney, 2000).

Finally, while the two countries from which the U.S. imports the most oil are Canada and Mexico, the next five countries by import volume are Saudi Arabia, Nigeria, Venezuela, Iraq, and Iran, all countries which are experiencing political instability or have disagreements with current U.S. leadership (EIA, 2006; CIA, 2006). The oil market is a global one, so even conflicts with which the U.S. is not involved, or for countries from which the U.S. doesn't import, will cause an increase in petroleum prices. But the fact that a large portion of reserves are in these unstable regions is a concern for future availability and price. All of these factors contribute to an increase in research and development for alternative fuels.

2.1.3 U.S. ethanol production

The primary use of biomass for energy production in the U.S. is the conversion of corn grain into ethanol. While the industry has existed for the past 25 years, the last five years has seen an expansion from a capacity of 1.5 billion gallons per year, to an expected capacity of 5.8 billion gal/yr by the end of 2006 (RFA, 2006). This growth has occurred for a number of reasons. First, methyl tert butyl ether (MTBE), an oxygenate additive used in gasoline to meet the federal regulations for oxygen content has been banned in 20 states, and is being phased out by gasoline blenders nationwide for fear of future liability. Second, an excise tax credit of $0.51/gal ethanol is awarded to blenders for using ethanol in gasoline (RFA, 2006). This also corresponds with the 2005 Energy Bill which requires a minimum of 7.5 Bgal/yr in renewable fuel production by 2012 (Energy Bill, 2005) and the call by President Bush to replace 75% of petroleum imports from the Middle East by 2005 (Bush, 2006). Finally, technology maturation has decreased the cost of producing ethanol while high energy costs have driven up its price. The result is that ethanol producers are making large profits (Kephart, 2006).

Figure 2.4 shows the growth of the ethanol industry over the past twenty five years. While the industry has been growing at a pace of 10% annually for the past five years with no signs of slowing down, producers are concerned about a couple of issues. First, the corn grain used for ethanol has increased to 15% of the total production (USDA, 2006). This also corresponds with constraints on the available land for future growth in corn production. The impacts of further expansion on the price or corn are uncertain. Moreover, the corn industry is facing possible modification of current subsidy programs based on upcoming legislation and current negotiations with the World Trade

Organization over the fairness of the large U.S. subsidies, amounting to $4B per year for corn farmers (EWG, 2006). The case studies later in the thesis investigate the above questions.

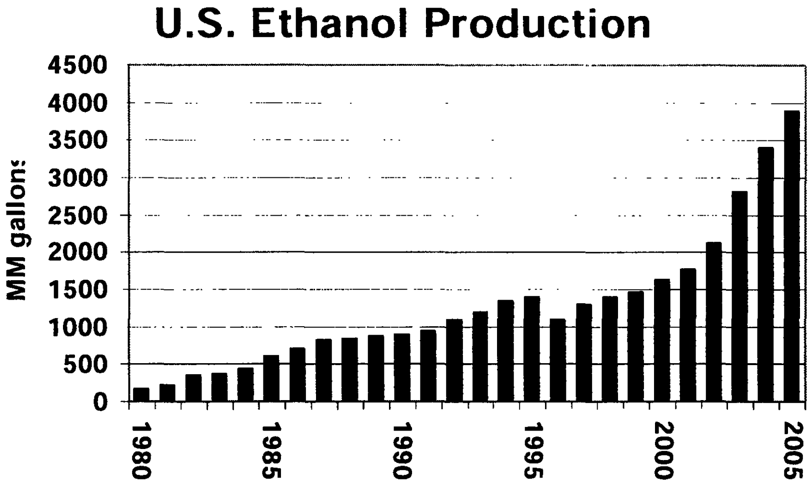

Figure 2.4 Capacity of U.S. ethanol industry over the past twenty five years.

Corn grain is not the only available biomass for energy production. In fact, it only makes up a small percentage of the over total. The rest of this chapter focuses on the rest of this available biomass and the processes and products for which biomass can by used.

2.2 Biomass description

Biomass is the term used to describe all plant-derived, non-fossil organic matter. It comprises all plants, trees, and residues from agriculture or forests. Processed organics such as municipal solid waste (MSW), sewage, manure, and milling wastes are also included. The chemical composition of biomass is primarily oxygenated hydrocarbons, and because of this similarity to fossil fuels, it is a possible energy source for heat and power, or for conversion to transportation fuels and other industrial products. Biomass is considered renewable because it replacement time scale is on the order of a year. While some trees can be centuries old, most vegetation regenerates annually. This section describes some of the advantages and disadvantages of using biomass for energy followed by details of the important considerations for assessing feedstocks, processes, and products.

2.2.1 Advantages and disadvantages

Biomass energy is being explored because of its benefits as a renewable, domestically available material which can be converted into many products, emits zero net carbon dioxide, and provides for rural development. However, the same characteristics which provide these advantages, also present a variety of challenges which much be overcome to enable implementation of large scale biomass facilities.

2.2.1.1 Composition

The chemical composition of lignocellulosic biomass is primarily cellulose, hemicellulose, and lignin – oxygenated hydrocarbons similar to fossil fuels. This similarity enables the conversion of biomass into transportation fuels, chemicals, power, and hydrogen. In fact, many of these conversion processes are derived from hydrocarbon based technologies. A significant advantage of this characteristic is that biomass becomes a form of stored energy, as opposed to other renewables such as solar and wind, which are intermittent and cannot be used on-demand without additional storage capability.

One drawback of the composition is that the oxygen and typically high moisture contents significantly lower the heating value of biomass, and it has a much lower energy intensity (7000-9000 Btu/lb) than coal, natural gas, and petroleum which have energy contents 50-75% higher (Tester, 2005). Another drawback of ethanol as an additive to fuel is its inability to be shipped via pipeline. The tendency of ethanol to pickup water means it typically needs to be hauled over rail or road, adding costs to the fuel end price.

2.2.1.2 Supply

Because of the vast land resources available in the United States, the agricultural and forest industries have the potential to supply a considerable amount of biomass for energy production. Additionally, the excessive amount of waste generated throughout the country provide another possible feedstock. Details of this availability is given later. These supplies are considered renewable as the plants which the biomass is derived from are continually replenishing. Moreover, the biomass in the U.S. is reasonably dispersed, suggesting the potential for local production and distributed generation could be a possible advantage. The following three advantages described in the next several subparagraphs: national security, agricultural development, and waste disposal, follow from this one.

Two possible disadvantages come from these supply characteristics. First, wide dispersion combined with low density cause a potential logistics problem. The economies of scale required for some of the conversion facilities would entail more concentration feedstocks, and the collection and distribution of the available biomass will be difficult. Second, as will be shown in the availability section, the U.S. produces significant biomass, but complete conversion of available lignocellulosic biomass will still only replace about 30% of the nation's current petroleum consumption. So biomass alone will not be able to supply the country's energy needs. This point should also be remembered when addressing national security impacts below.

2.2.1.3 National and energy security

Having a wealth of indigenous biomass energy could have a substantial impact on foreign petroleum imports. A decrease in this reliance would create an economic cushion against future oil shocks and possibly lessen the requirement for a significant defense presence in the Middle East. As was described in the supply section, the U.S. currently imports over 60% of its petroleum with nearly 20% of those imports coming from the Middle East. The continuing stability of oil markets has been identified as a plausible rationale for military intervention in that region (Tester, 2005).

The economic and social ramifications of this high level of importation has been described (Parry, 2003), and will not be discussed in more detail here, other than the identification of petroleum replacement as a metric for biomass energy technologies. Despite that, it is important to realize that complete energy independence is neither likely, nor in the best interest of the country as continued trade encourages development worldwide. Additionally, petroleum resides in a world market, and price shocks in countries from which the U.S. doesn't import oil will still cause the price of domestic gasoline to be high. Therefore, the primary point of increasing domestic energy supplies is to diversify the available options so price volatility does not cause quite the negative impact on the overall economy.

2.2.1.4 Agricultural development

The agricultural industry has long been a foundation of the U.S. economy. Recently though, the industry has required massive subsidies to keep farmers economically afloat. Developing a market for energy crops and agricultural residues can provide a method for diversifying the economic potential for the industry. Also, growth in agriculture often results in the creation of more jobs than in the fossil industries. Ideally, the further development of the biomass industry will increase the productivity of farmers and lower the need of these subsidies, which have amounted to over $150 billion over the past ten years (EWG, 2006).

Despite its potential impact on rural development, the implementation of biomass production and collection can have negative impacts on the environment because of the input requirements of intensive cultivation. The use of additional fertilizer and chemicals can impact downstream ecosystems, while increased water consumption continues to lower aquifer water levels in agricultural areas (Konikow, 2005; Horrigan, 2003). Studies have shown that biomass plantations have negative impacts on surface water flow (Jackson, 2005). Additionally, soil carbon levels can adversely be affected and erosion may lead to declines in subsequent productivity (Wilhem, 2004). Each of these concerns is addressed in the case studies, but much further research is required to ensure the sustainability of these biomass systems.

2.2.1.5 Solid waste disposal

Waste is generated in the United States at unprecedented rates. Landfills and incinerators are currently being used for disposal. The development of technologies to convert this waste into usable products would have significant impacts on land use and resource extraction. Initially landfill gas facilities have enabled power generation from anaerobic digestion, and groups have developed technology to convert animal renderings into liquid fuels (Lemley, 2003), but the potential for converting the lignocellulosic portions of landfills into fuels without incineration can provide fuels while decreasing the land requirements for future waste disposal.

2.2.1.6 Global warming

While the conversion of biomass derived fuels into energy results in carbon dioxide emissions, this carbon was initially incorporated as carbon dioxide from the atmosphere during the plant growth stage of the biomass as was shown in the photosynthesis equation. Therefore, the biomass results in a net zero emission of carbon dioxide from direct use. Emissions from other steps in the life cycle of the biomass must be considered; however, the overall emissions are often much less than fossil fuels. The ethanol case studies demonstrate this with a lowering of greenhouse gas emissions per energy unit of 10-50%. Large scale production of biofuels contributes to the stabilization wedges described by Pacala (2004).

The formation of policies for carbon emission reduction or trading must be careful to include the upstream processes, though. The production of ethanol from corn grain has a higher carbon dioxide emission rate than the production from corn stover. Therefore, the credits provided to ethanol from the two different manufacturing processes should be different.

2.2.1.7 Air/water pollution

Biomass derived ethanol used as a transportation fuel emits less carbon monoxide, nitrogen oxides, and sulfur dioxide than gasoline, primarily due to its low sulfur content and high oxygen content. Ethanol as an oxygenate compares favorably to MTBE because it is not persistent and doesn't cause the groundwater contamination which MTBE does (Powers, 2001). The lower air emissions are witnessed in power generation also, while the biodegradability of biomass based products is important related to issues of human health.

However, these emissions are actually higher for ethanol on a life cycle basis because of the increased number of combustion processes along the supply chain. The overall impact of these emissions is difficult to ascertain as the air pollution effects are localized in rural areas. There are concerns with the emissions of formaldehydes from ethanol and the increased volatile organic compounds emissions resulting from the 10% mixture of ethanol in gasoline (Deeb, 2003). Future mixtures of the fuel should probably be placed at a different point on the mixture curve utilizing the lower vapor pressure of ethanol. Moreover, as more ethanol is used in internal combustion engines, hopefully the designs for emission reductions will focus on the formaldehyde issues.

2.2.1.8 Hydrogen production

While biomass can be converted into a number of products as described below, the ability of biomass conversion to hydrogen is an advantage. As the energy future becomes more directed towards hydrogen as a primary energy carrier, the question of where the hydrogen will come from needs to be addressed. Biomass provides a renewable source for hydrogen. Technology has already been developed to produce hydrogen from biomass through thermochemical conversion such as pyrolysis and gasification (Ni, 2006; Spath, 2003). Further technological advances have been made to catalytically reform biomass directly to hydrogen at low temperatures and pressures (Davda, 2004).

2.2.2 Energetics of biomass growth and chemical composition

Biomass can be considered an energy carrier for solar energy. Intrinsic energy content in the vegetation is captured from solar energy via photosynthesis as carbon dioxide is incorporated as fixed carbon during the growth stage of all biomass. Using sunlight and chlorophyll as catalysts, photosynthesis takes place by the following reaction:

$$6CO_2 + 6H_2O \xrightarrow{h\upsilon} C_6H_{12}O_6 + 6O_2 \quad \Delta G^0 = 480\,\mathrm{KJ/mol} \qquad (2.1)$$

Average solar incidence in the U.S. is 4kWh/m^2/day, and average plant capture efficiency is 1%, suggesting a typical potential yield of biomass is 13 Mtonnes/acre annually. Many factors contribute to this yield, including photosynthetic efficiency, solar incidence, water, and nutrient availability. For example, while efficient ecosystems have a photosynthetic efficiency of 1%, that efficiency can range from the global mean of 0.3% to peak field efficiency of 5% to a theoretical maximum of about 10% (Tester, 2005).

Photosynthesis converts carbon dioxide and water into carbohydrates and other organic compounds. The carbohydrates produced are primarily glucose and sucrose, but can consist of other five and six carbon sugars. While sugarcane contains sucrose and the grains from rice, wheat, and corn contain starch, the largest fractions of global biomass production are cellulose, hemicellulose, and lignin. Other components such as oils, proteins, extractives, and ash compose a smaller fraction of biomass. For this analysis, the starch, cellulose, hemicellulose, and lignin components will be the most important.

Starch is composed of long polymers of α-glucose molecules connected together in chains of α-1,4 linkages with branches formed as a result of α-1,6 linkages. Starch is widely distributed and stored in all grains and tubers, and contributes 65-70% of the composition of corn grain. Due to the α-linkages in starch, this polymer is highly amorphous, and is more readily broken down by enzyme systems into glucose. This is a significant reason why the current ethanol industry utilized primarily corn grain. The gross heat of combustion of dry starch is 7560 Btu/lb (EERE, 2006).

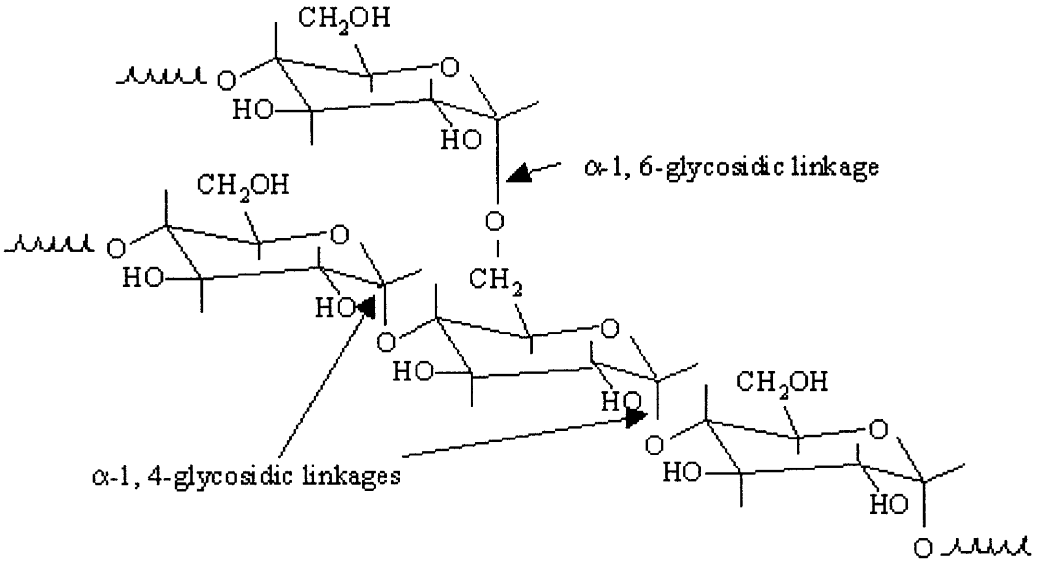

Figure 2.5 Schematic of starch composition

Cellulose is also a polymer of glucose, but as opposed to starch, the monomer units have β-glucose linkages. Cellulose is a principal constituent for the structural framework of wood and other biomass cells. In fact, it is the most prolific component in the global biomass supply. The ß-linkages form linear chains with significant hydrogen bonding leading to a high stability. The cellulose is resistant to chemical degradation as the hydrogen bonding inhibits the bending of the glucose molecules which would occur during the hydrolytic breaking of the polymer. This stability is important for the cellulose's role of providing structure to nearly all plants. Unfortunately, this recalcitrance is problematic for the degradation of cellulose for industrial products. Degradation of the cellulose can occur by its hydrolysis to a cellobiose (glucose dimer) and ultimately to glucose. However, this hydrolysis often requires severe temperature an pH conditions leading to expensive costs. This problem will be addressed in the case studies. The heating value of glucose is similar to starch on a dry basis, with a HHV of 7500 Btu/lb (EERE, 2006).

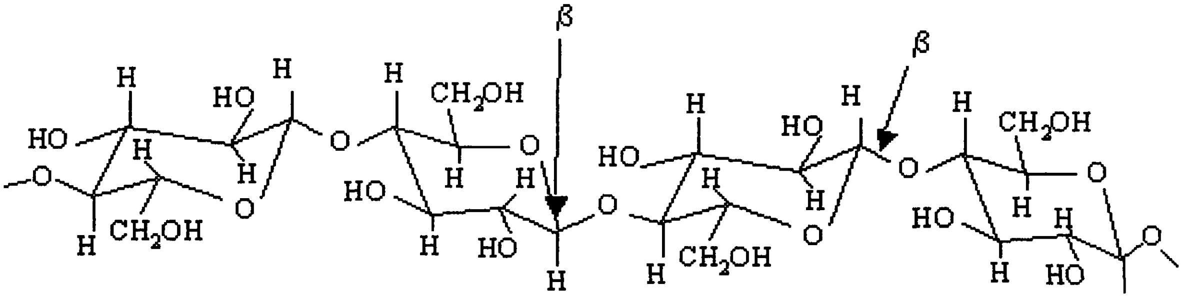

Figure 2.6 Schematic of cellulose composition

Hemicellulose is composed of short, highly branched chains of primarily five-carbon sugars, D-xylose and L-arabinose, and six-carbon sugars, D-galactose, D-glucose, and D-mannose. These component sugars are highly substituted with acetic acid and uronic acid (EERE, 2006). The branched nature of hemicellulose renders it amorphous and relatively easy to hydrolyze to its constituent sugars compared to cellulose. However, the hemicellulose is, along with lignin, wrapped around the cellulose matrix, causing more difficulty in the degradation of cellulose. Another problem with hemicellulose is that the component sugars, especially the pentoses, are much more difficult to ferment into ethanol.

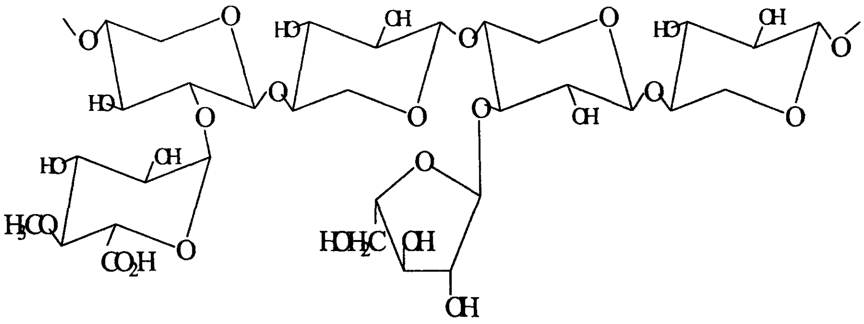

Figure 2.7 Schematic of hemicellulose composition

Lignin is the major non-carbohydrate, polyphenolic structural constituent of wood and other plant material that encrusts the cell walls and cements the cells together. It has a highly polymeric substance, with a cross-linked, highly aromatic structure derived principally from coniferyl alcohol ($C_{10}H_{12}O_3$) by extensive condensation polymerization. Lignin's higher heating value is 9111 Btu/lb (EERE, 2006). Because lignin is non fermentable, it is primarily useful in thermochemical processes, and is often simply combusted for heat and power. The pulp and paper industry has been using waste lignin as an energy supply for many years. Researchers have looked at potential higher value products based on its phenolic composition, but have not been terribly successful.

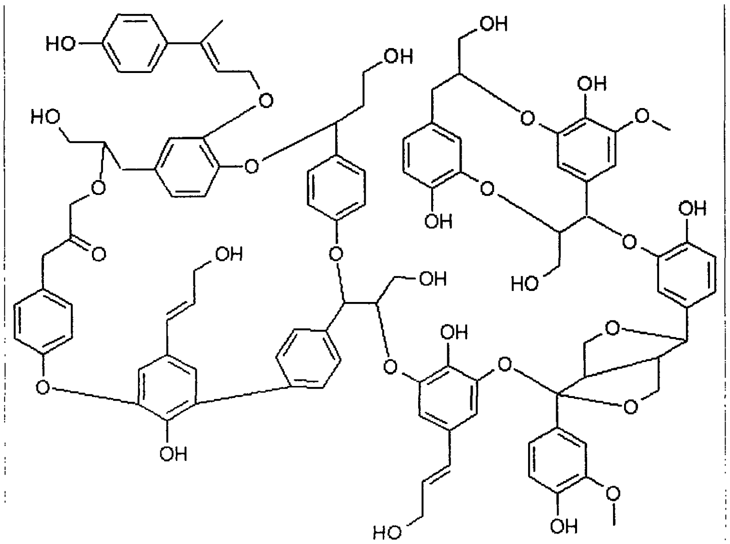

Figure 2.8 Schematic of lignin composition

These four components compose the majority of global biomass. The following section describes some of the different forms this biomass takes and the overall availability for energy production.

2.2.3 Biomass feedstocks

The primary feedstocks for current bioenergy utilization are corn grain and sugarcane for ethanol production, oilseeds for biodiesel production, wood chips and landfill gas for power generation, and wood and shrubs for household heating, primarily in developing countries. As the use of biomass for industrial production expands, the portfolio of biomass options will also increase. The above feedstocks will continue to provide niche roles in energy production, they are limited in their production capability to lignocellulosic materials. This biomass can be described by six primary categories: energy crops, agricultural residues, primary forest production, forest residues, mill wastes, and urban wastes.

	Corn grain	Corn stover	Switchgrass	Soybean	Poplar	Bagasse
Starch	72.4	0.0	0.0	17.4	0.0	0.0
Cellulose	6.0	36.2	32.0	8.7	42.7	40.3
Hemicellulose	6.0	23.2	25.2	8.7	18.7	25.7
Lignin	0.0	18.5	18.1	0.0	29.2	23.9
Protein	9.5	0.0	0.0	44.2	0.0	0.0
Oil	4.5	0.0	0.0	20.9	0.0	0.0
Extractives	0.0	8.1	17.5	0.0	2.6	3.9
Acids	0.0	3.2	1.2	0.0	4.9	2.3
Ash	1.5	10.7	6.0	0.0	2.0	3.8

Table 2.1 Composition of various biomass feedstocks (NREL, 2006)

Grains and oilseeds are the primary feedstocks for current ethanol and biodiesel production. The three primary examples are corn, wheat, and soybeans, which cumulatively account for 60% of total U.S. cropland (USDA, 2006). However, the continued growth of these crops for energy production is constrained by their input intensity compared to the available energy which can be derived from their products. Therefore, many expect that other crops dedicated to energy production will be further developed. Examples of these potential energy crops are switchgrass, or other herbaceous perennial grasses, and willow, or other fast growing trees. These lignocellulosic crops have the potential to provide higher biomass yields with much less energy and nutrient inputs. Additionally, these crops are native to different regions in the country and are hardy enough to grow on less fertile cropland. Despite these advantages, production of energy crops is limited at present because of a lack of markets.

Switchgrass is receiving the most attention form researchers, and a number of groups have published reports suggesting the viability of large scale production. Table 2.1 shows the breakdown in composition of switchgrass compared to other biomass feedstocks, and Figure 2.9 provides a review of the switchgrass yields for the various studies. Because development of the crop is still in preliminary stages, many expect improvements in the genetics of the crop to lead to even more yields. One caution to that expectation is that the switchgrass genome is considerably less understood than corn. Moreover, since the crop is perennial, the continual improvements from new plantings annually will not occur. However, using an average of the maximum yields in Figure 2.9, and assuming complete conversion of the sugars, the theoretical ethanol production from switchgrass is 1200 gallons/acre, compared to 400 gal/acre from corn, or 600 gal/acre if the entire corn plant is used. However, estimates of the cost of switchgrass production range from \$30 to \$150 per ton (Schmer, 2006, McLaughlin, 2005; Walsh, 1998), with the upper end of that range being too expensive for competitive ethanol production.

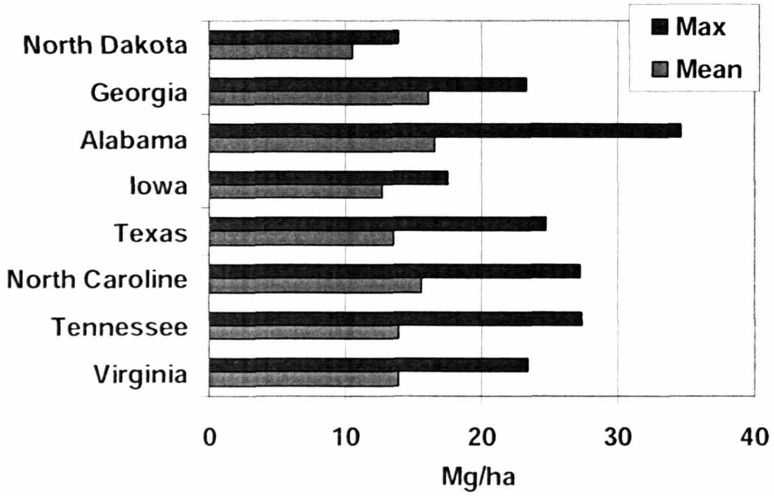

Figure 2.9 Switchgrass yields for test sites in multiple states (McLaughlin, 2005)

Along with energy crops, agriculture can provide potential bioenergy feedstocks through the utilization of residues, either material left on the field after grains and seeds have been harvested, or the manure from animal wastes. This lignocellulosic material can be collected and converted to industrial products. Potential agricultural residues are corn stover, wheat straw, rice straw, sorghum residue, and sugarcane bagasse. Collection of these materials may have additional benefits above the economic potential of products sales. The removal of crop residues is often associated with no-till cultivation practices, saving money on field work and limiting erosion. However, the removal can also be problematic because of the loss of nutrients and soil carbon. The impact on subsequent year yields or global warming might actually be detrimental.

Corn stover is considered the most widely available lignocellulosic material available today. The biomass from corn stover is typically equivalent to the dry mass of the corn grain for an individual corn plant. Groups are beginning to develop projects investigating the harvest and distribution logistics of the stover (Sokhansanj, 2003; Perlack, 2003; Glassner, 1999). However, the sustainability of this corn stover removal is still uncertain. Wilhem (2004) published a review looking at potential affects of the removal of corn stover, with reports varying from a requirement to put additional stover back onto the field after corn grain harvest, to the acceptability of removing 80% of the stover. More focus is given to corn stover and its potential conversion to ethanol in the case studies.

Much of the global biomass grows in the world's forests and jungles. In the U.S., forests cover 33% of total land area (ORNL, 2005). Some of this land is unreachable while some is reserved for parks and wilderness. Most of the remaining is open for harvest, primarily sawlogs and pulpwood for the timber and pulp and paper industries. While primary wood production from forests could conceivable be used for biomass energy, the wastes and residues within the forests and from wood processing mills are an attractive feedstock. Already, the forest product industry utilizes a small percentage of their waste stream for energy production, but the commercialization of improved biomass conversion technologies will provide outlets more complete utilization. Other potential forest base feedstocks are the residues generated by logging, cultivation, and forest clearing operations. Moreover, the US Forest Service believes that forest health may be improved by the removal non-merchantable biomass from rough and rotting trees and underbrush (ORNL, 2005). This removal could provide additional resources.

Potential wastes and residues are not limited to agricultural or forest production. Urban wastes are also potential sources. Municipal solid waste (MSW) is more-or-less trash, consisting of food wastes, grass clippings, pallets, discarded furniture, lumber scraps, etc. The organic fraction of this trash is available for potential biomass conversion, but collection and separation from non-usable materials may be difficult (Wiltsee, 1998). Another urban source which is receiving increase attention are waste oils from restaurants. While the supply of this material is limited, it can provide niche urban markets.

The utilization of these available feedstocks is inhibited by two general themes. First, the collection of distribution of the biomass may be difficult. For example, the collection of waste biomass from forests is fraught with problems of how to manage the removal economically, without causing external environmental impacts. Additionally, the density of this biomass is often very low leading to higher distribution costs (Kumar, 2005). Second, conversion processes for the biomass are not optimized. While simple combustion for heat and power is an option, resulting emissions may be a problem, and the economic value of that energy may not be high. Technology needs to be provided to overcome these two barriers before more complete utilization of available biomass occurs. Meanwhile, technology assessment of the biomass removal and conversion should be continuously undertaken. There is no clear answer as to whether the removal of forest or agricultural residues actually makes economic and environmental sense. The following case studies will attempt to elucidate information pertaining to that question for the specific example of corn grain and residue.

2.2.4 Feedstock availability

A number of researchers have estimated the overall potential for biomass production, both in the U.S. (ORNL, 2005) and globally (Giempietro, 1997; Berndes, 2001; Hoogwijk, 2003; Wolf, 2003). Berndes (2003) performed a review of the studies and found an incredible range from the various analyses. Estimating the total usage of bioenergy in the year 2050, value were reported from a low of 50 EJ to a high of 450 EJ, compared to an estimated overall consumption of 1200 EJ at mid-century. This high variance is due primarily to different assumptions for the uncertain parameters of land availability and biomass yield. A common concern for all of the studies is that they do not sufficiently investigate the interaction of biomass energy production with other land uses such as food production, biodiversity, conservation, and soil carbon sequestration (Berndes, 2003). While this thesis does not focus on the question of global supply, the questions relating to other land and biomass utilization is addressed.

Currently, the use of biomass for industrial products basically consists of ethanol production from sugarcane in Brazil and corn in the U.S. While the production of ethanol from the sucrose in sugarcane is very inexpensive, the North American climate is less suitable for sugarcane production. By contrast the corn grain comprises 70% starch, a sugar polymer which needs to be degraded into fermentable sugars. While this process is more expensive, it is still more feasible than using other sugar polymers, as will be shown later. However, with 15% of corn production devoted to ethanol production, constraints from corn demand for animal feed will begin to drive up prices as ethanol production continues to grow.

One suggestion is to expand the amount of corn acreage. This option may run into difficulties as farm land is already receding nationwide, and planting corn instead of other crops will affect the end use costs of those other products. A small percentage of acreage is currently set aside for the USDA Conservation Reserve Program, but that land is typically highly erodable and not the best for agricultural production. Moreover, the current usable biomass production rate for corn is only about 3 Mtonne/acre, considerably less than the theoretical yield calculated above.

Another suggestion is to move towards energy crop production combined with the utilization of the available agricultural and forest residues, and urban and mill wastes. This lignocellulosic biomass is more difficult to break down into fermentable sugars, but is much more plentiful and can be grown with much less input intensity than corn. The economic and environmental performance of this process will be described later, but right not the focus is on availability. A recent study (ORNL, 2005) estimates that the potential availability of this lignocellulosic biomass in the U.S. is over 1.3 billion tons annually. Figure 2.10 shows the breakdown of that potentially available biomass. Assuming complete utilization for conversion to ethanol using the optimized process suggested later, this biomass could contribute.120 billion gallons of ethanol per year, 25% the total transportation sector, with coproduct electricity amounting to 300,000 GWh, nearly 8% of the total power sector. While complete utilization would be difficult as simply construction the infrastructure for that level of production would approach $200 billion, the study shows that biomass is available and can contribute to the overall energy supply without requiring all of the available farmland. In the report, about 300 million tons of biomass are provided by energy crops from 30 million acres, less than half of current corn acreage and the amount of CRP land.

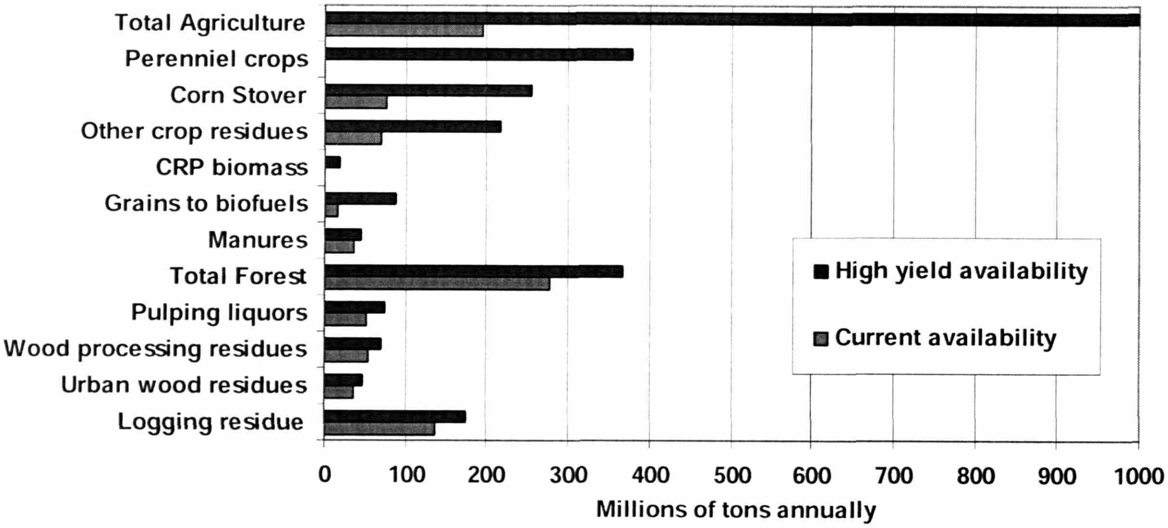

Figure 2.10 ORNL (2005) lignocellulosic biomass availability

2.2.5 Biomass processes and products

The conversion of biomass to fuels, power, or other industrial products proceeds through three primary types of processes: biochemical, thermochemical, and mechanical conversion. Within each of these general categories are many different technology alternatives. Most of these processes lead to specific products – fuels, chemicals, electricity; although there can be some variation. While some of the process options are specific to different types of biomass feedstock, others are ubiquitous. This chapter will given an overview of the basic concepts behind a few of these processes. Figure 2.11 charts out a number of the conversion technologies and potential products. More emphasis on ethanol production via sugar fermentation will be provided in the case studies that follow in subsequent chapters.

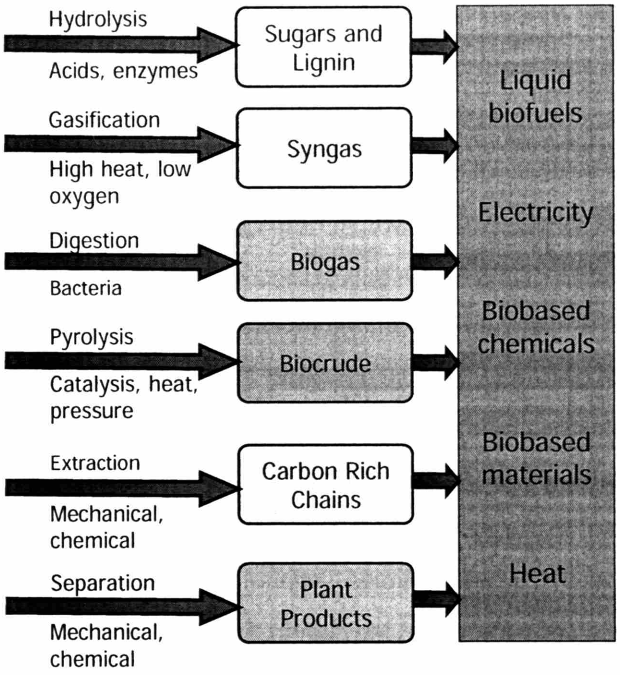

Figure 2.11 Technologies for biomass energy conversion

Thermochemical conversion pertains primarily to the processes which are operated at elevated temperatures with the most common being basic combustion, or the burning of biomass in the presence of oxygen. The heat provided by the combustion reaction can be used to generate steam and electricity either by itself or cofired with coal (Robinson, 2003). The combustion of biomass is limited by the lower heat value of the material (7000-9000 Btu/lb) as compared to fossil fuels and by the typically high moisture content. Additionally, electricity generation via combustion has a limited efficiency (20-25%) due to the Carnot efficiency (Tester, 2005).

Interest in the use of gasification technology has been increasing (DOE, 2001). In the gasification process, the biomass is partially oxidized at 800-900°C into a synthesis gas composed primarily of H_2, CO, and CO_2, but also including CH_4, tars, and other impurities. After the gasifier, the syngas is cleaned of impurities and the H_2/CO ratio is optimized using the water gas shift reaction. The syngas can be used downstream as a low heating value input to a combined cycle power generation unit. Additionally, the syngas can be converted into Fischer-Tropsch liquids or other chemicals. The gasification route has the disadvantage of having considerably high capital costs. Moreover, the complexity of the system makes operation difficult. Gasification technology has been commercialized by a few companies for the conversion of coal or petroleum coke to electricity, synthetic fuels, and chemicals; however the process is yet to be utilized on a large scale as of yet due largely to the high capital costs. Biomass gasification uses a lower energy value fuel, so future development of biomass gasifiers will probably be preceded by the coal industry (Dry, 2004).

Pyrolysis and hydrothermal conversion processes are also in various stages of development. Pyrolysis occurs in the absence of air at temperatures around 500°C, and produces a bio-crude which can be upgraded to usable fuel, but the economics of the process and the low quality of the fuel have limited its commercialization (McKendry, 2002). The hydrothermal processes use high temperature and pressure water as a solvent for the conversion process. Changing World Technology has utilized a hydrothermal process for the conversion of turkey ofal into liquid fuels and other coproducts (Lemley, 2003). Huber (2006) has demonstrated the reformation of biomass for hydrogen production and the hydrogenation into liquid fuels. Additionally, the gasification process has been studied in supercritical water (Yan, 2006). Except for a few cases, these process have yet to be commercialized, but process advancements and catalyst innovations may push the development.

Biological conversion of biomass occurs primarily through fermentation, with the conversion of corn grain and sugarcane to ethanol being the most significant route (Bothast, 2005). Fermentation is not limited to starch or sucrose, though as most any sugar can be used. Moreover, chemicals other than ethanol, such as sorbitol, levulinic acid and glycerol (Holladay, 2004). Moreover, metabolic engineering tools are allowing for the designed fermentation of products such as hydrogen (Woodward, 1996). Primary work in this area is focused on the production of ethanol from lignocellulosic material, and that will be a primary focus of the later chapters. A block flow diagram of the process being developed at NREL is given in Figure 2.12. While this process has not been commercialized on a large scale, Iogen is operating a pilot plant in Canada with wheat straw as the feedstock. (Lawford, 2003).

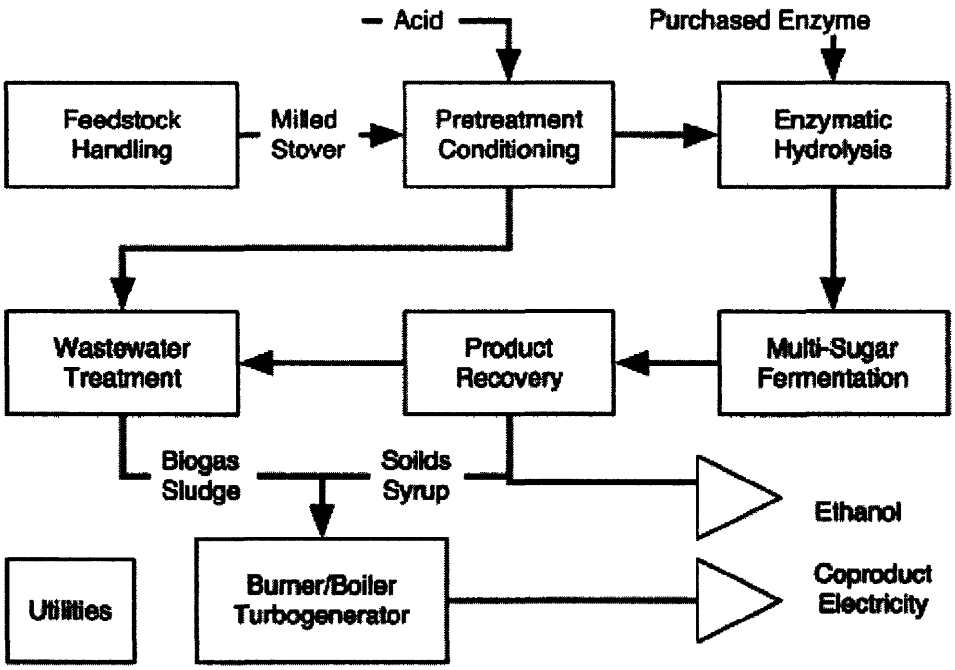

Figure 2.12 NREL lignocellulosic ethanol schematic (Sheehan, 2003)

Anaerobic digestion is another biological conversion where organic material is converted to biogas, primarily methane and carbon dioxide, by bacteria in the absence of oxygen. The biogas can then be used to operate a small generator. Small scale use of biogas has been demonstrated in villages in developing countries using dung and on farms using manure. A primary problem is maintaining operability with the low energy content fuel (McKendry, 2002). Larger scale implementations are becoming popular at landfills, where the landfill gas can be collected and converted to power.

The main example of mechanical conversion for bioenergy is the extraction and esterification of oilseeds and previously used oils for production of biodiesel. Biodiesel can be an adequate substitute for diesel, especially in large urban areas with significant waste cooking oil. However, on a large scale basis, biodiesel production is limited more by agricultural constraints than even corn grain ethanol (Giempietro, 1997).

While many of these conversion processes have made considerable progress in development, combustion, fermentation of starch and sucrose, and anaerobic digestion of landfill gas for power have been the only large scale commercialized processes. While some of the other technologies are better suited for distributive generation or other niche markets, major advancements of these conversion technologies must occur before biomass can be utilized on a significantly larger scale.

2.3 Future of biomass

The above description of important characteristics for biomass energy results in a number of questions for its potential implementation. Below are a number of questions, some of which will be addressed throughout this work, which need to be answered to properly assess the economic, environmental, and social performance of large scale bioenergy systems. Because this thesis focuses primarily on ethanol production, the initial questions will be addressed from the point of view of a policy maker or industrial leader looking at potential incentives, research and development, or technology deployment.

Current biomass energy production is concentrated in the corn ethanol industry and generates very polarized viewpoints because of uncertainties in overall energy balance and government subsidies. However, a much greater potential can be realized by the utilization of lignocellulosic biomass rather than starch from grains. Unfortunately, lignocellulosic biomass has disadvantages also. Primarily due to its heterogeneity and lower energy density, the collection and processing of biomass has large economic and energetic costs. Moreover, many of the environmental and health impacts of the processing and use phases for biomass are similar to those for fossil fuels.

2.4 Biomass questions

Before a transition to bioenergy requiring a heavy economic investment is made, the following questions must be answered: 1) Does the use of biomass as a feedstock for fuels, power, and chemicals, make sense socially, economically, and environmentally? If so, 2) What is the best supply chain configuration and process flowsheet for biomass conversion?

The goal of this case study is to use an expanded technology assessment methodology which is described in the next two chapters to provide answers to several specific questions:

Production cost

- What are the critical cost factors in ethanol production?
- Is ethanol competitive with petroleum?
- How much more corn can be used for ethanol?
- What are economic impacts of ethanol/corn subsidies?

Environmental impacts

- What is overall greenhouse gas abatement?
- Are local air impacts really improved?
- Does ethanol production lead to further intensification of agriculture?

Energy utilization

- Does the production of ethanol lower reliance of foreign petroleum?
- Is energy required for production greater than available energy?

Advanced feedstocks

- How do the above objectives change with cellulosic ethanol?
- What technology advances are most critical for commercialization?

2.4.1 Assessment methodology overview

The primary case study will assess the use of corn as a feedstock for the production of ethanol, which is currently a commercialized and expanding industry. An initial look will be taken at the current process as it has been studied extensively in the literature, with an emphasis on the variability and uncertainty of thee energy balance question. From there, an extensive investigation of the incorporation of lignocellulosic feedstocks such corn stover and switchgrass will be performed. While details of the assessment methodology are provided in the next chapter, an overview is provided here.

A life cycle approach is necessary for any analysis of biofuels because the feedstock production step – growing the agricultural crops, is incredibly energy intensive. Understanding the full environmental impacts is impossible without including the effects of farming. The supply chain for biofuel production can be simplified into three primary stages – biomass production, transportation, and processing. Specifically, an initial goal is to determine the relative magnitudes of the three stages between the three technologies. As proxies for overall environmental impact, the energy requirements for fertilizer production (corn production), diesel fuel (transportation), and utility requirements (processing), will help determine these relative effects.

Material and energy balances for the stages of processing will be simulated using Aspen and Excel models. These balances will then be input into a combined Access and Excel program which calculates the life cycle inventories and associated environmental impacts. Probability distributions for each of the impacts are generated to analyze the impact of uncertainty. The economic model will use standard chemical engineering costing for the facility. However, this analysis will be combined with the upstream costs for corn production and transportation to ensure economic sustainability throughout the process chain. After the initial analysis, a more thorough assessment will look at all impacts associated with the process to determine the feasibility of using the energy requirement proxy. Also, a more thorough analysis of the impact of the usage of genetically modified organisms as well as the soil sustainability of energy crops will eventually be attempted.

The case of using agricultural crops for fuels and chemicals presents an ideal example where these questions need to be investigated. The example covers interesting questions of energy and national security policy, rural economic development, and advanced science. While the phrase "green is good" is often used to suggest that bio-based products are renewable and should be expanded, a comprehensive and systematic analysis of these technologies must be performed to determine which conditions allow bioenergy to have an optimal economic and environmental performance. A number of assessments have been performed looking at the environmental impact of utilizing biomass feedstocks for ethanol or other products. As the primary commercialized technology, ethanol production from corn grain has received the most attention in the assessments with much focus on the energy balance around the life cycle of ethanol production. Other analyses have looked at similar environmental and economic assessments of potential, but not commercialized, technologies and products. However, the existing analyses lack a clear decision process, one which helps assess the various potential feedstocks, processes, and products, and determine which direction industry and government should take regarding research and development, environmental and economic policy, and process commercialization considering all uncertainty. While these concepts seem broad, a comprehensive methodology is able to address them all.

The renewed interest in utilizing agricultural materials for energy and products has been driven by a number of factors. The most important of these are high energy prices, environmental concerns, national security, interest in developing new agricultural markets, and the accelerated development of biotechnology. Additionally, it is the only renewable option with the foreseeable potential to provide liquid fuels for the transportation industry. The technology development has not yet reached an economically feasible point; however, a number of scenarios exist which would push bioenergy into the forefront. The following six sections discuss scenarios or areas of research which clearly will impact the future of bioenergy. Each of the scenarios also serve as a basis for the questions which need to be answered in the analysis of the use of agricultural products for fuels and chemicals.

As a note, these are a subset of the scenarios which have an important impact on the overall effect of biofuels. Decision makers may have other important considerations. Additionally, the answers to the questions will be different based on the utility and objective function of the decision makers. Therefore, this write-up simply illustrates a methodology for comprehensively assessing the overall system.

2.4.2 Important considerations

The following paragraphs list a handful of questions which are critical for the future of biomass energy, but which won't be a focus in this work. They are subjects which could be thought of as future work specific to biomass energy

2.4.2.1 Carbon taxes (Kyoto Protocol)

In the above discussion of economic competitiveness, the concern of externalities of energy production, and the lack of their contribution to the cost was briefly mentioned. One possible change to this status quo would be the implementation of any global warming policy which included the regulation of greenhouse gas emissions. One potential policy is the Kyoto Protocol (UN, 1997). This protocol is an international treaty which calls for the reduction of greenhouse gas emissions by individual countries of 10% under 1990 levels. Primary tools for this reduction will be increased energy conservation and efficiency. However, the substitution of fossil fuels by non carbon dioxide emitting energy sources such as solar and wind is another option. Finally, forestry and agricultural land use has an impact on a country's inventory as it effects the amount of carbon dioxide taken up by the biosphere. Although, how land use will be accounted for is not completely determined.

The use of biomass for fuels and chemicals relates to the issue of land use and its accounting in the treaty is also unclear at this stage. While bioenergy is considered a renewable energy, as opposed to solar and wind power, its use as a combustible fuel releases carbon dioxide. However, the carbon dioxide emitted during use is considered to be negated by the uptake of carbon dioxide by the plant during biomass growth. Currently, the proposed system would regard biofuels as carbon dioxide neutral fuels, meaning their use would not count as part of the carbon dioxide inventory. Unfortunately, this is a little simplistic as the upstream energy requirements of agriculture and production change the carbon balance.

To reconcile this, a proper accounting system for carbon dioxide emissions from different fuel sources needs to be developed to ensure that emissions and credits are not double counted. Once that is accomplished, the implementation of carbon taxes could be a policy for curbing carbon dioxide emissions to satisfy Kyoto. If implemented, this carbon tax would have a direct impact on the economic competition between petroleum and ethanol derived from agricultural sources.

Key questions – Should the Kyoto Protocol directives on biofuels be modified to better allocate greenhouse gas emissions? What impact will that have on the competition between ethanol and gasoline.

2.4.2.2 Soil carbon

A large uncertainty facing the developing of an accounting system for the greenhouse gas emissions of land use is how to treat soil carbon. The cycling of carbon between the atmosphere, vegetation, and the soil is important in understanding the overall fate of carbon dioxide and determining which policies should be implemented to lessen the impact of global warming. Complicating matters is that the stability in vegetation and land is not as well understood or controllable as in the atmosphere. Fires, tillage, deforestation, etc. have a considerable impact on how transport of carbon dioxide to and from the atmosphere takes place. Moreover, this uncertainty should be a major concern of researchers investigating the production of biomass, whether for agriculture and forestry for industrial products or for permanent growth.

Specifically, soil carbon cycling could have a major impact on how much biofuels reduce greenhouse gas emissions, and a true carbon tracking system would have to included the effect of soil carbon. Unfortunately, the research on this subject, especially predicting well into the future has not given adequate results on the impact of such important matters as greenhouse gas emissions, or more importantly, future crop yield. A parametric study needs to be performed which puts upper and lower bounds on the impacts of soil carbon specific to these concerns. Additionally, how these bounds relate to future economic and environmental performance of biomass energy should be determined.

Key questions – Will increased production of agricultural crops for industrial purposes significantly lower soil carbon and reduce future crop yields? What percentage of carbon dioxide emissions come from soil carbon and how does that change with modified land use?

2.4.2.3 Rural development subsidies

The agricultural industry in the United States is heavily subsidized (this is additional to the subsidies for ethanol blenders which was discussed above). With global free trade treaties which discourage production subsidies, the current system is not sustainable. Already, a WTO judgment has gone against the U.S. for their subsidies on certain crops. The impact of this on the rural economy is yet to be seen, but significant changes to the American agricultural system are certain to continue.

One possible solution is to develop new products for internal consumption which can be developed from the expansive rural lands in the country. Investing in crops other than the primary corn, soybean, wheat, and cotton could move the industry into a more sustainable direction. Energy crops for local use are an example. A new system of agricultural subsidies would have an impact on the viability of ethanol produced from a non corn feedstock.

Additionally, agricultural advances over the last century have had led to an incredible increase in productivity. A side effect has been the likewise increase in the energy intensity of this production. More recent technology advancements are looking at optimizing fertilizer and pesticide treatments to increase efficiency. A further concept is to begin taking advantage of the other resources on the farm, everything from wind and solar power to the utilization of the agricultural waste products. Subsidizing technologies to increase the overall energy efficiency of on the farm processes will help in decreasing the production costs of agriculture.

Key questions – How much energy efficiency can be gained in agriculture by growing different crops, capturing other energy sources, and utilizing wastes as coproducts? What monetary subsidies are necessary to achieve this increase in efficiency?

2.4.2.4 Development and acceptance of genetic engineering

The genetic modification of agricultural crops for drought resistance and self nitrogen fixation would be a huge step towards the decrease in energy intensity. Currently, half of the embodied energy in corn ethanol production is from nitrogen fertilizer. Significantly reducing this requirement while also keeping the nutrient level of soils high would be a major step. Additionally, another energy intensive aspect of large agricultural production is irrigation. Designing crops which can better utilize water would be a bonus not only for food production, but also for possible energy production. The economic impact of each of these technology developments would be big; however, the environmental impact would be huge.

2.4.2.5 Incorporation of waste and trash as feedstocks

The amount of waste produced by industry and personal consumption in the United States is immense. Decreased consumption is the best solution to this problem. However, the development of processes which can utilize this waste as a feedstock is a big step. A number of technologies are on the verge of commercialization. Biofuel production is an example of one that has the possibility to move from using agricultural products to the incorporation of cellulosic wastes from urban centers. The economics of the production would be considerably impacted by the use of a negative value feedstock, where a tipping fee would be paid to the producer rather than the other way around.

Key questions – What is the estimated economic value, locally and globally, for these technology advancements? How would other technologies or policy implementations compare?

Chapter 3 Technology assessment methodology

This thesis has two overarching objectives. 1) present a methodology for multi-objective technology assessment and decision making within a large scale energy system and 2) apply that methodology to an assessment of transportation fuels development and production, primarily biofuels. While the previous chapter provided an introduction to biomass energy systems, this chapter will focus on a review of technology assessment tools and a proposal for a methodology which integrates some of these tools together. Subsequent chapters will focus on the application of these integrated tools to the biomass energy problem.

The methodology development is based out of a chemical engineering framework, so the basis for the technology assessment will be traditional process design. However, four additional themes will be woven into the design structure.

- Expanded system boundaries
- Environmental performance assessment
- Hierarchical, multi-objective optimization
- Uncertainty propagation

Before describing the integration of the tools, an overview of these concepts, and others from the technology assessment literature is given.

3.1 Traditional chemical engineering process design

Throughout the thesis, the difference between technology assessment and process design is a fine line. More explicitly, the former includes varying levels of detail of the latter. While, the work does not propose a detailed engineering design for a biomass energy facility, the process simulation and economic assessment tools are used for a simplified process design. Because this framework is provided as an extension for chemical engineering process design, a short description is given here.

The method of hierarchical design developed by Douglas (1988) is a standard starting point for the complex task. Hierarchical process design is a system of generating flowsheets for specific processes, using block flows which are subsequently decomposed to finer detail until reaching unit operations, such as reactors, distillation towers, heat exchangers, etc. For example, ethanol is manufactured by the fermentation of corn, so the preliminary step would be a one block process with corn as the feedstock and ethanol as the product. The next step in the hierarchical process is successive refinement. In this step the block flow is expanded to include two stages; the first is the reaction block which is followed by the separation block. At this step the conversions for each of the flows into and out of the blocks are refined to better define the process.

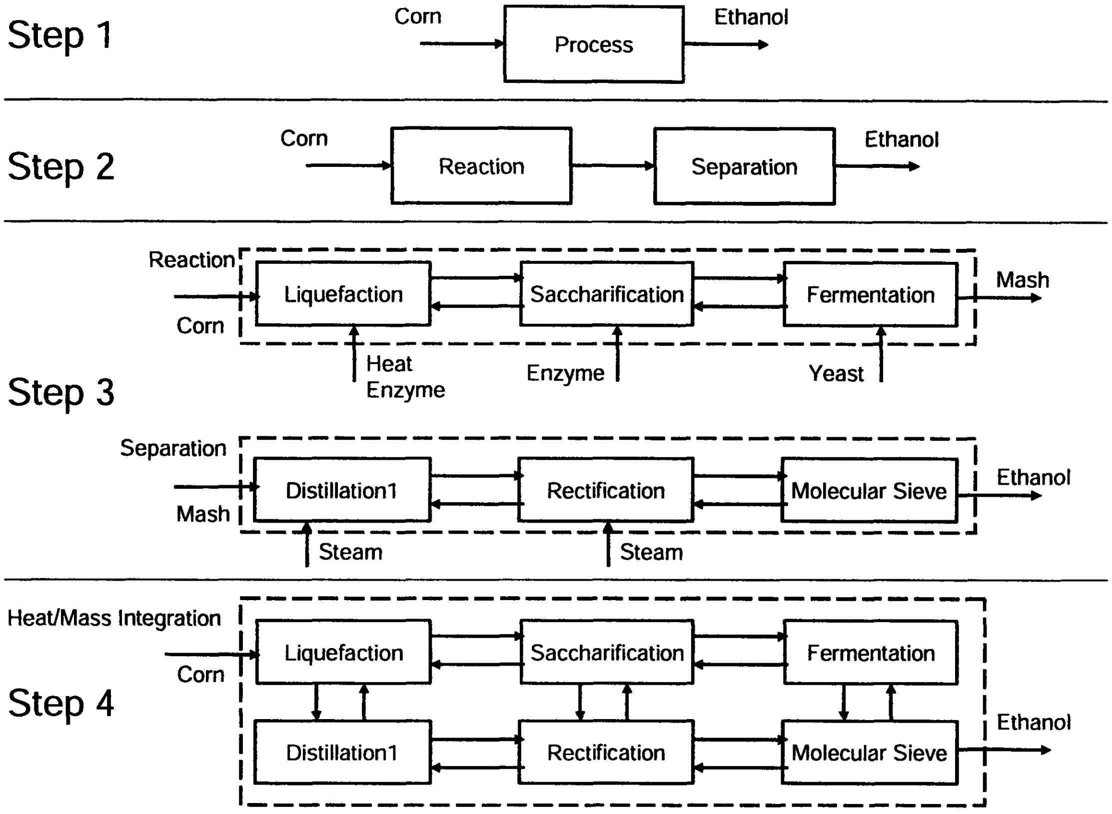

Figure 3.1 Hierarchical chemical engineering process design

In the example, the overall conversion is a combination of a hydrolysis reaction where the polymer starch in the corn grain is converted to its component glucose. This is followed by a fermentation reaction, where the glucose is converted to ethanol. The same structure is used for adding detail to the separations block to arrive at a series of distillation towers to break the azeotrope in the ethanol-water mixture (McAloon, 2000). Unit operations are defined for the various process steps, and optimization using heat integration, process intensification, and other tools is used to better define the process. This successive refinement is continued on until a detailed process flowsheet has been developed. Figure 3.1 shows the steps associated with this hierarchical analysis.

Once a detailed process flow sheet has been designed, a process simulator such as Aspen Plus (AspenTech, 2006) can be used to mathematically simulate the material and energy balances in the chemical process. Figure 3.2 depicts a simplified Aspen Plus process flowsheet for the corn grain ethanol process. These process flows are then used to design the specific unit operations for the entire process. For example, using vapor flow within a distillation column, the required diameter for that column can be estimated. Using the calculated diameter, along with the height from a different calculation, the overall size of the tower can be defined, and the construction cost can be evaluated using existing cost estimations from various textbooks and other source (Peters, 2002; Turton, 2003; Biegler, 1997) (see the economic assessment section for further details).

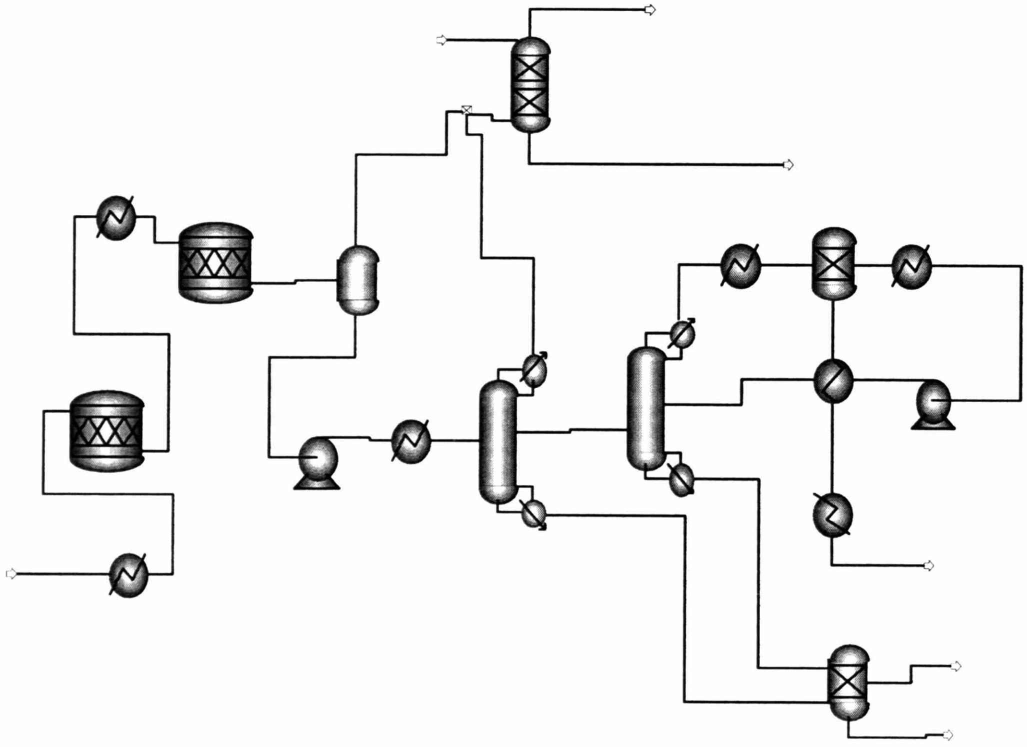

Figure 3.2 Aspen Plus flowsheet for ethanol production from corn grain

These calculations can be performed for all of the major equipment, and an estimate of the overall capital cost can be found with the appropriate additions for utilities, land, debt, etc. Operating costs can also be estimated using the material and energy balances combined with raw material costs, product prices, and other associated costs such as labor, overhead, administration, taxes, and insurance. The capital and operating costs are combined at attain an economic metric for the performance of the hypothetical facility.

This is the level of detail that most traditional chemical process designers use when making industrial level decisions as to whether a process is feasible or not, both technically and economically. At this point, the economic performance of the potential process is assessed with a Net Present Value (NPV) or similar calculation (see below). This economic assessment is used to optimize the process and make decisions as to whether the projects should go forward. However, because of the onset of more social and environmental concerns in industrial design, this paradigm is no longer sufficient. Process simulators are very powerful tools, but to this point they still are unable to evaluate all of the economic, environmental, and social implications of the processes of which they are models.

For example, as will be shown in the economic assessment section below, the initial process design results in an total annualized cost of production of $1.00/gallon of ethanol, while the current price of ethanol is more than twice that. Based on that information, a decision maker would be dumb not to go forward with the project. However, there are initial considerations. First of all, even though the capital would be paid back quickly, finding $50 million in available capital is not insignificant. Second, this production cost is based on specific prices for corn, coproduct DDGS, and natural gas, all of which have relatively high price uncertainties, especially with growing demand for corn and natural gas and a saturated DDGS market (Wald, 2006). Finally, the price of ethanol is dependent on currently high energy prices and is artificially boosted by a $0.51gallon subsidy (RFA, 2006). On the other hand, the price could rise even higher with potential carbon emission regulations All of a sudden, the decision moves beyond the technical aspects and into a realm of trying to predict commodity prices and future policies.

The traditional practice of chemical engineering process design needs to be expanded to include the themes listed at the beginning of the chapter. The following sections introduce frameworks and tools used to integrated these other considerations.

3.1.1 Decision framework

One of the primary shifts applied in this work is a transition from technology assessment being a "design problem" to a "decision problem" (Hoffmann, 2001). The decision becomes to maximize an objective function under the constraints of the system. In mathematical terms, this becomes an optimization problem as shown in Equation 3.1, but with the added complexity of multiple objectives, an expanded system, and uncertainty. Each of these added complexities will be described in more detail in the next section.

$$\begin{aligned} \text{Min} \quad & \mathbf{c}^T\mathbf{x} \\ \text{s.t.} \quad & \mathbf{A}\mathbf{x} \geq \mathbf{b} \\ & \mathbf{A}'\mathbf{x} = \mathbf{b}' \\ & \mathbf{x} > \mathbf{0} \end{aligned} \tag{3.1}$$

The first step in the decision process will be defining the objective function. Because of the multiple aspects of this function, it will vary considerably for the different decision makers and stakeholders affected by the resulting decision. Each of these individuals and groups will have unique utility functions describing their associated risks compared to the decision (Keeney, 1993). Because of the high uncertainty resulting from all of the possible combinations of utilities, the work in this thesis tries to present examples of two primary decision makers: 1) a policy maker who wants to devise the best policies for biomass energy which optimize economic and environmental impacts, both short-term and long-term. and 2) and an industry decision maker focused on making capital decisions that will improve the economic performance of his/her company. While environmental impacts may be important for satisfying investors and customers, the primary objective of the industry leader is the economic well-being of the company depending.. Other potential decision makers and stakeholders will be involved throughout the work but those are the two primary ones.

More importantly, though, because even the utility functions of these decision maker "types" will vary considerably from person to person, most of the assessment is based on indicators such as described by Hoffmann (2001). Figure 3.3 presents an example of a typical hierarchy of objectives. In the later discussion on multi-objective optimization, the use of Pareto curves is introduced as a method to demonstrate the potential tradeoffs between competing objectives.

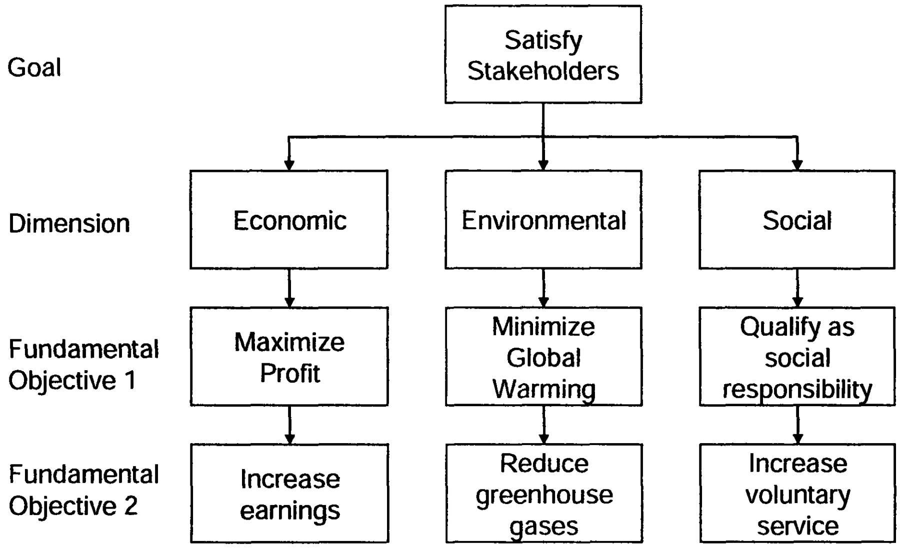

Figure 3.3 Indicators for decision problem optimization (Hoffman, 2001)

3.2 Multiple objectives

The first expansion of the traditional design framework is the inclusion of multiple objectives. Examples of these and methodologies for assessing the performance follow. While environmental and social concerns will be integrated, the economic bottom line will still drive the decision, and so that is where this section starts. This is not a new concept as many researchers have investigated methods for the incorporation of multiple objectives into chemical process design (Alexander, 2000; Azapagic, 1999; Cano-Ruiz, 2000; Hoffman, 2004; Diwekar, 2003; Chen, 2002; Shonnard, 2000, Steffans 1999). The primary contribution in this work is the integration of the Bayesian uncertainty analysis and the network programming framework as will be described in Chapters 5 and 7.

3.2.1 Economic assessment

For the production of ethanol to be profitable, the revenue from selling the products must be greater than the costs of production, but those costs must include capital cost and any financing, and these are often difficult to compute. Therefore, traditional tools such as net present value (NPV), internal rate of return (IRR), and payback period are applied to information provided in the above process design. These economic analysis tools use cash flows over the anticipated lifetime of the processing facility with an applied discount rate to take into consideration the time-value of money. More details on these and other economic assessments can be found in the following literature (Peters, 2002; Turton, 2003; Biegler, 1997).

Net present value is the most prominent tool used in the economic literature. By discounting the anticipated cash flows, a decision maker can compare the value of a project to an equivalent dollar value at the current time. The NPV for the production of corn grain ethanol is derived as follows

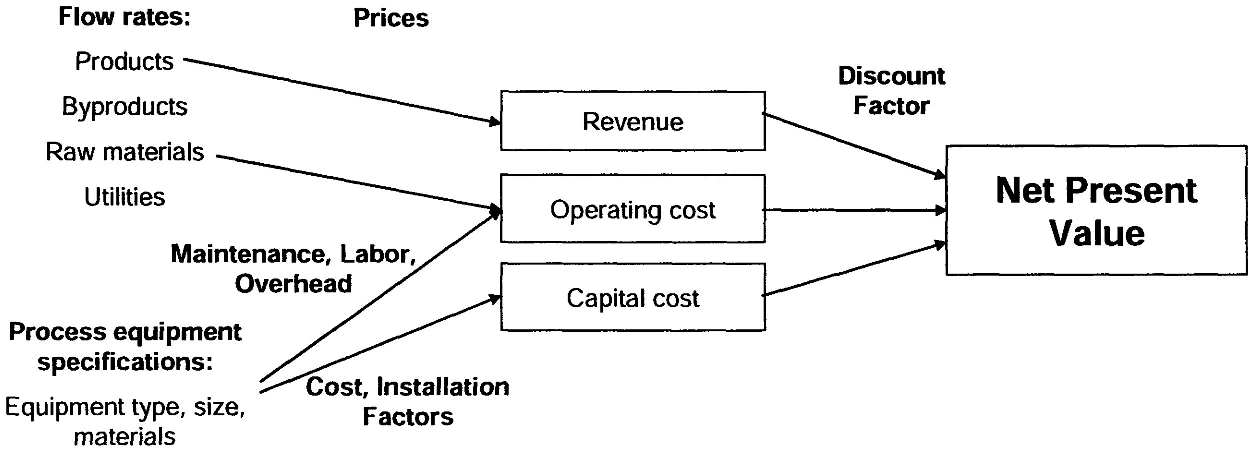

Figure 3.4 NPV calculation

While this may be useful when comparing alternative projects, NPV of cash flow sometimes lacks a connection to daily business variables. Therefore, the NPV of cost per unit sold is a better measure for comparing alternatives (Hoffmann, 2001). For the assessment of ethanol production, the total annualized cost per gallon of ethanol produced is used to define the economic performance of the facility. This TAC is derived by annualizing the original capital cost, assuming a debt/equity ratio and an interest rate as follows, and is discussed in further detail in Chapter 6.

$$NPV = \sum_{t=1}^{T} \frac{1}{(1+i)^t} \left(\begin{array}{l} \sum F_{prod} P_{prod} - \sum F_{raw\,mat} P_{raw\,mat} \\ - \sum F_{util} P_{util} - \sum OC_{fix} \end{array} \right) - \sum CCF * C_{equip} \qquad (3.2)$$

The resulting value is the required cost of ethanol over the lifetime of the plant for profitability. This economic value will be used to compare ethanol to other transportation fuels, and to assess emerging technologies for improved ethanol production. For the initial case study, the cost of production of ethanol using the parameters given in Table 3.1 along with the economic parameters in Table 3.2 is $1.00/gallon. Considering the spot rack price of ethanol in May 2006 is ~$3.00 (Axxis, 2006), today's ethanol producers are very profitable, which is confirmed by increased industrial investment (RFA, 2006) and in business news (Carlton, 2006).

3.2.2 Environmental assessment

In today's business climate, it is becoming increasingly more important to assess the environmental impacts of technology as well as its profitability. Policy makers, consumers, and society in general are becoming increasingly aware of how industry impacts the environment. This has resulted in a stricter environmental regulations, increased consumer advocacy, and even specialized investor groups which focus on socially responsible investments. How this will affect the production of transportation fuels is still highly uncertain. Energy production and transportation fuels specifically are the leading cause of anthropogenic carbon dioxide emissions into the atmosphere, the primary instigator of global warming. As policymakers are beginning to tackle the problem of global warming, special regulations on transportation fuels are sure to emerge.

A number of environmental impact assessment tools are being developed to help decision-makers determine the environmental performance of products and processes.

Cano-Ruiz (2000) and Allen (2002) provide comprehensive reviews of a number of assessment techniques and metrics. However, no one methodology has been defined as the best. Environmental assessment is hobbled by the lack of a consensus on what metric should be used to define environmental performance. The attempt to define environmental goods with economic values causes much uncertainty..

The most prevalent tool in development and use is life cycle assessment (LCA) or environmental impacts (Kniel, 1996; Wenzel, 1997; Heijungs, 1992; Guinee, 1993). The concept behind LCA is that environmental impacts not only come from the actual product or process, but additionally from the upstream and downstream processes involved. Another terminology used to describe LCA is cradle-to-grave assessment. This methodology takes into consideration all of the impacts from resource extraction to transportation to processing to use to disposal, with the results from the calculation being aggregated environmental impacts such as global warming impact, human toxicity, and eutrophication potential. The mathematical framework for calculating an LCA is reasonably straightforward. However, the data required for an accurate assessment is immense, and it is unclear how to treat relative preferences for weighting of the different emissions into impact categories. While other environmental impact assessment methodologies are available, LCA will be the primary tool used here. The details of the mathematics and the data collection and reconciliation are explained in detail in the following chapter.

For the case study, the primary environmental metrics used are net energy production and greenhouse gas emissions, but other air pollution and resource extraction values are calculated as well.

3.2.3 Social and political considerations

The implications of domestic corn grain ethanol on the U.S. energy sector, and the subsequent impacts on national security are even more uncertain than environmental performance. While industrial decision makers may not consider these impacts in all of their decisions, specific policies can influence the costs of production or prices of products. Another example is the further development of the rural economy. Currently, ethanol blenders receive a $0.51 per gallon federal excise tax credit when mixing ethanol into gasoline. While this doesn't directly affect the cost of production, it does have a significant impact on the price of ethanol. For long term profitability, a decision maker would have to consider the future of the tax credit and consider the implications of its potential removal

3.3 Expanded system boundaries

This concept is actually introduced in the above section on environmental life cycle assessment, where the environmental performance of a product includes the impacts of the upstream processes required for its production. However, this idea should not be limited to environmental performance. For example, a company which is trying to limit its environmental footprint by installing a natural gas combined cycle cogeneration power plant to avoid the addition carbon emissions associated with buying electricity off the grid where most of the production is via pulverized coal. The same decision may make sense solely from an economic standpoint, if the cost of power generation from the new facility is less than the grid price.

In the assessment of bioenergy, the upstream processes are critical in the analysis of economic, environmental, and social performance alike. Therefore, in addition to the process simulation model of the ethanol conversion processes, models are developed for corn production and feedstock distribution as well. The inclusion of these models suggest that the input intensity of corn production leads to the grain not being the most ideal raw material for energy production, from an economic as well as environmental viewpoint. See Chapter 5 for a description of the upstream model development and the details of the multi-objective performance assessment.

3.4 Multi-objective optimization

The integration of multiple objectives into the optimization problem given in Equation 3.1 leads to the problem of how to formulate a new objective function. Hoffman (2001) relates methods provided by others (Keeney, 1993; Clemen, 1995, Edgar 1988, Taha, 1997) on how to aggregate or reduce the different functions, before reaching the conclusion that it is best to keep the objectives separate. The information provided by the multiple optimizations are illustrated for the end decision maker so that the person can choose between the appropriate tradeoffs. This approach will be used in this thesis as well

An important tool for this illustration are plots of Pareto frontiers. A Pareto frontier is a graphical representation of the non-dominated points. Therefore, for each point on the Pareto frontier, a move to increase one objective must lead to a decrease in another objective. This tool will provide the decision maker a visual method for evaluating the possible configurations of the technology. Figure 3.5 shows an example of a Pareto frontier curve. In this example, Point A is on the Pareto frontier, Point B is a dominated point, and Point C is infeasible.

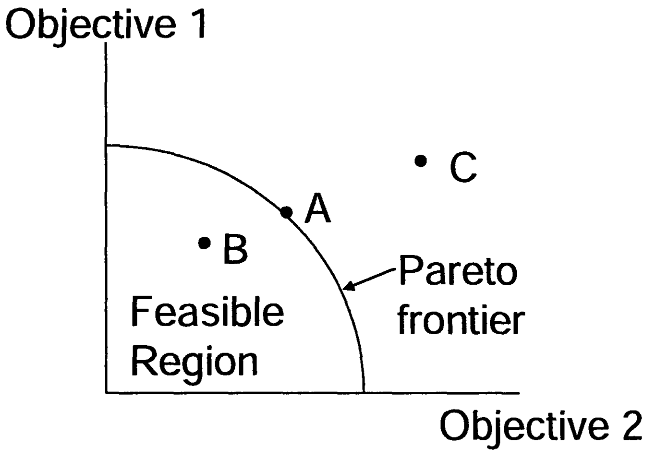

Figure 3.5 Example of a Pareto frontier curve

For more than two objectives, graphical demonstration of the Pareto frontiers can become difficult as a surface is required for three objectives, and a fourth is impossible to depict visually. The Pareto frontiers in this work will remain two dimensional with multiple graphs required for additional objectives. Moreover, the initial comparisons between different designs will simply use data points which represent specific operating positions.

3.4.1 Mathematical programming

In academic and research groups, another tool for the optimization process in chemical process design is the use of mathematical programming such as MINLP, Mixed Integer Non-Linear Programming (Daichendt, 1998; Guinand, 2001; Biegler, 1997, Bertsimas. 1997), a very rigorous mathematical tool for describing and optimizing the high non-linearities in chemical processes. In fact, the complexity of these algorithms do not necessarily lend it to the real time applications necessary for industrial and policy decisions. A more simplified example of mathematical programming which is used more prevalently in industry is linear programming. A specific example of the use of LP is in the optimization of petroleum refinery operations (Song, 2002; Zhang 2001).

Guinand (2001) also proposes a from of LP, network programming, as a tool for analyzing potential retrofits of existing manufacturing facilities. Network programming is a form of LP where the underlying mathematical formulation can be shown with a network structure. A network program is typically graphically presented as a system of nodes and arcs as is seen in Figure 3.6. Equation 3.3 gives the mathematical formulation of a standard network program. This tool is useful in transshipment, resource allocation, and multi-commodity flow problems. Because of the supply chain nature of biomass energy systems, the technology assessment methodology proposed here uses the network programming approach, but within the context of the multi-objective, life cycle approach.

$$\begin{aligned} &\text{Min } \mathbf{c}^T\mathbf{x} = \sum_{ij} c_{ij}x_{ij} \\ &\text{s.t.} \quad \mathbf{Nx} \le \mathbf{q} \text{ or } \left[\sum_{ij} x_{ij} - \sum_{ji} x_{ij}\right] = b_i \\ &\qquad \mathbf{Ax} \le \mathbf{b} \\ &\qquad 0 \le x_{ij} \le u_{ij} \end{aligned} \tag{3.3}$$

These mathematical tools become harder to use once more than one objective is required. As described in the above section, a Pareto frontier method is used to visualize the tradeoffs between the objectives. The formulation of this frontier becomes more challenging in the framework of an optimization routine. As in Hoffman (2001), a ε-constrain method is used, where each objective is optimized iteratively with the other objectives being considered constraints at different values. The optimization is performed multiple times to determine the frontier.

3.4.2 Sensitivity analysis for network model

Sensitivity analyses of the optimization are important tools for analyzing the resulting Pareto frontier. The first is a simple analysis of the slopes of the curve at different operating points gives the marginal environmental performance per economic cost. This is critical information for the decision maker. The other analyses are functions of the network programming mathematics. The calculation also results in the determination of shadow prices, the marginal impact of each constraint on the overall objective function, and reduced costs, the required change in a variables coefficient before it is utilized in the optimization.

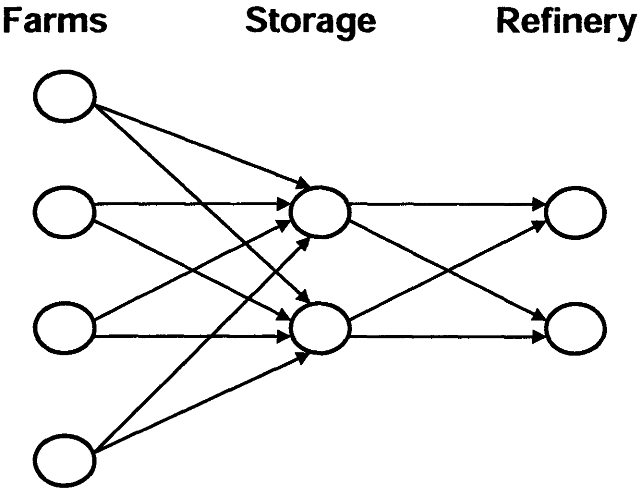

Figure 3.6 Nodes and arcs in network structure

For the case study, the network program will function as the overall structure for the biomass ethanol system, with the nodes being processes such as corn production and ethanol conversion, and the arcs representing shipments of the biomass as in Figure 3.6. In fact, this optimization model is performed for the entire supply chain, rather than simply the ethanol conversion process. Integrating the concept of expanded system boundaries, the optimizations in this step will look at models for resource extraction and transportation in addition to actual process model. This will allow for the decision maker to see the impacts of process developments along every stage of the supply chain. Because the network program is based more on input-output models, than the detailed process models themselves, the overall structure will be primarily suited for identifying parameters in the process which contribute most to overall economic and environmental costs. The next steps involve decomposition of the models to more detail.

3.5 Uncertainty Analysis

A concept which is often ignored in traditional technology assessment methodologies is how to manage the uncertainty implicit in the performance and impacts. These uncertainties come from 1) not knowing how well a technology will work, 2) not knowing what the price or other economic parameters involved in the process will be, and many other systematic and parametric uncertainties. A whole literature is devoted to descriptions of different kinds of uncertainty and methods for dealing with it within a process framework (Biegler, 2004; Rooney, 2003; Kheawhom, 2002; Pistikopoulus, 1995, Morgan, 1990). References for uncertainty analysis in life cycle assessment are provided in Chapter 4. In chemical engineering process design, the concept of uncertainty is difficult to comprehensively include, so it is often managed by performing simplistic sensitivity analyses, using higher required rates of return, or even adding large design factors making equipment much bigger than it needs to be. The methodology proposed in this work will incorporate tools which address the problem of uncertainty directly.

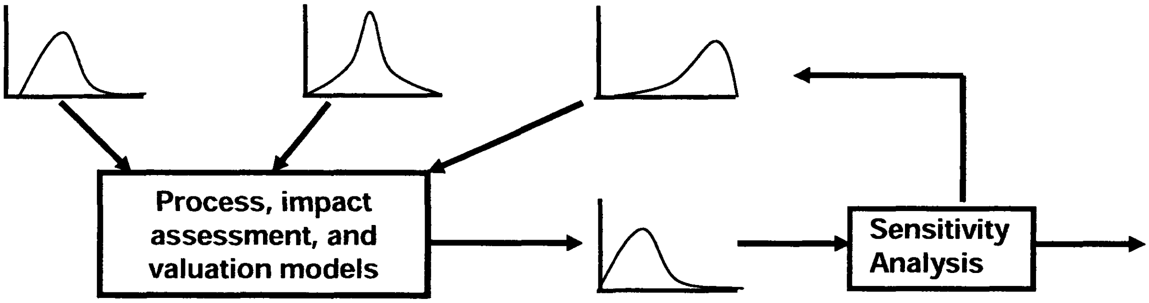

Figure 3.7 Process for uncertainty analysis

Rather then using deterministic representations of the parameters involved in the technology assessment, probability distributions will be utilized and propagated throughout the mathematical calculations using Monte Carlo simulations of the random variables representing process inputs and economic and environmental factors. Figure

3.7 presents a schematic of the steps for including this uncertainty. Note that specific processes for developing the prior distributions will be presented in the case studies. The use of probability distributions will present difficulties in the end as comparisons between probability distributions are much more vague than comparisons between deterministic values; however, the comparisons will be more realistic. Moreover, tools such as relative performance metrics and sensitivity analysis can be used to lessen the variance in the comparisons between competing alternatives.

Many tools for sensitivity analysis have been proposed in the literature. Chen (2005) gives a review of techniques. For simplicity, the method used here is the rank correlation procedure as described in more detail in Chapter 4. The resulting correlations are not true contributions to the variance, but relative ones representing the parameters which contribute most to the variance. By minimizing the variance of those critical parameters, the Monte Carlo simulation can be performed iteratively until the variance is at a point where significant information can be derived.

3.5.1 Bayesian analysis

A critical step in this process is the updating of the prior distributions after each Monte Carlo simulation. Once the decision maker has identified the critical parameters, more extensive investigation into those parameters will provide better information to the decision maker. For this step, Bayesian theory will be applied. Bayesian theory is a statistical method which assumes a prior knowledge of the probability that a random event may occur, and then updates that probability using experimental data. It is often at variance with the frequentist method which suggests that there is a true probability which will be determined given an infinite number of samples. The basic Bayes' rule is given in equation 3.6 and describes how conditional and marginal probabilities relate. See Chapter 4 for a more detailed description with examples …

$$f(x|y) = \frac{f(x,y)}{f(y)} = \frac{f(y|x)f(x)}{f(y)} \tag{3.4}$$

These concepts are applied here in the updating of probability distributions. For the initial iteration of the process assessment, prior distributions are proposed for the uncertain inputs into the system. These prior distributions can take any mathematical form and are often based on historical data, expert analysis, or simple estimations of lower and upper bounds. After being propagated through the system, and identified as critical parameters, however, these prior distributions must be updated to have lower variance. By finding data more specific to the case study being assessed, the Bayesian equation can be used to transform the prior distribution into a posterior. This process is iterative along with the rest of the analysis.

3.6 Specific applications

These are the primary tools which will be integrated into the technology assessment methodology. With the proper implementation and an understanding of the decision-makers objectives, these tools will allow for someone to decide which alternative is best between competing technologies. This section will briefly outline how the tools will be used to evaluate technologies and determine how best they can be improved and optimized.

3.6.1 Resource allocation for research and development portfolios

One application of this multi-objective optimization method is resource allocation. The definition of this could be determining how best to invest time, money, or other resources into product development. This is an important question for research and development programs. This is especially important for emerging technologies. In order for these technologies to become commercialized, they must be economically and environmentally sustainable. There are often many opportunities for improvement in these emerging technologies; however, each of the use improvements does not provide the same possibility for return. The utilization of the above tools for resource allocation can provide decision-makers a way of determining which technology advancement will provide the greatest process improvement.

While the Pareto frontier can provide the decision-maker the choice between competing objectives, to resource allocation tool will show how the Pareto frontier is improved by different technology advancements. Using this visualization, one can determine which improvement appears to be best and should be implemented.

3.6.2 Policy Decisions

Each of the above tools are important for making policy regarding the technology involved. For transportation fuels, these tools will allow policymakers to compare the economic and environmental performance of competing technologies; however, the tools can also be applied to scenario analyses. For example, the implementation of carbon taxes or other regulations on fuels can be incorporated into the economic and environmental models to simplistically evaluate how that will impact the comparisons. Obviously, more detailed economic models may be required to predict possible feedbacks and how of the changes would impact the overall economy, but this methodology allows for the estimation of the initial impact on production costs. Additionally, the resource allocation tool can be used for persons who are deciding on research budgets, especially where money is going to meet proposed objectives.

The above sections briefly outline how the methodology proposed in this thesis can be useful for decision-makers. And specific examples in the details of each of these tools will be described in later sections; however, this can be seen as an overview of how these tools can be implemented. The next chapter will start to describe the case studies involved, and how all these tools can be used to assess the technologies related to the production of biofuels and synthetic fuels from coal.

Chapter 4 Environmental Life Cycle Assessment

One of the primary tools currently utilized for assessing environmental performance is life cycle assessment (LCA). It is becoming increasingly used to examine the environmental impact of a product, process, or activity. As its name suggests, LCA includes the overall resource use and pollution generation for all phases of the product's life, everything from resource extraction to waste disposal, rather than simply assessing the emissions from the production process itself. Figure 4.1 provides a schematic of the processes, including upstream which would be included in LCA. Note that the figure does not show all of the process included, it is simply a representation. Once the cumulative material inputs and outputs are determined, the overall environmental impact can be determined. LCA is typically used for a relative environmental performance comparison between product alternatives; however, the methodology can also be used to specify problem areas in the product life cycle.

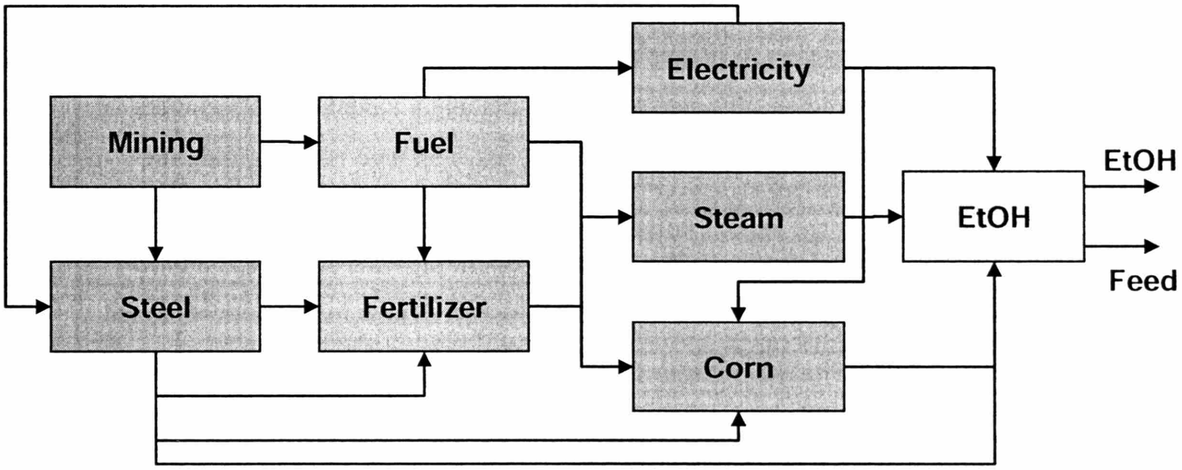

Figure 4.1 LCA schematic for corn grain ethanol production

4.1 Methodology

LCA has been under continual development over the past decade. Currently, the International Standards Organization has a framework for the procedure – ISO 14040; however, other groups have proposed similar guidelines with modifications. Most divide the methodology into four components which are listed below with short descriptions:

- **Goal definition and scoping** – Defines the purpose and extent of the study, including a description of the boundaries of the system, i.e., which upstream and downstream process will be included. Additionally, the functional unit – the basis for comparison between alternatives, and how impacts are allocated in multiple product systems are defined.
- **Life cycle inventory** – The pollutants, resources, and inter-process material and energy balances from each process related to the life cycle as defined in the system boundary are quantified. The data collection for this stage is typically the most difficult step in the LCA as the information requirements are very large.
- **Impact assessment** – The overall inputs and outputs from above are used to characterize the impacts of the life cycle on the ecosystem, resource depletion and human health using a number of different metrics such as global warming, ozone depletion, smog, particulate matter, human toxicity, eutrophication, acidification, and eco-toxicity. This step is the least straightforward, as translating an emission to its impact on the environment is not very well understood. Moreover, this step allows for placing a valuation on particular impacts. These valuations will be different bases on who is performing the evaluation.
- **Improvement assessment** – The last component presents an opportunity to find which processes in the life cycle contribute the most to the environmental impact. Once these are isolated, process improvements can be suggested to improve the overall environmental performance of the system.

A number of commercial software packages are available which contain input/output inventories for industrial systems (SimaPro 2006, Umberto 2006). The data in these inventories are typically generic and can be used as estimates for upstream processes. Combined with more detailed material and energy balances for the primary processing units, a matrix calculation based on input-output economics can be used to accumulate the overall life cycle inventory.

4.1.1 Matrix calculation derivation

Life cycle assessment is based on input-output economics, for which Lontief (1986) won the 1973 Nobel Prize in economics. The concept is that the delivery of a single product or services requires not only the production of that product, but all of the upstream production as well. Using the input-output derivation, the total accumulated throughput of those upstream processes can be calculated. LCA applies that same theory, but instead of using economic throughput, the metrics are material and energy throughputs.

The derivation of the LCA calculation is provided in the following section. The application of these equations is performed in a spreadsheet based tool called EnvEvalTool developed by Cano-Ruiz (2000). See his thesis for a more detailed explanation of the software package. For the calculation, matrices are required which contain data for all of the processes in the system regarding feedstock use, product make, and a emissions. The following list describes the important starting matrices and vectors.

Label	**Description**
B	use matrix (direct product inputs required per process throughput)
C	Make matrix (direct product outputs produced per process throughput)
E	environmental exchange matrix (emission factors for all processes)
F	market share matrix (percentage of overall product made by specific process)
H	characterization matrix (converts emissions to environmental impacts)
d	demand vector (products required)
p	price vector

Table 4.1 LCA Data Matrices

Label	Description
G	allocation matrix
D	process by product throughput matrix
A	product by product throughput matrix
T	product by product total requirements matrix
L	life cycle exchange by product matrix
X	direct throughput vector
Q	total throughput vector
E	life cycle environmental exchange vector
O	life cycle environmental impact vector

Table 4.2 LCA Calculated matrices

4.1.1.1 Process throughputs

The input-output calculations start with the formulation of the overall product by product throughput matrix, **A.** The matrices used for this calculation are **B**, **C**, and **F**. **B** and **C** describe the inputs for each of the processes respectively. For example Figure 4.2 shows a simple block flow for ethanol production with a couple of the raw materials and products shown.

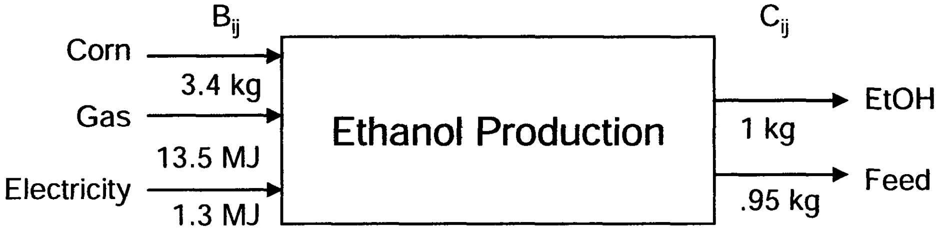

Figure 4.2 Inputs and outputs for ethanol production

For the jth process, B_{ij} represents how much of the ith product is used, and C_{ij} represents how much of the ith product is produced Therefore, the entry $B_{\text{corn, ethanol}}$ gives the amount of corn which is required to produce 1 kg of ethanol, $C_{\text{feed, ethanol}}$ gives the amount of animal feed which is produced as a byproduct in the production of 1 kg of ethanol. The process for filling these matrices with data is described in more detail later in this chapter and in Chapter 5, and the actual matrices are shown in the Appendices.

The matrix **C** needs to be transformed to take into consideration how much of the inputs and emissions are allocated to the coproducts in a multi-product process. For example, with both ethanol and DDGS produced, how much energy is allocated to either. A simple calculation is to use economic values of the products. In this case, **C** (actually the inverse of **C**) is transformed into the allocation matrix, **G**, by the following calculation:

$$G_{ji} = \begin{cases} \dfrac{p_i}{\sum_{i'} C_{i'j} p_{i'}} & \forall C_{ij} \neq 0 \\ 0 & \forall C_{ij} = 0 \end{cases} \tag{4.1}$$

For this work, the allocation procedure is based on system expansion (Kim, 2005) where the corn grain ethanol byproduct, DDGS, is assumed to be a replacement for soybean meal. In this case, the calculation uses the life cycle energy replacement, rather than price as the allocation metric. The same formula is used, with the p_i replaced. For all products which have single products, $G_{ji}=1/C_{ij}$.

Another transformation is required for the products which are supplied by multiple processes, with electricity being the primary example. The power generated throughout the economy comes from a number of sources: coal, natural gas, and nuclear being the most prominent. To take this into a consideration, a market share matrix, **F**, is provided where F_{ij} represents the percentage of the i^{th} process which contributes to the j^{th} product. $F_{\text{coal,electricity}}$ is 57% which suggests that 57% of the electricity in the economy is supplied by coal. The market share matrix is included in the calculation by taking the dot product of the **F** and **G** matrices to form the process by product throughput matrix.

$$\mathbf{D} = \mathbf{F} \bullet \mathbf{G} \tag{4.2}$$

D_{ij} represents the amount of product j produced by an individual throughput of process i. Now, the use matrix must be integrated into the information provided in **D**. This is accomplished by multiplying **D** by the use matrix to give the product by product throughput matrix.

$$\mathbf{A} = \mathbf{BD} \tag{4.3}$$

This matrix describes the direct inputs required for the production of each product, i.e., A_{ij} represents the amount of the i^{th} product required to produce the j^{th} product. For example, the column for corn grain lists the amounts of fuel, fertilizer, chemicals, etc. required to produce 1 kg of corn. Now, the primary equation in input-output economics shows that the total throughput of an economy can be calculated by starting with the identity matrix plus the product by product matrix, multiplied by the demand vector:

$$\mathbf{x} = (\mathbf{I} + \mathbf{A})\mathbf{d} \tag{4.4}$$

However, this only calculates the direct requirements for the demand vector. For example, requiring 1 MJ of ethanol energy requires 0.04 kg ethanol. However, to further calculate the inputs required for producing the ethanol, one must add the second tier inputs which is represented by the square of the product by product matrix multiplied by the demand vector. This calculates the products required to meet the first tier requirements. The third tier is the cube of the matrix multiplied by the demand vector, and so on. For the total requirements, the sum of all or these tiers must be calculated, but the continuous sum converges to the following equation.

$$\mathbf{T} = (\mathbf{I} + \mathbf{A} + \mathbf{A}^2 + \mathbf{A}^3 + \mathbf{A}^4 + \cdots) = (\mathbf{I} - \mathbf{A})^{-1} \tag{4.5}$$

Multiplying this by the demand vector gives the overall products required to meet the products in the demand vector. Each of the entries in the vector **q** represents the amount of the i^{th} product which is required through the life cycle.

$$\mathbf{q} = (\mathbf{I} - \mathbf{A})^{-1}\mathbf{d} = \mathbf{Td} \tag{4.6}$$

The matrix **T** is the critical matrix as its entries, Tij, represent the life cycle total of the ith product required to produce one unit of the jth product.

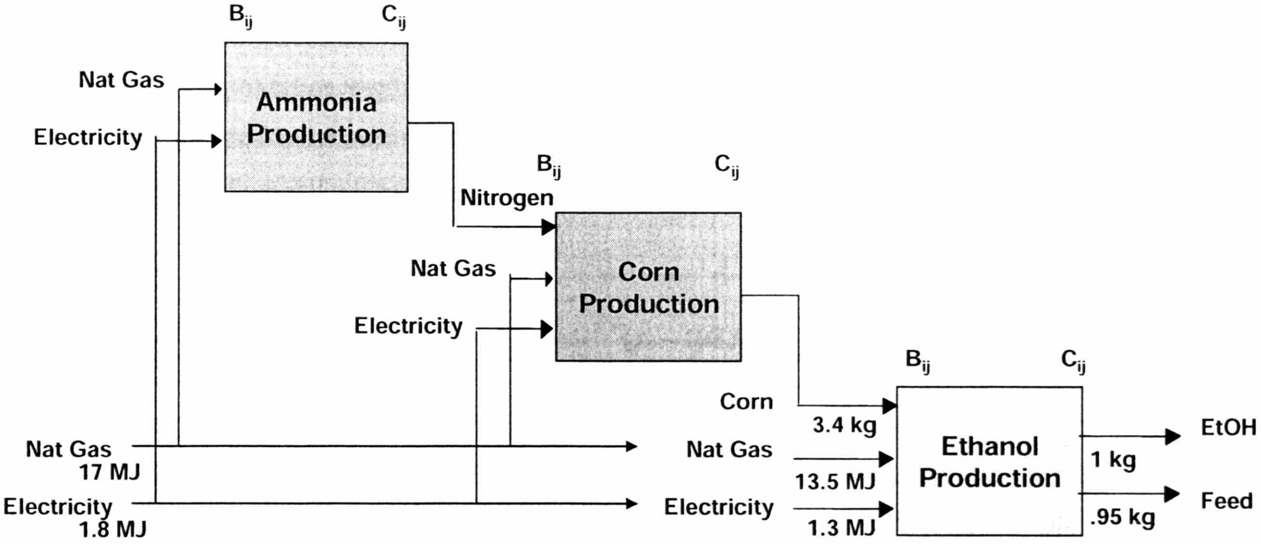

Figure 4.3 Example of including upstream processes in total requirements calculation

As Figure 4.3 graphically shows, the B_{ij} and C_{ij} can be utilized in each of the processes to calculate the overall requirements. The **T** matrix is the primary tool used for the calculation of the energy balance and for separating the contributions from each sub-process, and it is found in the Appendix. Solely investigating $T_{i,ethanol}$, the energy carriers can be multiplied be their heating values and summed to achieve the overall energy inputs.

$$Energy_{etoh} = \sum_{i} \mathrm{LHV}_i T_{i,etoh} \tag{4.7}$$

where i includes non-fossil electricity, natural gas, oil, and coal. This energy calculation can be performed for other processes in the supply chain to get the energy breakdown by process as well. The results of these calculations are provided below.

4.1.1.2 Life cycle emissions

The above calculations are a part of the life cycle inventory stage. The following ones move onto the impact assessment stage. The above matrices need to be transformed from material and energy balances into environmental exchanges by multiplying be the environmental exchange matrix **E**.

The entries E_{ij} represent the amount of emission i from process j. First, this matrix must by multiplied by **D** to transform it from an emission by process to an emission by product matrix. This is followed by a multiplication by **T** and **d** to give the overall emissions vector for the life cycle. gives the life cycle environmental exchange vector. This vector calculates the sum of all of each emissions over the life cycle of the process.

$$\mathbf{e} = \mathbf{ED}(\mathbf{I} - \mathbf{A})^{-1}\mathbf{d} = \mathbf{Ld} \tag{4.8}$$

The i^{th} entry of **e** represents the overall emissions of material i due to the demand vector. Figure 4.4 demonstrates this calculation for carbon dioxide. As in the throughput calculations, the matrix $\mathbf{L} = \mathbf{ED}(\mathbf{I} - \mathbf{A})^{-1}$ is useful for separating out these emissions be the sub-processes.

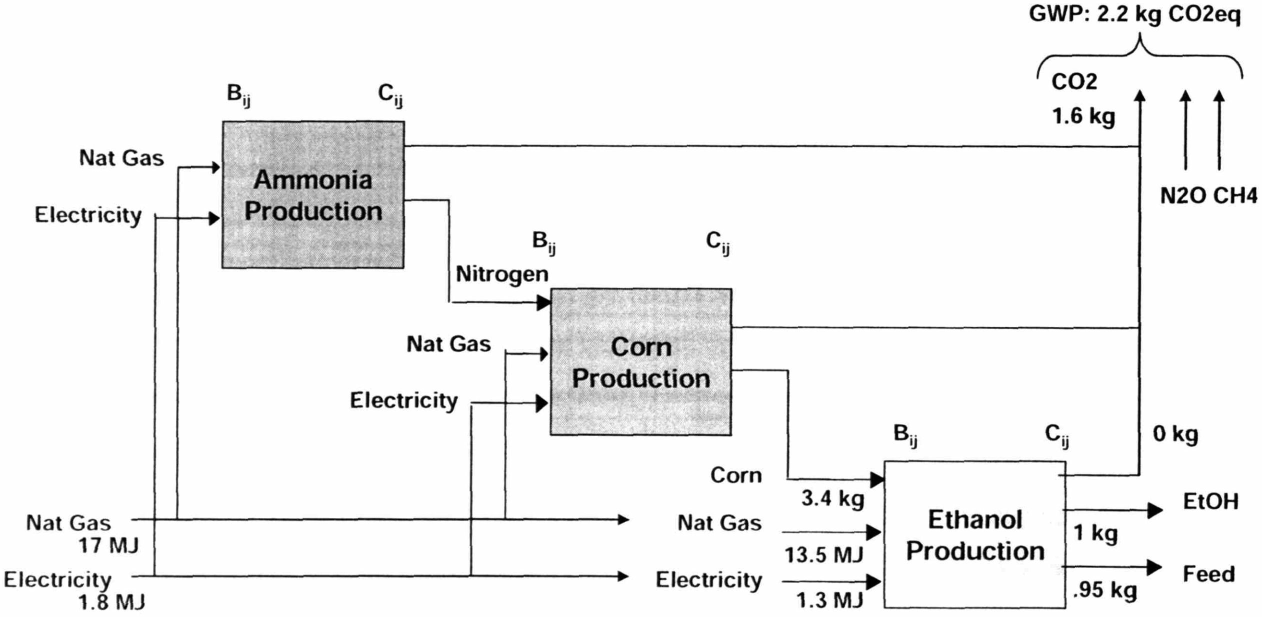

Figure 4.4 Example of life cycle emissions from ethanol production

Finally, the overall environmental impacts can be calculated by multiplying the transpose of **H** by **e,** where the entry H_{ij} represents the contribution of emission i to impact category j. This accumulates each of the total emissions into the respective impact categories. For example, the global warming potential entry multiplies each emission by its relative radiative forcing coefficient, with carbon dioxide being the basis. This is the calculation used to determine the carbon dioxide equivalent of ethanol and gasoline.

$$\mathbf{o} = \mathbf{H}^T\mathbf{E}\mathbf{D}(\mathbf{I} - \mathbf{A})^{-1}\mathbf{d} \qquad (4.9)$$

Returning to Figure 4.4, the overall carbon dioxide emissions are added to the overall nitrous oxide, methane, and other greenhouse gases to calculate the overall impact relative to carbon dioxide emissions. Note again that these figures do not represent the overall products, processes, emissions, and impacts; they are simple examples. The full matrices can be found in the appendix. A fuller description of the spreadsheet and database tools which make up the EnvEvalTool can be found in Cano-Ruiz (2000).

4.2 Problems and challenges

While environmental life cycle assessment is a powerful tool, providing insights to decision makers on which technologies have better environmental performance or which are the critical processes in the overall supply chain, it does have several significant drawbacks, some relating to the uncertainty in the system and some relating to the process itself

4.2.1 Uncertainty in LCA

Proper LCA calculations have significant data requirements. Not only are material and energy flows required for the process in question, but also for all the processes which provide the inputs to the initial one. In the ethanol case study, the primary raw material to the production facility is corn. Thus all of the inputs into corn production must be quantified. Moving further upstream, agricultural inputs such as fertilizer must also have defined material and energy balances. It doesn't take too many inputs before the data requirements become very large. Moreover, many of these process have uncertain and variable inputs and outputs. The combination of the data requirements and uncertainties add considerable complexity to the system. Most LCA calculations make significant assumptions in these data and their quality. A number of techniques to manage the uncertainty have been developed and some will be described later in this chapter.

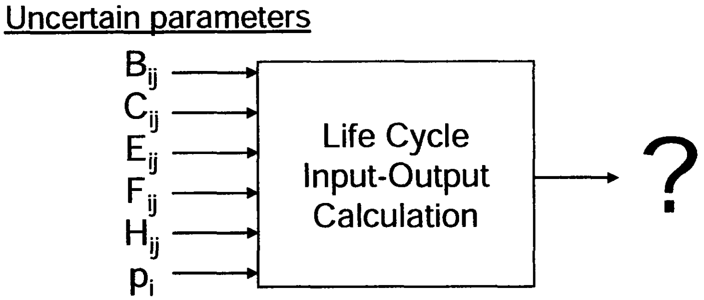

Figure 4.5 Uncertain inputs in LCA

Another significant source of uncertainty comes from the impact assessment stage. All life cycle emissions are aggregated into a number of impact categories such as global warming potential or human toxicity. These categories are proxies for actual environmental impacts and their aggregation is a subjective calculation with differing opinions on the real impact. Human toxicity is especially difficult as it entails a combination of fate and transport models along with epidemiological data on the effect of the substance once it is taken into the human body. Cano-Ruiz (2000) provided a comprehensive review of a number of the techniques in the literature with the development of a probabilistic approach to the human toxicity calculation. Figure 4.5 gives a representation of the uncertain inputs in the LCA calculation. For the corn grain ethanol case study, these amount to close to 1000 uncertain inputs.

4.2.2 Structural shortcomings

Because of the large data requirements, LCA is typically performed, if at all, during the last stages of process design. Unfortunately, at this stage, there is little time and money for significant design changes. Hoffman (2001) presents a framework for moving the LCA calculation upstream in the design process. Another shortcoming is the lack of integration of cost or social factors into the process. Norris (2006) is developing the technique of life cycle attributes to bring in concepts of fair trade and other non-environmental socially responsible attributes of production processes.

4.3 Preliminary case study

Before introducing the uncertainty propagation aspect of the methodology, an example of a standard LCA is performed using the corn grain ethanol case study. The following describes the performance of each of the steps required in the methodology.

4.3.1 Goal definition and scoping

The goal of this LCA is to compare the greenhouse gas emissions of driving one mile in a standard automobile using ethanol derived from corn grain versus regular gasoline. Energy values from Wang (1999) were used to determine the fuel needed to travel that distance. Based on the average mileage of the U.S. fleet, the amount of energy required was 5.4 MJ/mile The results could be useful under a carbon emissions trading scheme, such as the Kyoto protocol which was introduced at the end of Chapter 3. Additionally, carbon and energy balances will be performed on the fuels to track the efficiency of the upstream processes used for production. The system boundary for ethanol is given above Figure 4.1. A similar figure is shown for gasoline production in Figure 4.6. Both processes have multiple products.

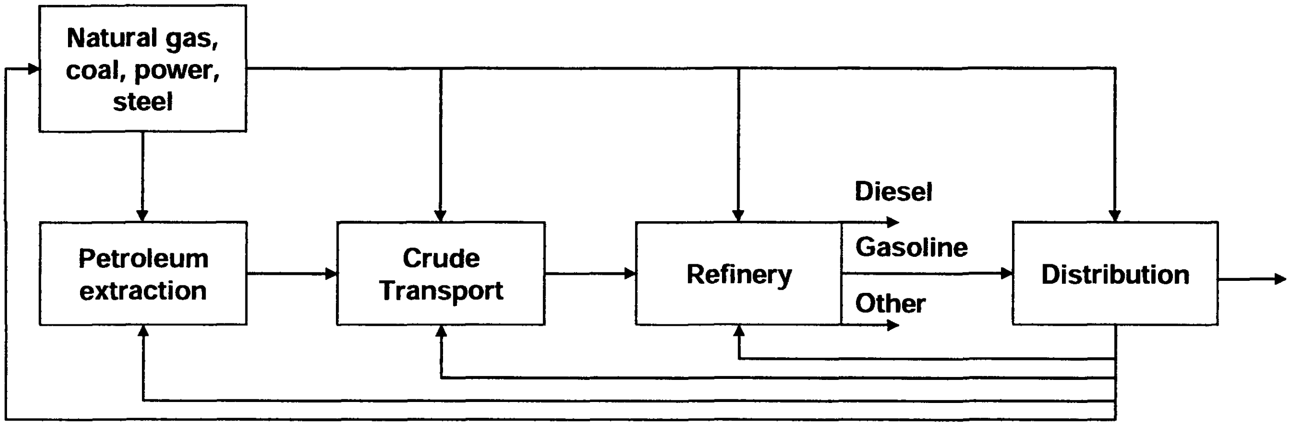

Figure 4.6 LCA schematic for gasoline production

The allocation of impacts to the coproduct is based on the system expansion model where the DDGS is assumed to be a replacement for soybean meal. Therefore, the inputs for soybean meal production are subtracted out in the matrix calculation. Other possible allocation procedures can be based on the economic value or energy content of the coproduct. With the system expansion model, the LCA impacts of DDGS are approximately 80% of the total. Likewise, gasoline production in a petroleum refinery consists of about 45% of the economic and energy value.

4.3.2 Life cycle inventory

This is typically the most straightforward step, yet at the same time, the most time consuming, because of the data requirements and the uncertainty. Because uncertainty is integrated in detail in Chapter 5, the detailed methodology for obtaining the inventory data is provided there. While the data sources are referenced in this chapter, the data used are simple averages from the probability distributions derived in the next chapter.

The description of the life cycle inputs will be given in tiers where the definition of a tier is the degree of separation from the actual production process. Therefore, with ethanol production being the primary process, a quick process description is given here. A process flow diagram is given in Figure 4.7.

Ethanol is produced from corn using a biological reaction. The corn is milled, heated, and mixed with enzymes to start the process of degrading the starch, a polysaccharide in the corn kernel into its component glucose sugars. These sugars are then fermented with yeast to a low concentration ethanol product. To purify the ethanol, a series of steam heated distillation columns are used. Finally, a molecular sieve is used to dehydrate the ethanol. The primary waste from the first distillation column is dewatered using a centrifuge and then dried further to produce a co-product called distiller's dried grains (DDGS), which can be fed to livestock. Note that this is the primary process analyzed here. Ethanol can also be produced from corn using a wet mill process. However, all the manufacturing facilities built over the past decade have been dry mills.

The first tier inputs are corn grain, electricity, natural gas, liquid propane gas (LPG), gasoline, enzymes, yeasts, processing chemicals and antibiotics, boiling and cooling tower chemicals, and water. These inputs and their quantities are accessible from several sources: an Aspen Plus simulation of a corn ethanol dry mill (Taylor, 2002), a report on corn ethanol economics (Tiffany, 2003), and a survey of U.S. ethanol producers (Shapouri, 2002)). Emissions from the process are CO, CO_2, NOx, VOC, and particulate matter. Producers have been very successful at recycling all of the wastewater and converting all of the solid waste to coproduct animal feed. The primary products from the process are ethanol and distillers dried grain (DDGS), an animal feed product. The Appendix includes tables for all the tiers' inputs, outputs, and emissions on a per gallon ethanol basis for a 50MM gal/yr processing facility, which is the standard size for the new plants being built.

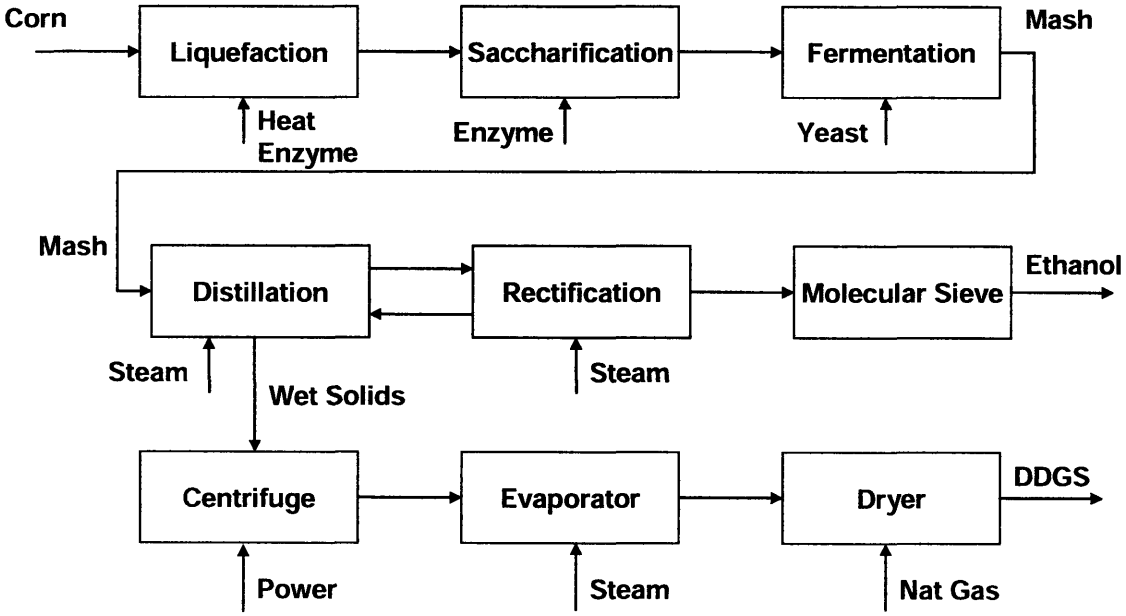

Figure 4.7 Process flow diagram for ethanol production from corn grain

With the material and energy balance determined for the first tier, most of the inputs are generic and the upstream tiers can be described with standard inventory data. For example, the LCA for the production of electricity or natural gas have been evaluated many times, and the input-output matrix from previous studies can be repeated. The inventory database developed by Cano-Ruiz (2000) is used.

The production of corn requires a little more research and discussion. Production requirements and costs vary from region to region which will impact the life cycle inventory. Using data from the USDA Economic Research Service (ERS, 2006), average values for the inputs required for corn production are acquired. Figure 4.8 shows the inputs required for corn production. The impact of soil carbon on overall carbon dioxide cycling is not well understood and will be left out of the preliminary assessment.

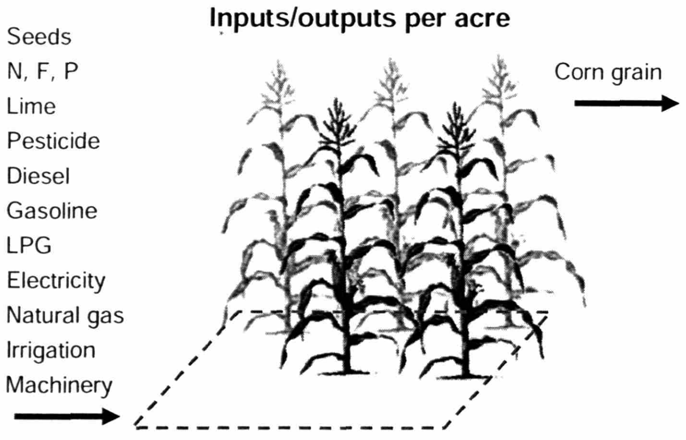

Figure 4.8 Inputs required for corn production

Once again, the upstream tiers inventories for the fossil fuels will be taken from generic inventories. Likewise, the pesticides have a lower input level, and generic data from other agricultural environmental assessment studies can be used. Seeds will be represented as corn production with 1/3 the yield, but with additional fuel use for activities such as packaging and distribution (Corn, 2004) This leaves the fertilizer production as the remaining inputs. Because the application rates are not trivial, a detailed look at the material and energy balances for the upstream processes is performed. The requirements for fertilizer production have been reported by a number of researchers and manufacturing organizations (Worrell, 2000; Bhat, 2004; Kongshaug, 1998; Ullmann's 2005).

Chapter 5 includes a detailed analysis of the inputs required for fertilizer production, and the average values from that analysis are presented here. As with the other inventories, tables in the appendix list the actual data values. Additionally, the actual matrices used for the calculations are shown

4.3.3 Preliminary results

The inventory data listed above was input into the EnvEvalTool, an LCA tool constructed by Cano-Ruiz (2000). The tool already has an existing database for fossil fuel production and combustion, which is used for the upstream processes, as well as for comparing the corn ethanol to gasoline. EnvEvalTool has a spreadsheet component which accesses the database and performs the matrix calculations required for impact assessment. Figure C.1 and Figure C.2 show the product by process use and make matrices for the corn grain ethanol case study while Figure C.5 shows the total requirements matrix in the Appendix.

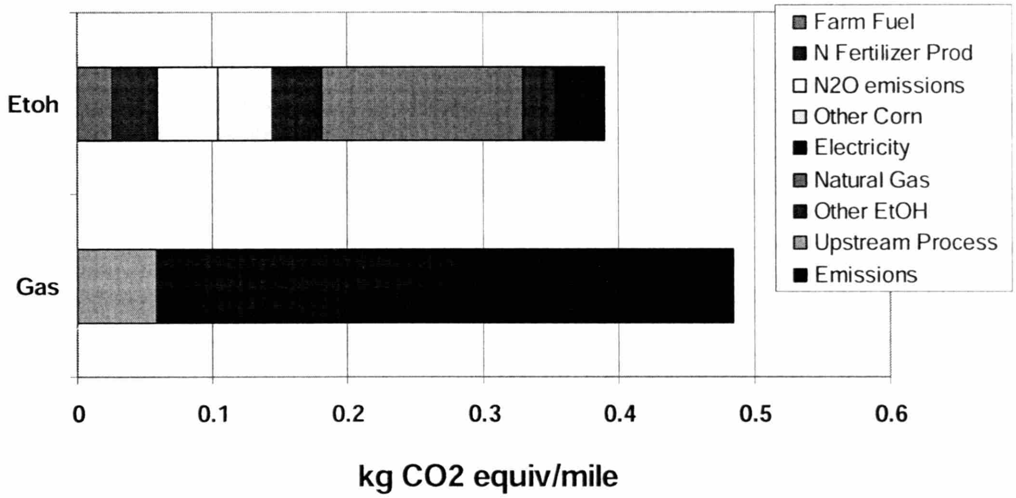

Figure 4.9 Global Warming Potential for corn grain ethanol vs. gasoline

Figure 4.9 shows the preliminary life cycle global warming potential for driving one mile using corn ethanol versus gasoline. The global warming potential is a proxy calculation defined by the Intergovernmental Panel on Climate Change (IPCC) which uses carbon dioxide as the basis, but assigns values to other greenhouse gases based on their relative radiative forcing.

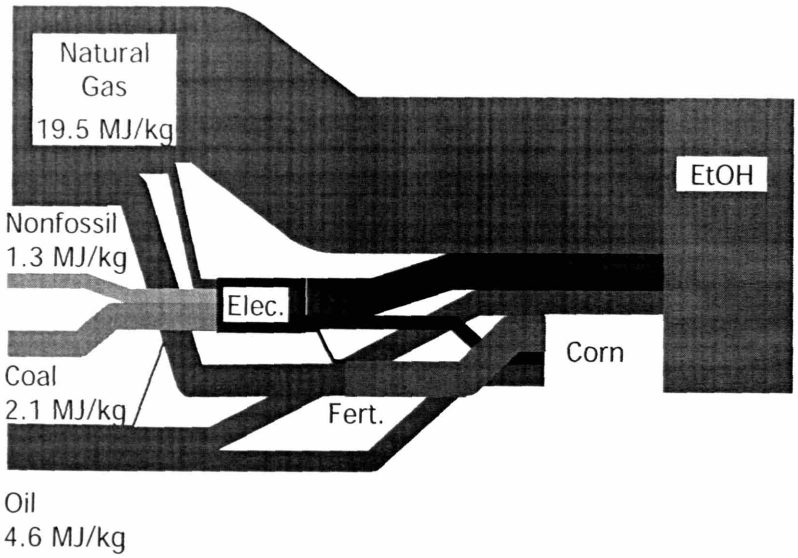

Figure 4.10 Total energy in corn grain ethanol production without coproduct credit

Figure 4.10 is a chart showing the embodied energy in ethanol production. The calculations show the relative amounts of coal, natural gas, and oil used in the production of ethanol. Figure 4.11 breaks down the ethanol production by process while Figure 4.12 does the same for corn production. This is the total energy requirement and does not include the coproduct credit. Considering the energy content of ethanol is 26.7 MJ/kg LHV, and the coproduct credit is ~5MJ/kg, this preliminary analysis shows that the energy balance of corn grain ethanol is positive, i.e., the energy required for production is less than the energy in the fuel itself. This is a controversial subject and is dealt with in more detail in the discussion of uncertainty below and the case study in Chapter 5.

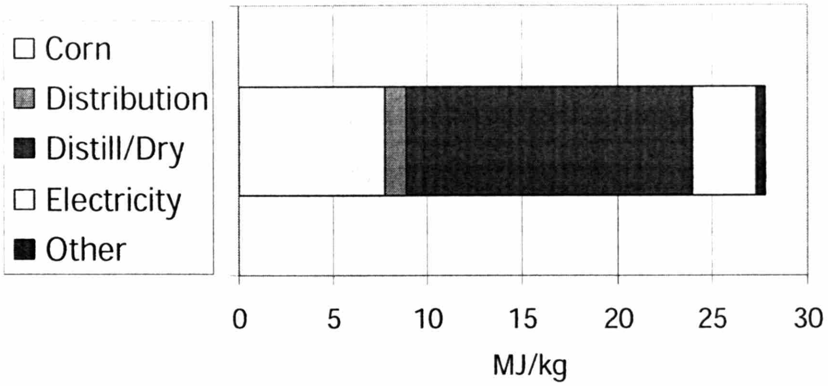

Figure 4.11 Total energy in ethanol by process without coproduct credit

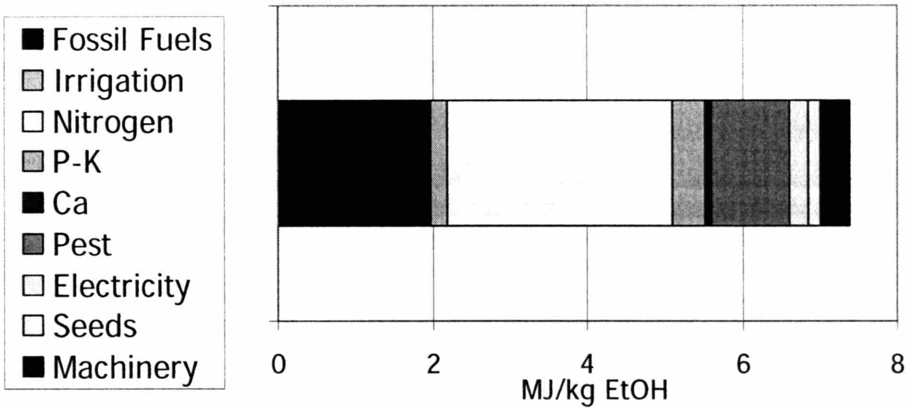

Figure 4.12 Total energy in corn production by input

Returning to the Kyoto protocol discussion which was introduced in the goal definition step, the environmental impacts calculated above – life cycle carbon dioxide emissions or life cycle global warming potential can be used for policy implementations. For example, rather than specifying ethanol as carbon dioxide neutral fuel, this calculation shows the actual carbon dioxide avoided as compared to gasoline. Additionally, other environmental impacts such as life cycle potentials for ozone depletion, photochemical smog formation, acidification, etc. are calculated for the corn grain ethanol process relative to gasoline. See Figure 6.4 in Chapter 6 for a demonstration of the calculation of these other impact categories.

The problem with these preliminary results is that they in no way reflect the uncertainty about the true values of the LCA calculations (the above figure notwithstanding). As a simple example, Figure 4.13 shows the variation in energy requirements for corn production in different states and different years as reported by Shapouri (2002, 2004). An average value may not be representative as the inputs vary from location to location and year to year by as much as a 50%. This variation can considerably impact the results of ethanol production and should be included in industrial and policy decisions. While the results are promising and give an idea of the impact of a switch from gasoline to corn ethanol, the whole picture is not shown. Only with the incorporation of uncertainty throughout the process will a better understanding of the environmental impacts be gained. The following sections and comprehensive case study in Chapter 5 give an example of how this can be performed and the knowledge that can be gained.

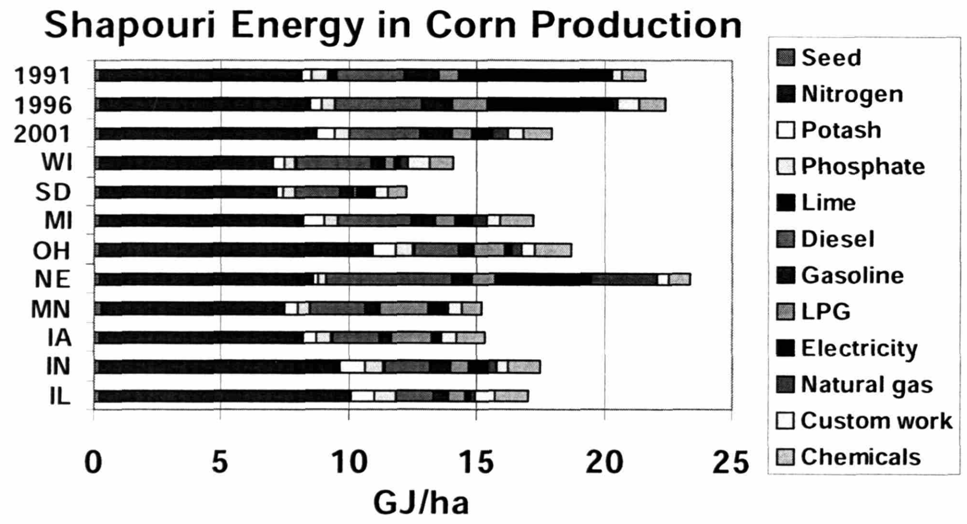

Figure 4.13 Variation of energy consumption in corn production by state and year

4.4 Uncertainty in Life Cycle Assessment

A critical question in the continued methodological development of life cycle assessment (LCA) is how best to manage the large amount of uncertainty throughout the process and in the final results (Huijbregts, 2001). An LCA calculation is affected by the uncertainty in the input-output data available for inventory collection, in the fate and transport models which are used to determine environmental damage, and in the choices for system definition. All of these uncertainties can contribute significantly to the conclusions which are drawn from the LCA. Therefore, it is critical to have an understanding of how the uncertainty implicit in the data, models, and system can affect the outcomes. To this point, most LCA case studies still do not rigorously deal with possible uncertainties or suggest methods for narrowing those uncertainties. Most include basic sensitivity analyses, but these are usually performed on only a handful of parameters, leaving significant opportunity for improvements in the methodology.

Failing to address the uncertainty in the system can call into question the conclusions from those assessments. LCA is used as a decision tool for comparing competing processes or products or for determining which elements of an individual product's life cycle contribute most to its environmental impact. When simple deterministic values are used, these comparisons are easy to make, but this hides the reality that the results are actually highly uncertain. This simplistic representation can lead to misleading results. When different assumptions regarding the data and models are made, the question remains: do comparisons between alternative processes still show the same conclusions?

One way of dealing with uncertainty is to use probability distributions to describe inputs, outputs, and damage characterization factors. The disadvantages are that data collection stages consume more time and resources while the results presented with uncertainty become more difficult to interpret. This often makes the comparison between competing technologies difficult. This is a reality that decision makers must face, but tools can be implemented to help elucidate the uncertainty as best as possible. A number of researchers have been investigating possible approaches to this problem (Cano-Ruiz, 2000; Lo, 2005; Heijungs, 2005; Geisler, 2005; Huijbregts, 2003; Huijbregts, 2001; Sakai, 2002; Ross, 2002; Andrae, 2004; Sonnemann, 2003).

This section will review some of the alternatives and will propose a new methodology which integrates a couple of the tools while adding one new one. The proposed method will consist of an initial perturbation analysis which captures the most important parameters relative to the expected value of the outputs. These critical parameters will be transformed from deterministic values to probabilistic representations. The next step will be to perform a Monte Carlo simulation. Subsequently, a sensitivity analysis of the LCA will show which of these parameters contribute most to the variance of the output data. Finally, the remaining critical parameters from the sensitivity analysis of the Monte Carlo simulation will be further refined using Bayesian analysis with more detailed data. While the first two steps have been demonstrated in the literature, this combination along with the addition of the new approach – Bayesian analysis, has not been.

4.4.1 Sources of Uncertainty

Life cycle assessment can be thought of as a model to describe the environmental performance of the production system for a specific process or product. As in any other model, LCA will consist of uncertainties where the model differs from the real system. As in any other model, uncertainty in LCA can be classified into a number of sources. Huijbregts (1998) describes six types of uncertainty which are specific to life cycle assessment: parametric, model, system, temporal, spatial, and process differences. For this work, we will focus on the initial three sources. The latter three can be thought of as specific examples of the first source, parameter uncertainty.

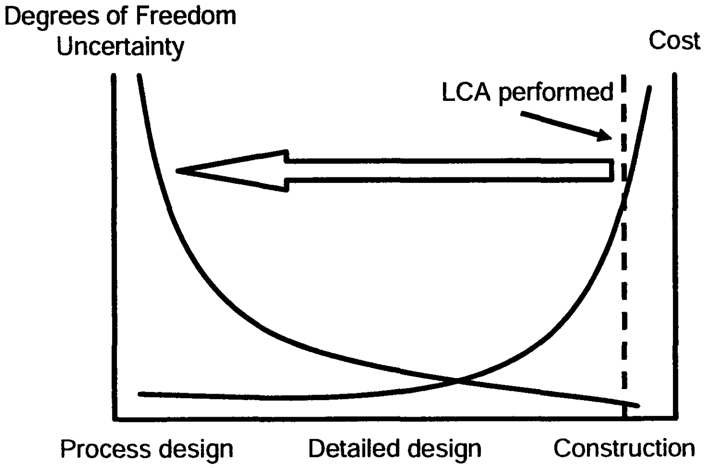

Figure 4.14 Uncertainty progression in chemical process design

4.4.1.1 Parametric uncertainty

Life cycle assessment is heavily data dependent, leading the inventory stage to be both time consuming and challenging to find the appropriate information. During this inventory, data is required for all of the material and energy inputs, outputs, and emissions for each of the multiple processes which make up the life cycle. There are many variations in these processes from facility to facility. For example, nitrogen fertilizer is an important input to agriculture. However, farmers have the choice of a number of different nitrogen forms – ammonia, urea, ammonium nitrate, etc. Moreover, even the process to make ammonia can be different depending on the age of the facility and the technology used for manufacture. Many of the processes are protected by intellectual property rights and trade secrets such that retrieving any data is impossible. Therefore, industry wide economic parameters or process simulations are often used to represent specific processes. Finally, in some cases, little or no information is available to estimate the inputs and outputs for a process, and the assessor is left to guess what those values may be.

Generic life cycle inventories have been published for many processes, especially upstream ones for energy production or resources extraction. These can be helpful, but a decision maker still needs to have an understanding how differences in the inventories for these upstream processes can impact the final results of an assessment. For the specific processes under investigation, more detailed models are typically available to describe the material and energy balances for the system. Even still, how the production will occur in the physical world will vary based on inefficiencies in the facility and other deviations from the model. While the data for these processes may be more reliable than data from the generic databases, it is still critical to take into consideration the variations which occur in the day to day operation of a production facility.

4.4.1.2 Model uncertainty

The impact assessment stage consists of even more highly uncertain data. Once the inventory is determined, the outputs to the environment or the resource consumption from inputs to the process are transformed into their specific environmental impacts. For example, the emission of a certain amount of SO_2 is related to acid rain. These relations rely on fate and transport or other models and can actually differ markedly from the real world occurrences. Another example is the impact of a chemical release on human health. To transform the inventory to an impact, models for the transfer of the chemical to the environment and subsequently to human uptake must be developed. Additionally, epidemiological studies which investigate how those chemicals affect health once in the human body are combined with the other models to determine the final impact.

The combination of uncertainties in these models leads to highly dispersed probability distributions for the actual impact. Some of the representations are more precise than others. For example, global warming potential (GWP) has a much tighter distribution than human toxicity. Therefore, decisions using GWP as an objective may be more trustworthy than those based on human toxicity, which can span several orders of magnitude. Understanding the contribution of these models to the overall uncertainty is critical for a decision maker.

4.4.1.3 System uncertainty

Finally, how the overall system is modeled can be variable. Researchers may draw the boundaries at different points. This involves a tradeoff of comprehensiveness versus effort. While being as complete as possible in the inclusion of upstream systems, at some point, the additional time and money required for completeness will be a greater cost than the benefits. Another systematic uncertainty arises when making the choice of how to allocate the environmental impacts to multiple products. When a process includes the production of a co-product, a decision needs to be made as to how much of the life cycle impacts should be allocated to the co-product versus the primary product. How this allocation is made can lead to considerably different comparisons between alternatives.

This type of uncertainty needs to be dealt with differently than the ones discussed above. In most cases, the uncertainty relates to how to make decisions between discrete alternatives, whereas the parametric and model uncertainties are more associated with continuous parameters. The discussion below will highlight the methods used for uncertainty analysis with these different types.

4.5 Methods for Managing Uncertainty.

Uncertainty within LCA has been recognized as a problem (Huijbregts, 2001). A short literature review is given to describe some of the tools which have been investigated along with examples of their implementation. Note that the terminology for this section can be confusing as a number of the techniques may share the same name. For reference, a short definition of the terms used here is given (Morgan, 1990).

- Sensitivity Analysis – A method of computing the effects of changes in input parameters on the expected value of the output.
- Uncertainty Propagation – A method for calculating the probability distributions of output values, based on using uncertainty within the input parameters.
- Uncertainty Analysis – A method for comparing the relative importance of the input parameters uncertainty measured as relative contributions to the output value variance.

4.5.1 Sensitivity Analysis

The most prevalent method is single parameter sensitivity analysis. This corresponds to the variation of a single input or parameter in the model to see how the results are affected. The sensitivity analysis can be repeated for a number of parameters to see the relative impact of those variations This tool is useful in seeing the influence of the particular parameters on the overall system. However, the process is somewhat limited in that the sensitivity of each uncertain parameter is tested one at a time. The following derivation demonstrates the use of sensitivity analysis and its limitations. This is just an introduction into the analysis for uncertainty in experimental design. Chen (2005), Saltelli (1993), and Homma (1996) provide reviews with much more detail.

For

$$y = f(\theta) \tag{4.10}$$

where $\theta = \{\theta_1 \ldots \theta_m\}$ is the vector input and $y = \{y_1 \ldots y_n\}$ is the output, sensitivity analysis is a method to characterize the influence of θ on the model prediction $y(\theta)$ and to compare the relative importance of θ_i around a nominal point θ'.

The sensitivity of y_i to θ_i is defined as:

$$S_{i,j} = \left.\frac{\partial y_i}{\partial \theta_j}\right|_{\theta'} \tag{4.11}$$

A normalized sensitivity analysis is used to compare the relative importance of the percentage changes of θ_i to the percentage change of y rather than absolute values. This is defined as:

$$S^n_{i,j} = \frac{\theta_j}{y_i}\frac{\partial y_i}{\partial \theta_j}\bigg|_{\theta'} = \frac{\partial \ln y_i}{\partial \ln \theta_j}\bigg|_{\theta'} \cong \frac{\theta_j}{y_i}\frac{y_i(\theta'+\Delta\theta_j)-y_i(\theta')}{\Delta\theta_j} \qquad (4.12)$$

However, for the life cycle assessment calculation, **θ** includes all of the B_{ij}, C_{ij}, E_{ij}, F_{ij}, H_{ij}, and p_i, so many sensitivity analysis calculations are required. Additionally, the sensitivity analysis is performed at a local point, and the impact at other places may be different. The following example displays the problematic nature of this.

Figure 4.15 illustrates the sensitivity analysis graphically. At the nominal value, **θ'**, as θ_i increases, S_i is positive representing an increase in the model response $y(\theta_i)$.

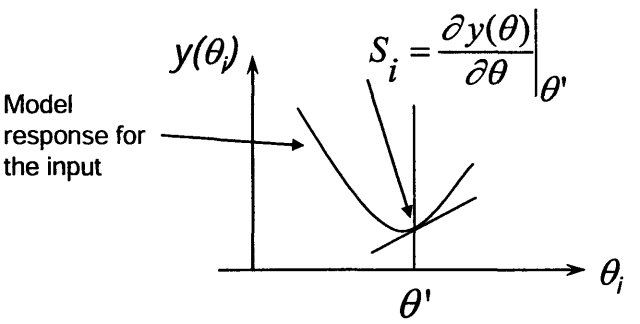

Figure 4.15 Schematic picture of sensitivity analysis

However, for uncertain θ_i, the actual value may **θ"** at which point S_i is negative and the model response would be in the opposite direction, as shown in Figure 4.16. With this uncertainty, there is a possibility that θ_i will occur with values smaller than the nominal value, and as θ_i increases, $y(\theta_i)$ decreases, which is the opposite trend of what was shown in the sensitivity analysis around the nominal value **θ'**.

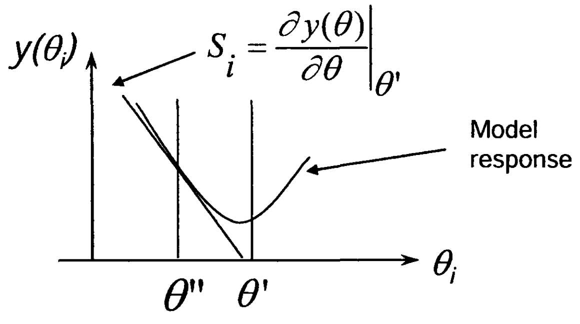

Figure 4.16 Schematic picture of sensitivity analysis

This example illustrates the limitation of local sensitivity analysis. It is suitable for differential variation of the parameters, but when the parameters vary along a large range, or the model responses have sharp change, sensitivity analysis is incapable of capturing the effect of parameters on model responses.

A sensitivity analysis can be applied for the case study of using corn grain for ethanol production. Figure 4.9 showed the abated carbon dioxide emissions for the utilization of 1 mile driven with ethanol relative to the same output using gasoline. A surprisingly high contribution is provided by the nitrous oxide which is emitted to the atmosphere after volatizing from applied nitrogen. Because of the relatively high radiative forcing of N_2O, its global warming potential is 300 times that of carbon dioxide. Therefore, it is a relatively important greenhouse gas. However, the amount of N_2O which is emitted is relatively uncertain with a range of 1-2% of the nitrogen applied as fertilizer being volatilized.

A sensitivity analysis is performed by varying this percentage across the data range, and recalculating the life cycle greenhouse gas emissions for each rate, shown in Figure 4.17. For this sensitivity analysis, θ_i represents the percentage of nitrogen which is volatilized after application into N_2O, requiring a modification of the E_{ij} where the i^{th} emission is nitrous oxide and the j^{th} process is corn production. Meanwhile, $y_i(\theta)$ is the total GWP for the process, o_i, where the i^{th} impact category is global warming potential.

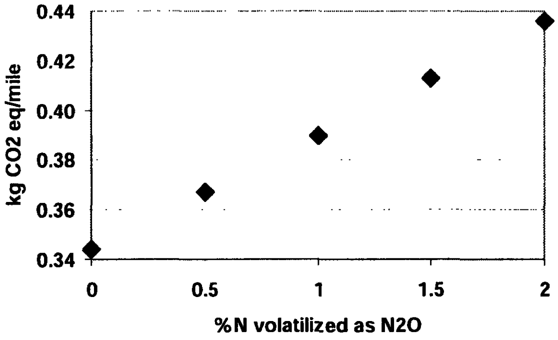

Figure 4.17 Global Warming Potential sensitivity to N2O emission rate

This analysis shows the high sensitivity of the overall emissions to the uncertainty in the volatilization rate in nitrogen fertilizer as using a rate of 2% versus 1% increase the overall greenhouse gas emissions by more than 10%. Moreover, this single parameter analysis ignores the many other uncertainties. For example, nitrogen application to the field is one of the more variable parameters to the system and its variability will significantly add to the sensitivity of the N_2O volatilization. is not the only uncertain parameter in the system. More rigorous tools are required to investigate the multiple uncertainties.

4.5.2 Perturbation analysis

The primary disadvantage of the parameter sensitivity analysis described above is its non-comprehensiveness. While the impact of the parameter θ_i on the $y(\boldsymbol{\theta})$ can be elucidated, if many parameters are uncertain, performing sensitivity analysis on each of these will become very time consuming.

A more rigorous perturbation method makes use of the matrix form of life cycle assessment, and allows for a calculation of a perturbation of all of the input parameters at once. This tool allows for comparisons between all parameters at once using a single calculation. The drawback still remains that the sensitivity applies to a local point, rather than to the global parameter space. This might not be as critical of a drawback for the inputs and outputs of the primary tier, though, as that system is linear. However, as variations are made to upstream systems, this linearity no longer exists, and the perturbation analysis can be informative. An additional disadvantage of the perturbation method, is that the tool is more useful to compare how variations in the parameters affect the mean value of the final impact value of consideration. How the uncertainty in the input variables for the input-output model affects the variance of the output parameter is not addressed.

To perform a perturbation analysis, a simple matrix calculation is required. What follows is a derivation of that calculation based on the above sensitivity analysis section and Sakai (2002). The goal is to determine **Δq** from ΔA_{ij} around **A'**, the original throughput matrix. Start by defining the change in **A'** as

$$\mathbf{\Delta A} = \mathbf{A}^{\mathbf{I}} \Delta A_{ij} \tag{4.13}$$

where $\mathbf{A}^{\mathbf{I}} = 1$ for entry A_{ij} and 0 for all others. Therefore, after the variation in demand, the new throughput vector can be defined as

$$\mathbf{A}'\mathbf{q} + \mathbf{A}^{\mathbf{I}} \Delta A_{ij} = \mathbf{d} \tag{4.14}$$

The goal is to solve for **q** and the perturbation expansion gives

$$\mathbf{q} = \mathbf{q}' + \mathbf{q}^{\mathbf{I}} \Delta A_{ij} + \mathbf{q}^{\mathbf{II}} \Delta A_{ij}^{2} + \mathbf{q}^{\mathbf{III}} \Delta A_{ij}^{3} + \cdots \tag{4.15}$$

where $q^{I}, q^{II}, \ldots$ are unknown constants. Replacing 4.14 with equation 4.15 and using only the first order decomposition gives the following for q^{I}

$$\mathbf{q}^{\mathbf{I}} = -\mathbf{A}'^{-1}\mathbf{A}^{1}\mathbf{q}' \tag{4.16}$$

Now, q^{I} can be substituted back into equation 4.15 to get the following approximation

$$\mathbf{\Delta q} = -\mathbf{A}'^{-1}\mathbf{A}^{\mathbf{I}}\mathbf{q}'\Delta A_{ij} \tag{4.17}$$

which is the sensitivity of **q** to ΔA_{ij}, the goal of the exercise. This can be extended to assess the sensitivity of each q_l in a matrix form by the following derivation which gives the relative change for slight changes in the input-output matrix.

$$\frac{\dfrac{\Delta q_l}{q_l'}}{\dfrac{\Delta A_{ij}}{A_{ij}'}} = -\frac{q_j'}{q_l'}A_{ij}'A^{-1}_{li} \tag{4.18}$$

The derivation can also be extended to include the relative sensitivity of the environmental impact categories.

$$\frac{\dfrac{\Delta o_k}{o_k'}}{\dfrac{\Delta A_{ij}}{A_{ij}'}} = -\frac{A_{ij}'}{o_k'}q_j'\sum_l E_{kl}A^{-1}_{li} \tag{4.19}$$

These equations are used in the spreadsheet calculation to form two more matrices, a perturbation matrix for the throughput matrix and a perturbation matrix for the environmental exchange matrix.

The application of a perturbation analysis for the corn ethanol example is demonstrated here. In the initial LCA calculation, the **A** matrix and **o** and **q** vectors are already calculated to determine the overall requirements through the system. These requirements were then used to calculate the energy balance. Using this same matrix, we can now calculate how a relative change to each of the possible parameters in the input-output matrix can cause a relative change in the energy required for the production of ethanol. Table 4.3 shows a subset of the Δp matrix. Under the column N production, and on the row Natural gas, Δpi,j = -0.06. This means that a 100% change in natural gas required for nitrogen production causes a 6% change in the energy requirements over the entire life cycle. The rest of the matrix entries may be interpreted in the same way. We can limit the number of important parameters by specification of a threshold below which overall impact is assumed to be negligible.

	process	Coal (p	Corn (p	Diesel	Electric	Ethano	Gasolin	Mecha	Mecha	**N fertilizer (per kg)**
product										
Coal (kg)		0.10								
Corn (kg)			0.17			-0.17				
DDGS (kg)										
Diesel fuel (kg)				0.08				-0.08		
Electricity (MJ)					0.13	-0.10				
Ethanol (kg)						0.80			-0.80	
Gasoline (kg)						-0.08	0.08			
Mechanical energy fr			-0.03					0.08		
Mechanical energy fr									0.80	
N fertilizer (kg)			-0.08							0.09
Natural gas (kg)										-0.06

Table 4.3 Perturbation analysis matrix

As was mentioned above, this method says nothing about variance. Thus, a parameter which has a variance of an order of magnitude, rather than simply two times the mean value may be left out. For example, the amount of irrigation used in corn production has a very low Δq_{ij}. However, its variance is extremely high, and it must be considered in any uncertainty analysis. This would be missed by using perturbation analysis alone.

4.5.3 Monte Carlo Simulation.

Direct incorporation of uncertainty through stochastic approaches allows the user to address the variance by combining parametric input uncertainty with model responses. Numerical tools such as Monte Carlo simulations are the most prevalent for this analysis. Rather than using deterministic values, the inventory and impact parameters are presented in probabilistic terms. The matrix calculations are then performed repeatedly using different samples from those probability distributions. The output data can then be displayed as probability distributions themselves. While the stochastic process is more challenging, it presents the most information to the decision maker.

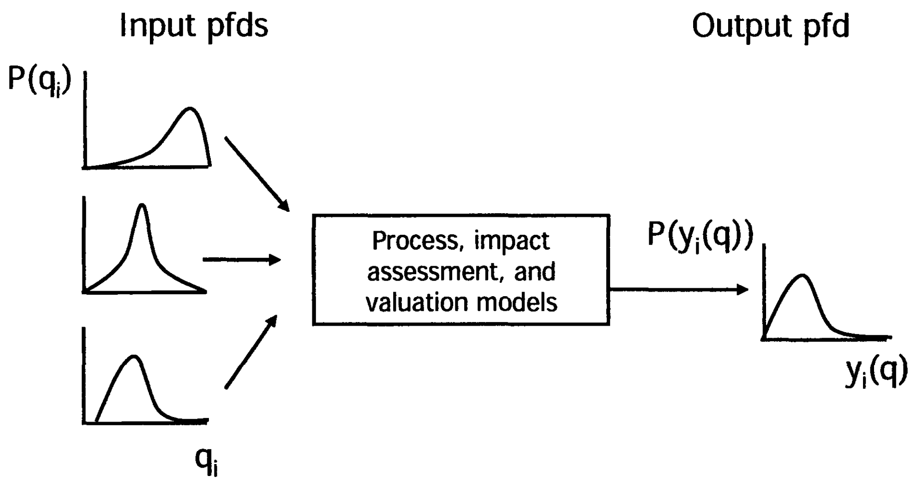

Figure 4.18 Graphical representation of Monte Carlo simulations

Monte Carlo methods are algorithms for computationally simulating stochastic models based on random sampling of the inputs to the process. As a simple introduction, a two-parameter simulation is described here. Let

$$y(\boldsymbol{\theta}) = \theta_1 + \theta_2 \tag{4.20}$$

where θ_1 can be described by a normal random variable, with a mean of 0 and a standard deviation of 1, while θ_2 can be described by a lognormal random variable, with a mean of 0 and a geometric standard deviation of 1. The probability density functions of these variables are given here.

$$f_{\theta_1}(x) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{1}{2}\frac{(x-\mu)^2}{\sigma^2}} \tag{4.21}$$

$$f_{\theta_2}(x) = \frac{1}{\sqrt{2\pi}\phi x} e^{-\frac{1}{2\phi^2}(\ln(x) - \xi)^2} \tag{4.22}$$

where μ is the mean and σ is the standard deviation of the normal distribution and ζ is the mean and ϕ is the standard deviation of the lognormal distribution.

To solve this problem, Monte Carlo methods sample a set of random numbers θ_{1j} and θ_{2j} from the normal distribution N(μ, σ) and the lognormal distribution Log-N(ζ, ϕ), respectively. Each of these samples are taken by using a random number generator to generate both x_{1j} and x_{2j} from U[0,1]. Using the inverse of the cumulative distribution function, x_{1j} and x_{2j} can be transformed to the appropriate θ_{ij}. An example is given in Figure 4.19.

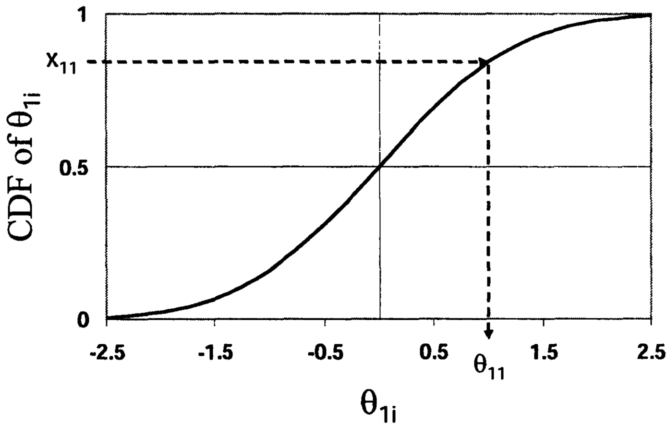

Figure 4.19 Monte Carlo sampling

This sampling is performed many *N* times, where *N* is a large number. (For this thesis, *N* is typically 2000.) For this example, $\{\boldsymbol{\theta}_1,\ldots,\boldsymbol{\theta}_{2000}$ are substituted into y($\boldsymbol{\theta}$) to compute a $\{y_1,\ldots,y_{2000}\}$. As *N* approaches infinity, the collection of these random numbers represents the probability distribution for y. The collection $\{y_1, y_2,\ldots, y_n, y_{n+1},\ldots,y_{2000}\}$ are transformed into a histogram as is shown in Figure 4.20. Throughout the rest of the thesis, most of the output distributions are described using percentiles, where the Monte Carlo simulation results are divided in the 5th, 25th, 50th, 75th, and 95th percentiles and displayed in a box chart as is shown in Figure 4.21.

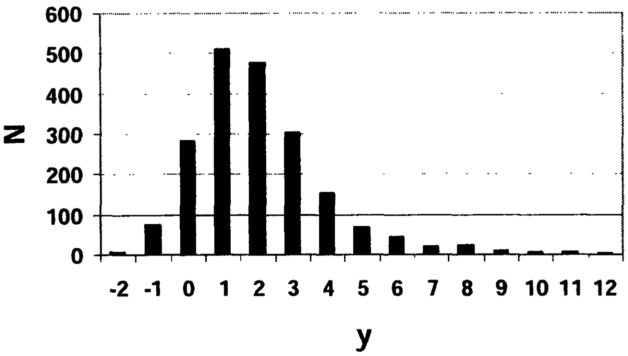

Figure 4.20 Histogram of Monte Carlo simulation

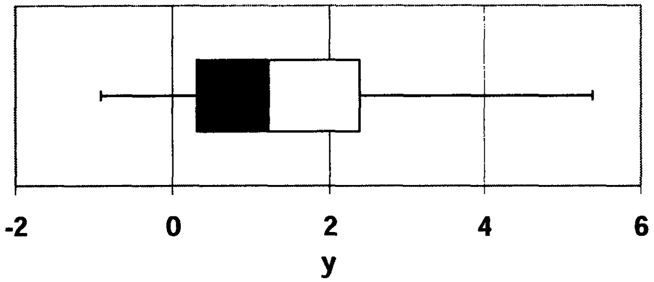

Figure 4.21 Percentiles of Monte Carlo simulation

These tools graphically represent the output distribution, but another powerful tool of the simulation is the ability to estimate the expected value or maximum likelihood of the initial model. To calculate the expect value of y, Monte Carlo methods transform

$$E\{y(\theta)\}=\int_{\infty}^{\infty} y(\theta)f_{y(\theta)}(y(\theta))dy(\theta)=\int\ldots\int y(\theta)f_{\theta}(\theta)\theta_1\ldots d\theta_n \tag{4.23}$$

into

$$E\{y(\theta)\}\approx\frac{1}{N}\sum_{i=1}^{N} y\left(\theta_1^{\,i},\theta_2^{\,i},\ldots\theta_n^{\,i}\right) \tag{4.24}$$

For our initial example, the expected value becomes

$$E\{y(\theta)\}\approx\frac{1}{N}\sum_{i=1}^{N}(\theta_{1i}+\theta_{2i})=1.64 \tag{4.25}$$

which makes sense because, independently, the expected value of $\theta_1=0$ and the expected value of $\theta_2=1.64$.

Returning to LCA, y(θ) becomes the equations described above for calculating the total energy utilization, the global warming potential, or any other output parameter of interest. The EnvEvalTool includes the capability to perform uncertainty analysis using Monte Carlo simulation using commercially available computer software. Instead of using deterministic values, the data are represented by probability distribution functions using the @Risk add-in program from Palisade Tools in an Excel spreadsheet. These prior distributions are limited to normal, lognormal, uniform, and triangular function, and are typically represented by their mean and standard deviation.

Unfortunately, the Monte Carlo method doesn't solve the time constraint problem of determining the life cycle inventory. In fact, it increases the required time, because probability distributions are required for the input parameters rather than simple data points. Note though that the inputs can be a mix of deterministic and probabilistic values. The methodology described here uses perturbation analysis initially to identify a subset of the uncertain parameters which are then described using probability distributions.

A more detailed description of the development of the prior distributions for the LCA calculation is given in the next chapter, but as an example, the graph in Figure 4.12 showing the energy inputs to corn production can be redrawn as in Figure 4.22 using the results from a Monte Carlo simulation of the LCA to show the uncertainty in the system.

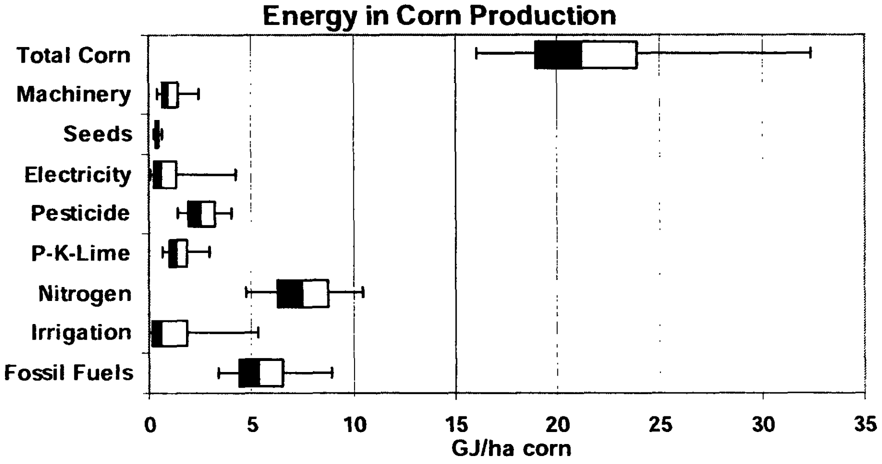

Figure 4.22 Monte Carlo results of life cycle energy inputs for corn production

4.5.4 Uncertainty Analysis

As the above figure demonstrates, the uncertainty in fuel and electricity use, nitrogen fertilizer application, and irrigation lead to significant uncertainties in the calculation of life cycle energy usage for corn production. The next section describes the methodology for reducing this variance to better inform decision makers.

4.5.4.1 Sensitivity analysis

The data collected in the Monte Carlo simulation can be used to correlate the input parameters to the output uncertainty. Chen (2005) described a number of these techniques, but for simplicity in use, the method of rank correlations is used in this thesis. A demonstration of this technique is provided here for the simple example presented earlier in this chapter. Note that the methods for this sensitivity analysis are slightly different than the above discussion on sensitivity. Whereas the analysis is section 4.5.1 deals with the sensitivity of an input on the output response, this sensitivity analysis investigates the impact of input uncertainty on the output variance.

The rank correlation method provides a robust measure of the degree of association between random variables by comparing sample ranks rather than sample values. In the example from above let, $R_i = \text{Rank}(\theta_{1i})$ and $S_i = \text{Rank}(\theta_{2i})$ where $\text{Rank}(\theta_i)$ assigns the numerical rank of θ_i from smallest to largest of all the $\{\theta_1, \theta_2, \ldots\}$. Now applying the standard correlation coefficient equation to R_i and S_i yields

$$r_S = \frac{\sum_{i=1}^{N} (R_i - \bar{R})(S_i - \bar{S})}{\sum_{i=1}^{N} (R_i - \bar{R})^2 \sum_{i=1}^{N} (S_i - \bar{S})^2} = 1 - \frac{6\sum_{N} (R_i - S_i)^2}{N(N^2 - 1)} \tag{4.26}$$

Applying these equation to θ_{1i} and θ_{2i}) above yields $r_{\theta 1} = 0.63$ and $r_{\theta 2} = 0.70$. While the rank correlation numerical value does not represent a specific contribution to variance, it does give a relative account. For example, $r_{\theta 1} < r_{\theta 2}$ suggests that θ_2 contributes more to the variance of y then θ_1 which makes sense as the former is a lognormal distribution compared to the latter with a standard normal.

This technique is applied to all of the inputs in the LCA case study to identify the ones which contribute most to the overall output variance. See Chapter 5 for the application of the sensitivity analysis to the corn grain ethanol case study.

4.5.4.2 Relative comparisons

Another variance reduction technique that can be helpful when using Monte Carlo simulation is to compare relative impacts versus straight comparisons. Rather than showing the impacts of alternative A, X_A, next to alternative B, X_B, the visual demonstration can be shown as X_A-X_B or X_A/ X_B. The result is that many of the uncertainties are correlated between the two alternatives and thus the overall uncertainty is lowered.

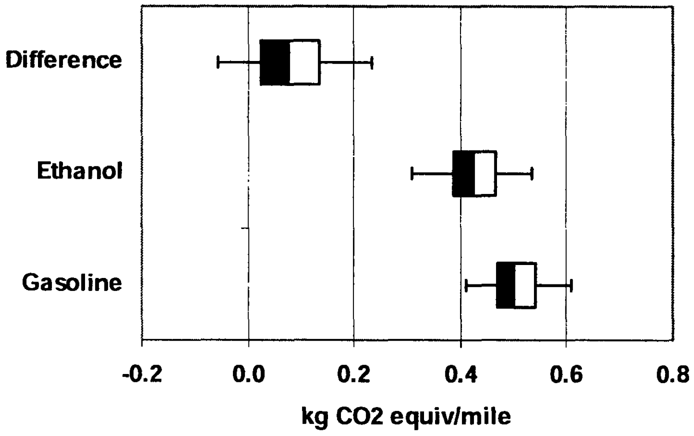

Figure 4.23 Greenhouse gas emissions with uncertainty

Using the corn grain ethanol versus gasoline example, Figure 4.23 shows the global warming potential with uncertainty for each fuel, along with a simulation of the difference between the two. While the probability that ethanol is less than gasoline is reasonably high when looking at the alternatives individually, that probability is considerably higher, 80%, when looking at the difference.

4.5.4.3 Bayesian analysis

One tool which hasn't been involved much in the development of uncertainty analysis for LCA is Bayesian analysis. This method allows for the updating of prior knowledge with new data. This may be especially useful in LCA as many inventories already exist for the process data which is required. If these inventories are revised to contain probabilistic data rather than deterministic data, an assessor could use the probabilistic inventory for a baseline assessment, but then update the analysis using the Bayesian approach with new data which is specific to the process being investigated.

Within the demonstrations of uncertainty analysis, the Bayesian approach will be used in the last step of the proposed methodology. Once the analysis has been refined to highlight just a handful of important parameters, more detailed data can be retrieved for the specific processes of consideration. This detailed data can be used to update and narrow the prior probability distributions. The goal is that updated distributions will decrease the uncertainty of the final outputs for a decision maker to accurately understand the environmental impacts.

Bayes' theorem is used in probability to relate conditional distributions of random variables. As the methodology presented here treats the uncertain inputs into LCA as random variables, Bayesian concepts can be useful. While a more detailed discussion of Bayesian theory can be found elsewhere (de Man, 2006), the basic ideas are presented here. Bayes' rule states that

$$p(\theta|y) = \frac{p(y|\theta)p(\theta)}{\int p(y|\theta)p(\theta)d\theta} \tag{4.28}$$

Where θ is a random variable, y is information, $p(\theta|y)$ is the posterior probability distribution of the parameter θ, given the data y, $p(y|\ \theta)$ is the likelihood function of the data, given the parameter θ, and $p(\theta)$ is the prior distribution The procedures for evaluating data with the Bayesian approach are very flexible. Typically, Bayes' theorem can be considered as an updating algorithm as the posterior distribution becomes the new prior and new information is provided, as illustrated in Figure 4.24.

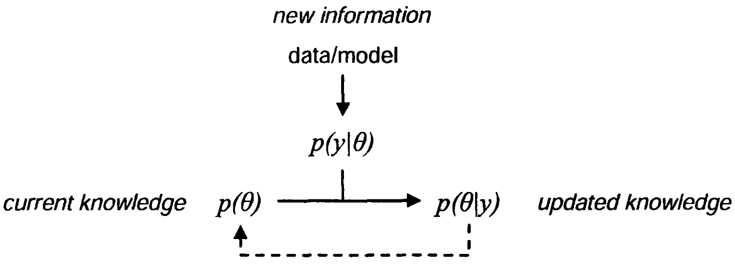

Figure 4.24 Bayesian approach for updating prior distributions

Returning to the simple case study, assume that further investigation into θ_2 results in data with a normal distribution with a mean of 1.5 and a standard deviation of 0.5. The original Monte Carlo simulation can be updated such that the probability for each θ_2 is represented by the following distribution (Lo, 2005).

$$p(\theta_{2i}|y) = \frac{p(y|\theta_{2i})p(\theta_{2i})}{\sum_{i=1}^{N} p(y|\theta_{2i})p(\theta_{21})} \tag{4.28}$$

After updating, the new output response distribution is shown in Figure 4.25. Note that the variance has been considerably reduced with the incorporation of the new data.

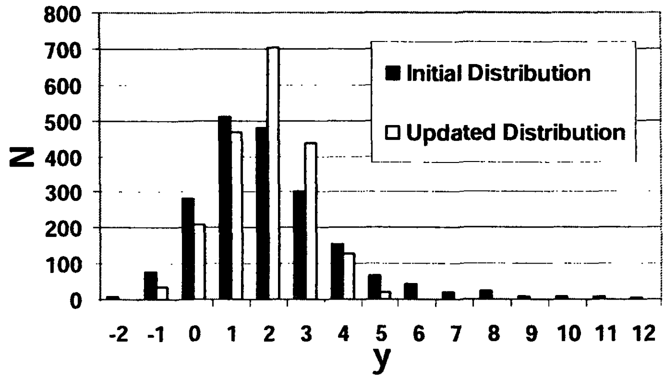

Figure 4.25 Histogram of Monte Carlo simulation after Bayesian updating

4.6 Methodology development for managing uncertainty

Figure 4.26 shows a block flow diagram of the methodology for the LCA uncertainty analysis. As shown in the figure, three separate tools are used with finer levels of detail. Because the initial LCA was performed using matrix calculations, the tools can simply be applied seamlessly to the original assessment.

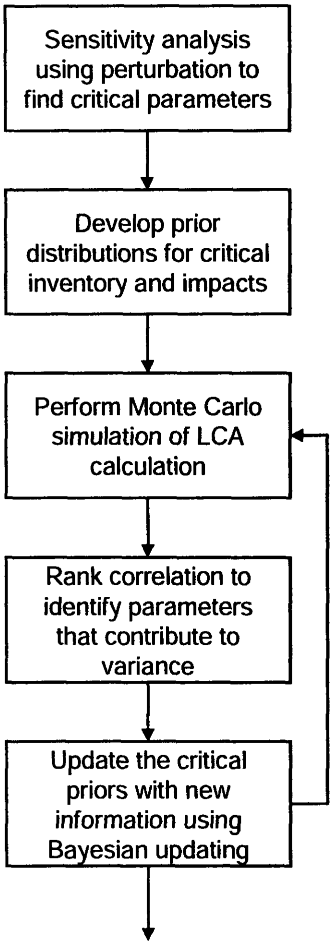

Figure 4.26 Block flow diagram of uncertainty propagation methodology

Step 1. The top-level approach for addressing uncertainty uses the analytical approach for perturbation analysis. Using the derivation provided, the variables in the equation are already contained in the EnvEvalTool, and adding this next step simply requires an additional spreadsheet page.

Because the matrix calculation is a linear system, the inputs to the first tier of inputs and outputs in the system will each have the same impact. Therefore, the perturbation will be trivial, suggesting that each input is equally significant and their uncertainties will have to be analyzed with further detail. The advantage of this approach for the initial screening becomes more obvious when looking at the second and higher tiers of the life cycle. At this point, the parameters will have different contributions to the expected value of the outputs being considered. Once again, it is important to note that this analysis only looks at the expected value not the variance. Therefore, the actual contribution to uncertainty in the final answer is not addressed here and a large enough sample of uncertain parameters must be carried over to the next step.

Step 2. Once the initial set of critical parameters is identified, the next phase is to find probability distributions which better represent the parameters than deterministic values such as averages. While it is desirably to have an accurate portrayal of the distribution, this first pass can be a little rougher of an estimate as the later sensitivity analysis will suggest if the prior distribution needs to be tightened. For parameters where much data is available, a statistical analysis can be performed to find a distribution which best fits that data. For simplicity, standard distributions are used to describe the uncertain parameters. Typically, the distributions are defined as a lognormal function to avoid any problems with negative values. Making an assumption for a distribution is more tricky when there is not a wealth of data. In these cases, engineering judgment is required to make lower and upper constraints for uniform or triangular distributions. If the later stage sensitivity analysis displays that the results are heavily dependent on that uncertain parameter, then a decision maker would have to allocate resources towards learning more about that parameter.

Step 3. After the distributions have been defined, they should be input into the life cycle assessment and a Monte Carlo simulation should be performed. The EnvEvalTool has the functionality of allowing for probabilistic distributions and stochastic simulations by using the Excel Add-in program @Risk. The simulation is performed using Latin Hypercube sampling and 2000 iterations. The @Risk interface calculates the simulation statistics for the output parameters. Using a graphical approach, the user can visually assess the variance in the outputs. This calculation allows for the determination of the distribution for the energy utilization for the overall process and for each sub-process. In addition to overall energy, the type and quality of the energy flows can also be accumulated. Note that this uncertainty propagation can also be used for the calculation of probability distributions for other environmental impacts such as global warming potential and greenhouse gas emissions.

Step 4. Following the Monte Carlo simulation, a sensitivity analysis of the results helps to illuminate information on which input parameters contribute most to the output variance. A number of sensitivity analysis methods can be used for this task (Chen, 2005), but for the sake of simplicity, a rank correlation is used to give a quick idea of the relative contributions between the parameters. While the correlation does not give an exact representation of the contribution to the uncertainty, this approach estimates which parameters are the strongest contributors to the overall variance. At this second level of detail, the simulation approach is able to narrow down the critical parameters further, beyond what was identified in the perturbation analysis.

Step 5. The final step requires a further refinement of the distributions, possibly including further data retrieval. In the Bayesian approach, the distributions utilized in step 2 for the Monte Carlo simulation will be the prior distributions. The updating data will depend on the parameter being considered. For parameters which had a large amount of original data, the updating may be a subset of the data which is more representative of the specific process being analyzed. Other sources, may be expert solicitations, data from new experiments, etc.

The prior distributions and new data can be plugged into the Bayesian equation to calculate the posterior distribution. In most cases the posterior will be narrow then the prior which is beneficial to limit the variance of the LCA. This posterior distribution is then used to replace the prior. Once again a Monte Carlo simulation is performed followed by a sensitivity analysis. The goal is to limit the variance in the output to the point that a decision maker can make a confident judgment between the available options. If the variance is still too great, a further refinement by performing another Bayesian iteration may need to be required. While this iterative process may not refine the resulting probability distribution to the most desirable range, the resulting information can inform a decision maker where to allocate resources to make sure the process is optimized. The above methodology was applied to the original corn ethanol case study and the results can be found in the next chapter.

Chapter 5 Corn Ethanol Case Study

5.1 Introduction

The corn ethanol industry has been expanding at a fast pace over the past decade. The production capacity in the United States has more than doubled over the past five years to over 4 billion gallons annually (RFA, 2006). While advocates label corn ethanol as a clean and renewable fuel important for energy security and the rural economy, a number of questions remain regarding its economic and environmental performance. These questions pertain to ethanol's role in local air emissions, its potential reliance on subsidies for continued economic feasibility, and whether or not the production of ethanol requires more energy than what is contained in the heating value of the product. The first two questions will be briefly outlines here, but the primary focus of this chapter is the third question – What is the energy balance of corn ethanol, and why do different researchers come up with very different answers to that question?

While many studies investigating the environmental performance of the corn ethanol system have been published, the energy balance, still remains contentious. Many of the researchers (Shapouri, 2004; Wang, 1999) show that the life cycle energy required to produce a gallon of ethanol is less than the heating value of that gallon. However, a couple of others (Pimentel, 2005; Patzek, 2004), still maintain the opposite. Figure 5.1 shows the range associated with the different studies. The results from the LCA calculation performed in Chapter 4 is included at the bottom. Using net energy ratio as the metric, the studies vary from 0.75 to 1.45. The net energy ratio is defined in Equation 5.1. In simplistic terms, a value greater than one means that there is more energy in the ethanol than is required to produce it and vice versa for a value less than one. In this chapter, an independent calculation of the energy balance of corn ethanol will be performed, with a discussion of the discrepancies between the other studies. Additionally, this new calculation will include a comprehensive analysis of the uncertainty and variability in the underlying data.

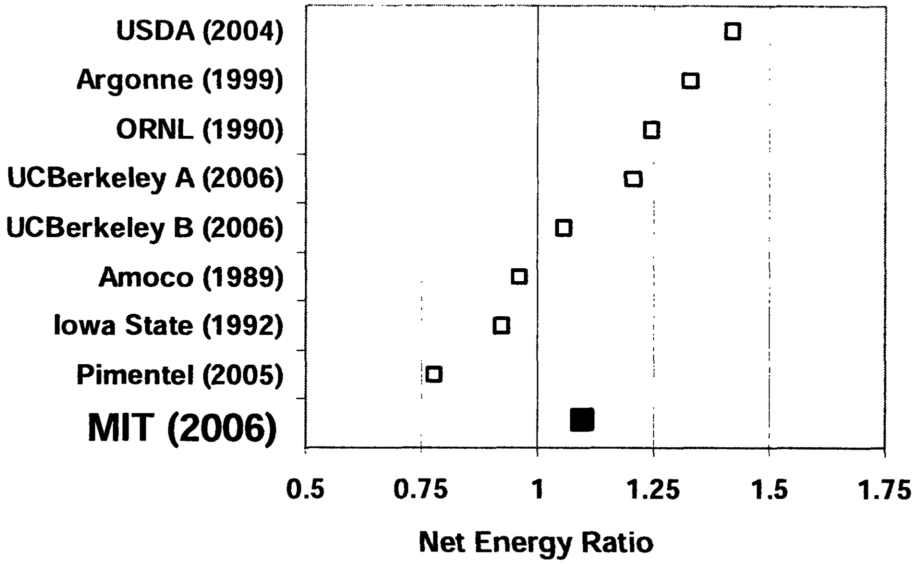

Figure 5.1 Energy balance results from previous studies

The net energy ratio is defined as

$$NER = \frac{\text{EtOH} + \sum \text{Coproducts}}{\sum \text{Inputs}} \tag{5.1}$$

where EtOH – heating value of ethanol, Inputs – heating value of the energy inputs (oil, coal, natural gas, and non-fossil electricity) to the life cycle of the system, and Coproducts – heating value of the energy inputs required for the production of the animal feed (soybean meal) which is replaced by the coproduct distiller's dried grains. The lower heating values of the fuels are used for all of the energy calculations Figure 5.2 graphically demonstrates these parameters.

5.1.1 Application of Methodology to Energy Balance Case Study

The next three chapters demonstrate the basic framework for technology assessment which is proposed in this thesis. The methodology is applied in this chapter to an analysis of the energy efficiency of corn ethanol using the methods for uncertainty analysis in life cycle assessment described in Chapter 4, the framework is generalized and extended to the economic and environmental assessments of the larger biomass energy picture in Chapters 6 and 7.

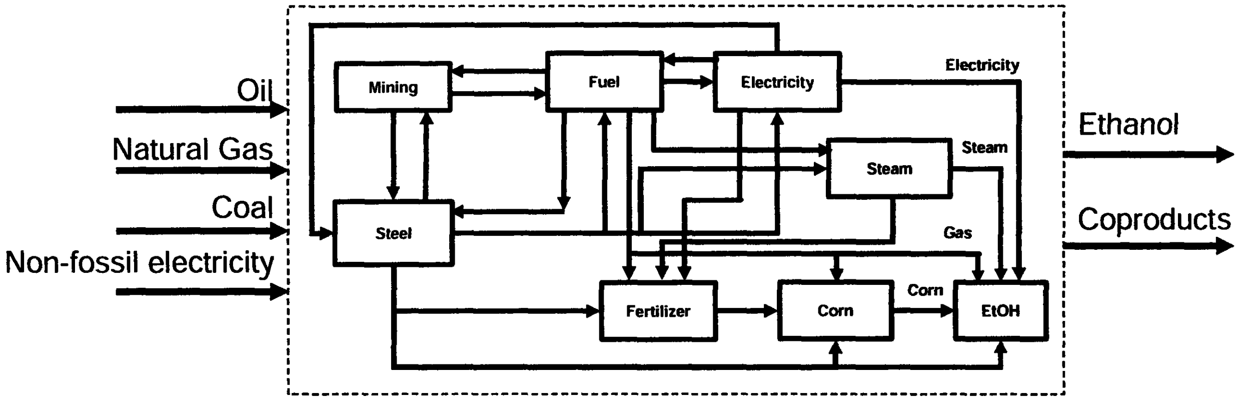

Figure 5.2 Parameters for net energy ratio calculation

A primary goal of this work is to provide some elucidation to the confusion which results from the differences in the energy balance studies as shown in Figure 5.1. Some of the overall results are impacted by differences in system boundary definition. In these cases, a decision making individual or group will simply have to decide which boundary provides the best information. However, most of the discrepancies are caused by differences in input data for the same systems. The primary shortcoming of most previous studies is that they use averages or even single data points as inputs. This hides uncertainty and poses a problem in that two very different values can be accurate for the specific situations they are describing while being an inappropriate indicator of the industry as a whole. For example, assuming a fertilizer application rate based on the average value from a subset of states for a particular year or choosing a single data point from a report on the energy use in a particular ethanol manufacturing facility will hide the fact that these values change from location to location and year to year.

For these situations it is critical to have a method that determines the accuracy of parameter estimates. Unfortunately, simply providing large ranges for all of the inputs results in vague output results. Therefore, determining appropriate data ranges and providing tools for sifting through the results is also important. This can become problematic for an energy system which is so large and non-uniform. Corn farmers work with different production practices from state to state. The weather affecting corn yield varies from year to year. A 40 year old fertilizer production facility is most likely less energy efficient than one which is only 10 years old. These are simply examples of the uncertainty and variability in the system, and many more could be stated.

This chapter provides a quick demonstration of the methodology used for this uncertainty propagation and analysis. A more detailed analysis of the mathematical tools can be found in Chapter 4 with the following procedure being diagramed in Figure 4.27. The methodology begins in section 5.3 at step 2 after the perturbation analysis described in the previous chapter.

5.2 Previous Energy Balance Calculations

A number of researchers have published analyses of the energy requirements for ethanol production (Keeney, 1992; Lorenz, 1995; Marland, 1990; Pimental, 2005; Wang, 1999). While few of them have been based on the specific guidelines for LCA, their calculations have followed the same concept. In addition to including the energy inputs for the primary processes, the energy requirements for upstream processes such as electricity generation, fertilizer production, fuel processing, etc. are included. For the most part, the various assessors choose similar boundaries on what to include in the energy requirement estimates although one exception is a variance in whether or not to include the energy embodied in farm machinery and the ethanol manufacturing facility equipment.

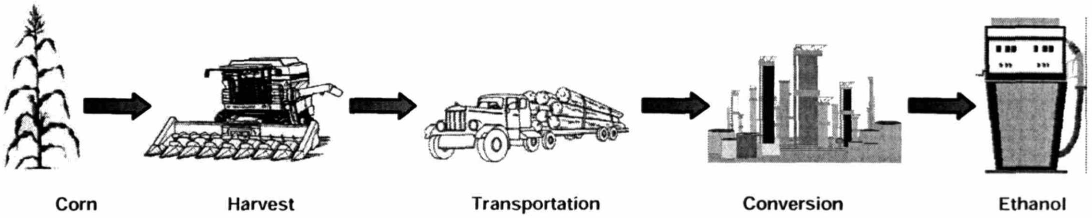

Figure 5.3 Corn grain ethanol supply chain

The supply chain consists of three primary processes: corn production, ethanol production, and the distribution of both corn and ethanol. Figure 5.3 gives a flowchart of the inputs to the system which are commonly included in these assessments. A short description of this supply chain is given here, while more details can be found in Chapters 2 and 4 and below when describing the input definitions.

The primary inputs for ethanol production are corn, natural gas which is used to dry the DDGS and produce steam for distillation, electricity for the centrifuge, pumps and other utilities, and a combination of other enzymes, yeasts, and chemicals. These last inputs do not contribute significantly to the overall energy utilization and our lumped together as "Other" in the following figures. The transportation inputs are labeled as "Distribution" in the figures below and comprise the fuel costs for hauling in the corn feedstock from farms and agricultural storage sites and for hauling out the ethanol to gasoline blenders. These are accomplished using a combination of trucks, rail cars, and barges.

The corn feedstock is typically planted in the spring and harvested in the fall. After harvest, a number of field operations consisting of tilling the soil and applying fertilizer must be performed before the next season of seed corn can be planted. For the inputs to the system, the amount of fossil fuel which is required is a summation of all of these field operations. Additionally, the fertilizer which is applied or the seed which is planted have embodied energies which are added. For corn production, the major fertilizer requirement is nitrogen; however, potassium, and phosphate are also needed. Moreover, depending on the acidity of the soil, a lime conditioner may be applied to raise the pH. Various herbicides and insecticides are necessary in certain locations and years to prevent pests from damaging the crop. Finally, in drier climates, water must be added to the fields in the form of irrigation.

5.3 Energy Balance Calculation with Uncertainty

This section serves two primary purposes. First, it provides a step by step procedure for defining the probability distributions for the critical parameters. However, the details of the definition step are framed as a comparison to the inputs for the Pimentel (2005) and USDA (Shapouri, 2004) reports, as they are at either extreme in Figure 5.1. Therefore, the initial focus is on the parameters which display the most discrepancy between these two reports and how they compare to the MIT result (this thesis).

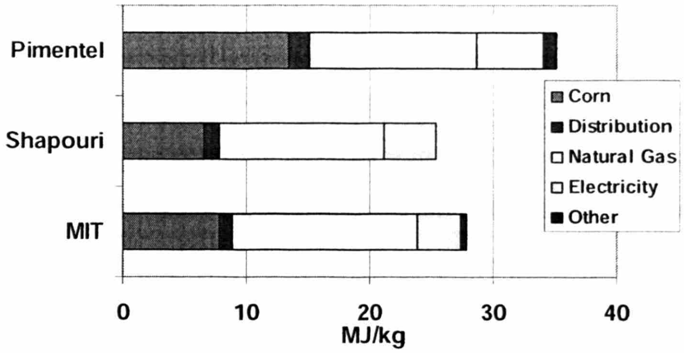

Figure 5.4 Life cycle energy required for ethanol production

The charts in Figure 5.4 and Figure 5.5 show the cumulative energy required from each subsystem for the three reports. Figure 5.4 shows energy required for ethanol production, whereas Figure 5.5 breaks down the component flows for the production of corn which is converted to ethanol. For this initial assessment, the uncertainty ranges have been stripped out of the results for this work with only the expected value being shown. Additionally, this is solely energy input, without coproduct consideration. As can be seen, the values from this assessment are somewhere between the Pimentel and Shapouri numbers, but are closer to the latter.

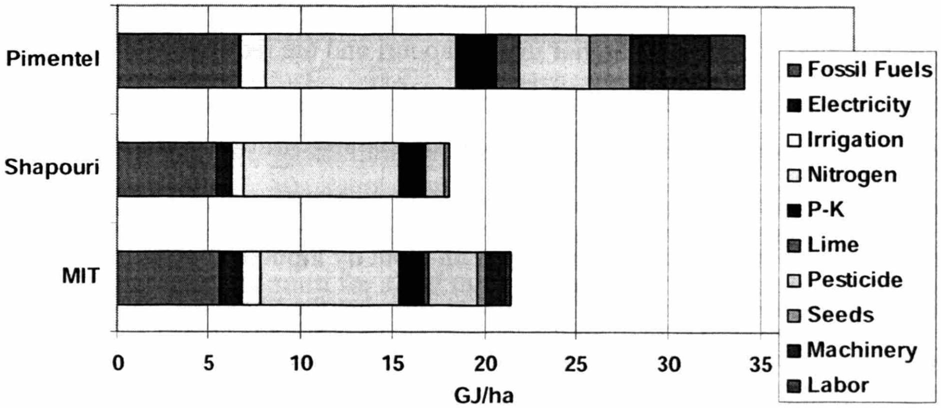

Figure 5.5 Life cycle energy required for corn production

Figure 5.4 shows the cumulative energy required to produce 1 kg of ethanol. Note that the lower heating value of ethanol is 26.7 MJ/kg. The first thing to note from the graph is that the difference in energy values between the Pimentel and Shapouri studies does not seem as great as is shown in Figure 5.1. This variance is created by differences in treating the co-product animal feed which is produced during the ethanol manufacture process. As in any LCA with multi-product processes, how the environmental impacts are allocated to the different products can be a contentious issue. In this initial comparison, the entire energy requirement is allocated to the ethanol. The variance in these results due to different allocation comparisons will be discussed later.

Further investigation into these top level results shows that while natural gas utilization in the ethanol process is the most significant contributor to the overall energy requirements, the primary contributor to the variance between the three studies is actually in the corn production. Additionally, there are slight differences in the other inputs – electricity, natural gas, and distribution. However, nearly 2/3 of the disparity comes from the agricultural process. Therefore, to understand the differences between the two studies the corn production process needs to be studied in greater detail; however, an improvement assessment with a goal of determining the best way to lower the overall energy input into the system would focus more on the ethanol production facility and the steam that is required to separate the ethanol from water in distillation or the natural gas which is used to dry the DDGS.

Variations in corn production are highlighted in Figure 5.5. As can be seen, the estimate by Pimentel is over 80% higher than Shapouri and the requirements from his study are consistently higher for most of the inputs into corn production. Because these estimates contribute most to the differences in the overall energy requirements for ethanol production, the sources of the estimates for fertilizers, pesticides, machinery, and seeds will be explored for both studies. Following is an input by input look at the energy requirements for the various upstream systems, comparing the Shapouri and Pimentel values to the prior distributions which are developed in this work. The methodology for the formation of the nitrogen production and application probability distributions will be given in the next section; however, the details of the other inputs can be found in the Appendix.

5.3.1 Inputs for Corn Production

The US Department of Agriculture has several databases with information for the fertilizer, chemicals, seeds, and fuel inputs required for corn production. How this data is integrated into the probabilistic corn production model for this thesis, the following demonstrates how the fertilizer and chemical inputs, specifically nitrogen, are developed for the model, as these combined categories contribute the greatest amount towards the overall energy requirement in corn production. The inputs can be broken down further into subcomponents – nitrogen, potassium, phosphorous, lime, herbicide, and insecticide. Table 5.1 presents all of these inputs for the Pimentel and Shapouri studies with the relevant parameters for determining overall energy input: 1) application rate and 2) embodied energy. The cells which are highlighted represent the values with a significant discrepancy between the two studies and will be the focus of the investigation in this section.

	Pimentel			Shapouri			Difference
	Rate	Energy	Total Energy	Rate	Energy	Total Energy	Total Energy
	kg/ha	MJ/kg	GJ/ha	kg/ha	MJ/kg	GJ/ha	GJ/ha
Nitrogen	153.0	**67.2**	10.3	149.9	**56.7**	8.5	**1.8**
Phosphorous	65.0	17.4	1.1	63.8	9.3	0.6	0.5
Potassium	77.0	13.7	1.1	99.0	6.9	0.7	0.4
Lime	**1120.0**	1.2	1.3	**18.0**	1.3	0.02	**1.3**
Herbicide	**6.2**	420.0	2.6	**2.4**	356.7	0.9	**1.8**
Insecticide	**2.8**	420.0	1.2	**0.6**	356.7	0.2	**1.0**
P-K-Ca-Pest			7.3			2.4	4.9
Fert/Chem			17.6			10.9	6.7

Table 5.1 Input data for fertilizer and pesticide production

As can be seen, Pimentel estimates both the application rates and the embodied energy to be higher than Shapouri for all of these inputs. The difficulty becomes determining which values are accurate, or at least, which values have the highest probability of being accurate. As will be shown later, the actual values for these variables are not fixed, but follow a distribution because of temporal and spatial differences, not to mention changes in technology development. The advantage of using a probabilistic viewpoint will be demonstrated soon. For now, the goal is to track down the sources of the values and make judgments on their accuracy. For the fertilizers, the application rates are reasonably similar; however, the embodied energies are considerably different. For the lime, the application rate is the disparate number, while for pesticides, both the rate and energy are in disagreement. The embodied energy of nitrogen leads to the most drastic difference between the studies. Therefore, the next level of decomposition in the comparison will investigate the energy utilized for nitrogen fertilizer production. (Nitrogen application rates will also be included to demonstrate the probability definition step using available USDA data)

5.3.1.1 Nitrogen fertilizer production

Nitrogen is the most significant fertilizer used in corn production. Without an adequate supply of the nutrient, the corn will exhibit a poor yield with a low protein content. In most soils, the nitrogen has been depleted with year after year production and an exogenous source is required. Nitrogen can be applied to a field in a number of forms, such as ammonium nitrate, ammonium sulfate, urea, and anhydrous ammonia. For each of these fertilizers, the nitrogen is originally converted into ammonia which can be upgraded downstream to the other forms. The worldwide ammonia industry is a large energy consumer, with an estimated annual production of 100 Mtonnes N and an estimated consumption of 1-2% of the world's energy (Worrell, 2000). Ammonia is produced by the reaction of nitrogen and hydrogen in the Haber-Bosch process. The production process is energy intensive because the primary feedstock for the hydrogen is natural gas. The nitrogen is reacted with hydrogen from natural gas reforming to produce the ammonia.

Because the industry is so large, there is quite a variation between different nitrogen producers. These variations are due primarily to the different products and to the ages of the production facilities. The ammonia industry has seen drastic improvements in efficiency over the past forty years, with the overall energy consumption of modern facilities being 30% less than the older generation. Meanwhile, downstream fertilizer producers can use the ammonia to produce upgraded products such as urea, ammonium nitrate, ammonium sulfate, and combinations of these and other fertilizer sources. These upgraded products can either consume more energy, such as the case for urea production, or produce excess energy such as with the exothermic reaction in ammonium nitrate production. However, much of the nitrogen fertilizer worldwide is still produced in lower efficiency manufacturing processes, and this fact must be considered when determining the embodied energy in nitrogen. Many of the analyses of nitrogen fertilizer production in the literature do not state assumptions for how they manage the variation in the data. Furthermore, the studies do not clearly state which of the upstream inputs and processes are included. Each of these factors are critical when comparing the overall energy utilization.

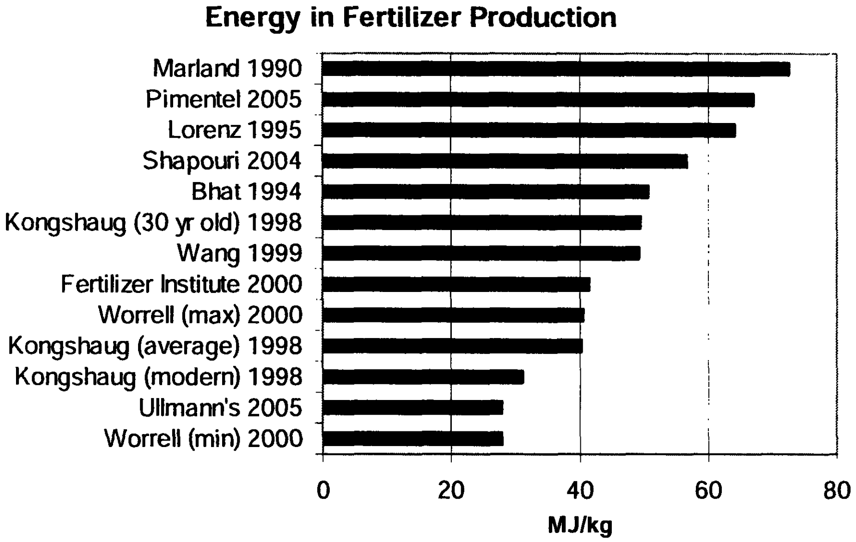

Figure 5.6 Energy required for nitrogen fertilizer production

To comprehensively assess the values for the embodied energy in nitrogen fertilizer production, probability distributions will be determines for the various inputs along with values for the mean, variance, and maximum likelihood. A problem arises in stipulated distributions because the sample size which is used is full of data from different sources using different assumptions. Therefore, these distributions should not be viewed as exact distributions. Instead, they are more representative of prior distributions in the Bayesian sense. These priors represent an estimation of the degree of belief in what is known, but this estimation can be updated with more pertinent data.

Figure 5.6 gives an example of the different recorded values for the energy required for nitrogen production. One important note is that excepting Pimentel, all of the data points greater than 50 MJ/kg are from 1994 or earlier, while the more current reports all indicate lower energy requirements for ammonia production, even for older manufacturing facilities. This is sensible because as modern facilities are built, the older facilities will make incremental improvements by using modified catalysts or heat integration networks. Therefore, the older facilities will still lag behind the modern ammonia production; however, their efficiency will be improved over where it was 30 years ago. In his energy requirement calculation, Pimentel cites a value (Patzek, 2004) which is based on the efficiency of a 45 year old plant which has not been upgraded. Facilities such as this do exist; however, they represent the extreme in fertilizer production, not the standard. Meanwhile, Shapouri has picked a value from a recent, unpublished study by Stokes (2004) which based on the more modern U.S. plants.

Rather than average all of the values in Figure 5.6, the probability distributions are formed by analyzing the process material and energy balances from the most current sources. Data was analyzed and collected from the following sources: the Worrell (2000) and Fertilizer Institute (2000) information were used because of their basis in actual U.S. industry data. Kongshaug (1998) was chosen because the data is representative of an actual fertilizer manufacturing company in Europe, Hydro Agri. Finally, the Ullmann's Encyclopedia of Industrial Chemistry (2005) contains information which represents both the theoretical minimum energy utilization and the best available technology option for modern facilities. It must be noted that fertilizer manufacturing in the developing world rather than in the U.S. or Europe can be much more energy intensive. However, most of the fertilizer used in U.S. agriculture is manufactured domestically and in surrounding countries such that the more efficient processes are representative of the actual fertilizer which is applied for corn production (Graboski, 2002).

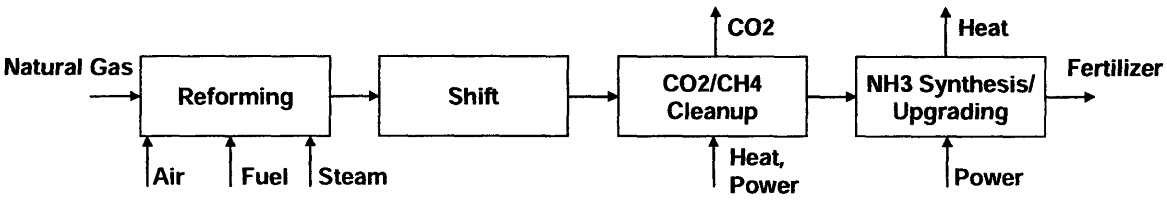

Figure 5.7 Process flow for nitrogen fertilizer production

Nitrogen production is formed from the reaction of hydrogen (typically from natural gas reforming, although coal and coke gasification is becoming more prevalent) and nitrogen in the Haber-Bosch process. Equation 5.2 gives the theoretical conversion of natural gas to ammonia. By looking at a simplified process flow in Figure 5.7, data for the specific inputs – natural gas feed, natural gas fuel, electricity, product upgrading, and packaging, can be identified in the underlying process data. Table 5.2 displays the data ranges chosen for this analysis.

$$0.89CH_4 + 1.27Air + 1.22H_2O \rightarrow 0.89CO_2 + 2NH_3 \qquad (5.2)$$

Input	Distribution	Min	Mode	Min
		MJ/kg N		
Natgas feed	Triangular	24	28	40
Natgas fuel	Triangular	6	12	20
Electricity	Uniform	0.56	0.75	1.50
Upgrading	Triangular	-5	5	5
Packaging	Uniform	1	2	3

Table 5.2 Probability distribution inputs into nitrogen fertilizer production

Using the above inputs in a Monte Carlo simulation of an LCA results in a total energy consumption with a distribution as shown in Figure 5.8. The representative distribution is lognormal with a geometric mean of 51 MJ/kg and a geometric variance of 1.1. Note that this value includes all of the upstream extraction and distribution for the fuel and electricity. Simply using the expected value, both the Shapouri and Pimentel values for embodied energy in fertilizer production are higher. Shapouri's is closer with a value which is within one standard deviation, whereas the Pimentel number is outside the 95th percentile. Comparing the estimates of Shapouri and Pimentel to the approximated probability distribution provides some information on the relative "goodness" of their respective values. Despite a slight overestimation, the Shapouri value appears closer to the real value. However, the actual value will vary depending on where and how the fertilizer is produced.

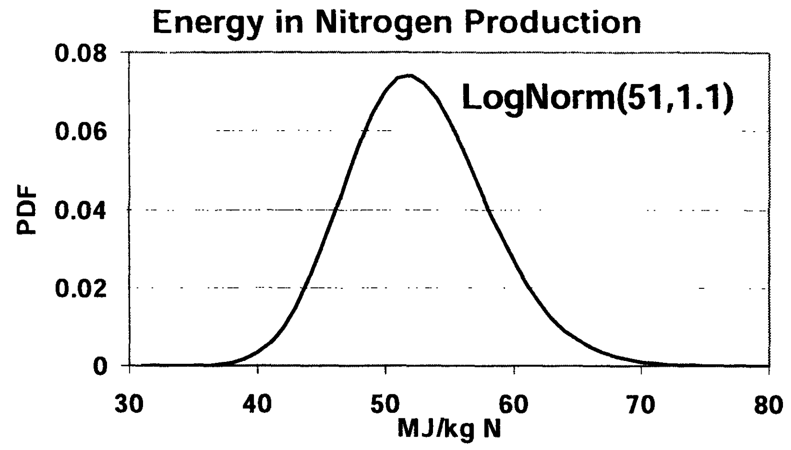

Figure 5.8 Life cycle energy requirements for nitrogen production

This same methodology is used to describe the production steps of the other inputs to corn production, and the details of this can be found in the Appendix.

5.3.1.2 Nitrogen application rates

For the application rates of fertilizers and pesticides, both Shapouri and Pimentel cite USDA data, from the Economic Research Service and the National Agricultural Statistics Service (ERS, 2006; NASS, 2006); however, the numbers chosen are sometimes still significantly different. The differences in how the available statistics are used lead to these discrepancies, and must be understood to avoid this confusion. These and other data from the ERS and the NASS are important as they represent the underlying data which is used for much of the corn production inputs, including fertilizers, chemicals, seeds, and fuels – diesel, gasoline, LPG, natural gas, and electricity. A critical difference between the use of the data for this work versus the other previous studies is that here, the complete data sets are used, rather than simply taking average values from a subset of states for a single year. These data are presented as state and regional statistics for each of these inputs. Using these statistics, prior probability distributions were developed for each of the inputs. The process will be demonstrated using nitrogen fertilizer application as a model.

Statistics for nitrogen application rates in corn production are given by NASS (2006) for each state over the last 30 years. For this analysis, only the last five years were used as the application rate has been trending upwards over time. Using the average for each set {state, year}, an overall mean and variance were calculated using a weighted methodology.

For a given year i, X_{ij} = the application rate in state j. We assume that $X_1, \ldots, X_J$ are normally distributed and mutually independent for each i. Therefore, we define

$$X \equiv w_{11}X_{11} + \cdots + w_{1J}X_{1J} + w_{21}X_{21} + \cdots + w_{2J}X_{2J} + \cdots + w_{IJ}X_{IJ} \tag{5.3}$$

which has mean and variance defined as

$$\mu = \sum_i \sum_j w_{ij} E(X_{ij}) = \sum_i \sum_j w_{ij} \mu_{ij} \tag{5.4}$$

$$\sigma^2 = \sum_i \sum_j w_{ij}^2 Var(X_{ij}) = \sum_i \sum_j w_{ij}^2 \sigma_{ij}^2 \tag{5.5}$$

Where i is the state, region, or county, j is the year or other time period, w_{ij} is the percentage of total corn acres in the region and time period, and μ_{ij} is the average nitrogen application. For the nitrogen application, the result is a normal distribution with $N(149, 30)$ kg/ha.

For many inputs, instead of assuming normal distributions, we assume lognormal distributions to avoid the possibility of sampling inputs in the negative range. With this assumption, the same calculations can be made, with the following modifications, and the same calculation can be performed using $\ln(\mu_{ij})$ instead, to find a lognormal prior distribution with the following parameters.

$$\mu = \sum_i \sum_j w_{ij} e^{\mu_{ij} + \sigma_{ij}^2 / 2} \tag{5.6}$$

$$\sigma^2 = \sum_i \sum_j w_{ij} \mu_{ij}^2 \left(e^{\sigma_{ij}^2} - 1\right) \tag{5.7}$$

For instances where not enough data is available, either uniform or triangular distributions can be defined using the lower and upper bounds of the limited information. Triangular priors are chosen if the limit data seems to be concentrated with a few outliers. The pdfs for these distributions are as follows.

$$f(x) = \frac{1}{b-a} \text{ for a < x < b, 0 otherwise} \tag{5.9}$$

$$f(x) = \begin{cases} \dfrac{2(x-a)}{(b-a)(c-a)} \text{ for } a \le x \le c \\ \dfrac{2(b-x)}{(b-a)(b-c)} \text{ for } c \le x \le b \end{cases} \tag{5.10}$$

Inputs	Units	Distribution	mean/min	stdev/max
Diesel	MJ/acre	lognormal	6.8	0.43
Gasoline	MJ/acre	lognormal	5.7	0.38
LPG	MJ/acre	lognormal	6	0.65
Electricity	MJ/acre	lognormal	4.6	1.16
Natural gas	MJ/acre	lognormal	5.4	1.72
Seeds	kg/acre	uniform	9.3	10
Insecticide	kg/acre	uniform	0.1	0.45
Herbicide	kg/acre	uniform	2.3	3.64
N fertilizer	kg/acre	normal	60.3	12.64
K fertilizer	kg/acre	lognormal	3.3	0.78
P fertilizer	kg/acre	lognormal	3.2	0.32
Lime	kg/acre	uniform	81.8	818.18
Steel	kg/acre	lognormal	1.8	0.5
Outputs				
Corn	kg/acre	normal	3611	537.01

Table 5.3 Corn production input parameters for one acre of land

The application of these techniques for the remaining inputs into corn production are in the Appendix. The resulting parameters for the input distributions are given in Table 5.3. Note that lognormal parameters are the mean and standard deviation of ln(x).

5.3.2 Inputs for Ethanol Production

The conversion of the corn grain into ethanol accounts for nearly 2/3 of the energy requirements in the life cycle of ethanol production. Up until this point, though, the focus has been on the energy in corn production, as the discrepancy in the previous studies has been driven by differences in assumptions on the agricultural inputs to corn farming. While there are slight differences in the material and energy inputs for ethanol manufacture in the former studies, those differences have been less significant. However, the values and probability distributions for these processing inputs need to be analyzed for a complete LCA under uncertainty. Moreover, as the assessment methodology moves to the improvement step, the actual process will be a significant target for energy efficiency gains simply because the magnitude of the energy utilization is highest for the process.

The process for converting corn grain into ethanol is described in more detail in Chapters 2 and 4. This section will simply highlight the overall process inputs. Ethanol conversion uses two primary energy sources: 1) natural gas which is used to generate steam for heat to the facility (although coal or other fuels sources can potentially be used for this process heat), primarily distillation and evaporation, and to fire the dryer for the production of the DDGS, and 2) electricity for the centrifuge, pumps, and other utilities. Other materials and chemicals, such as enzymes, urea, sulfuric acid, cooling water, etc. are put into the process, but they amount to very small contributions to the energy utilization and are not described in more detail here.

The LCA input-output data is drawn from two principal sources. The first is an industrial survey in which individual ethanol production facilities submitted their overall natural gas and electricity usage (Shapouri, 2002). This data includes a significant sample size and is used to generate the probability distributions for the natural gas and electricity inputs based on the above methodology. Table 5.4 lists the distributions for these inputs, along with the other inputs derived from the process model defined below. As before, this input data does not include the upstream energy costs for those carriers. That information is calculated in the overall LCA. The natural gas input into the process amounts to approximately 13.5 MJ/kg ethanol. This one input is half of the energy embodied in the ethanol.

Inputs	Units	Distribution	mean/min	stdev/max	mode	ASPEN
Corn	kg/kg	Triangular	3.2	3.6	3.5	3.15
Electricity	MJ/kg	Lognormal	1.3	1.3		1
Natural Gas	MJ/kg	Lognormal	13.5	1.1		11.8
Cooling water	m3/kg	None				0.134
Lime	kg/kg	None				0.004
Urea/Enzymes	kg/kg	None				0.006

Table 5.4 Ethanol production input parameters for 1 kg of ethanol

The second data source is an ASPEN Plus (Aspen, 2006) process simulation of a dry mill, a modification of a simulation from the USDA (Taylor, 2002). The simulation is a detailed mathematical model of the material and energy flows through the equipment in the actual process. The model relies on thermodynamic properties to describe how the various chemical components interact under the specified processing conditions. The Aspen process model is linked to a spreadsheet which uses the material and energy balance to calculate the economics of the process including capital and operating costs. Details of the process simulation and corresponding economic model can be found in McAloon (2002). A screen capture of the process flowsheet is given in Figure 5.9. A detailed description of the lignocellulosic ethanol process and corresponding Aspen flowsheet is given in the appendix.

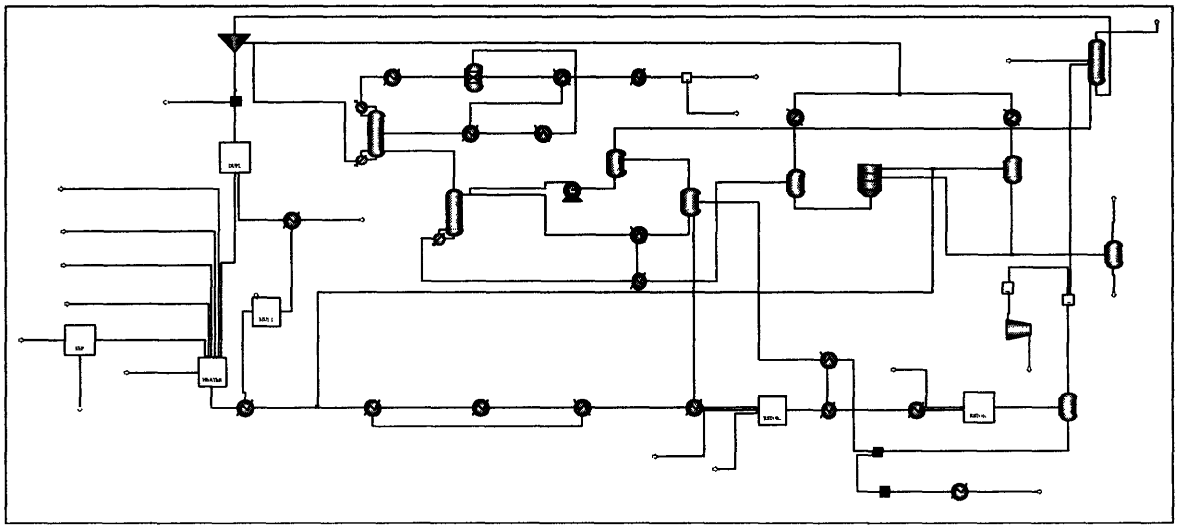

Figure 5.9 Aspen flowsheet of corn grain ethanol process

The process model can be used to calculate the natural gas and electricity requirements for ethanol production independently without relying on survey data. As can be seen in the far right column of Table 5.4, the input estimates from the model are slightly lower than those from the surveys. Because surveys rely on anonymous data, there are no assurances that the info is accurate; however, a likely conclusion is that the actual operation of the dry mills is not as efficient as possible. Once again, this information could be used in the improvement step to find inefficiencies in the process, but for now, the inputs are assumed to be based on the survey rather than the process model.

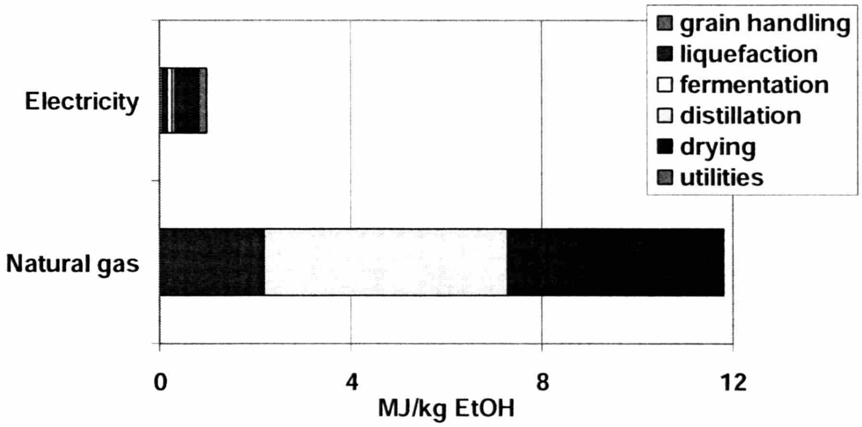

Figure 5.10 Energy usage in ethanol production by subsystem

To investigate with a finer level of detail, the process simulation can be used to determine how the energy is used by different sections within the process. For example, the natural gas usage can be divided between distillation, drying, and all of the other sub-processes. Figure 5.10 breaks down the energy usage by the respective subsection within the ethanol manufacturing process. As can be seen the critical sections are distillation (the separation and purification of the ethanol from water and drying) and the evaporation of the water from the remaining solids for the production of the dried animal feed, with each process accounting for about 1/5 of the life cycle energy utilization in ethanol production.

The data values used by Pimentel and Shapouri for energy inputs into ethanol manufacturing are reasonably close and do not cause much discrepancy between the two reports; however, one significant difference between the two studies is the conversion rate, with Pimentel assuming a yield of 2.5 gallons ethanol per bushel of corn, while Shapouri chooses 2.65 bu/gal. While the Shapouri value is representative of the expected yield, as is modeled with the Aspen simulation, the actual yields reported within the study are slightly lower, being closer to Pimentel's value. This difference actually affects the energy value for corn input as 5% more corn is required when assuming the lower conversion rate.

5.3.3 Conclusions from previous studies

With a detailed analysis of the previous energy balance studies compare to the work here, it is clear that each of the two extreme studies exhibit instances where the data chosen is at the extreme of the feasible data. As a whole it appears that the Pimentel study probably overestimates the required energy while the Shapouri study underestimates. The following section moves from a comparison of previous studies to how the currently described framework can be used to analyze specific systems.

5.4 Application of Sensitivity Analysis and Bayesian Updating

The previous section described the development of the probability distributions for the inputs into the supply chain of the corn grain ethanol system. By comparing individual subsystems to the value from previous studies, the "goodness" of those assessments was addressed. However, as an independent assessment of an energy system the uncertainty analysis is a powerful tool.

A recent report in Science (Farrell, 2006) also addressed the question of the energy balance. Their net energy balance results are labeled in Figure 5.1 as Berkeley A,B. The report clarified many of the misunderstandings and shortcomings in data from previous analyses and added metrics for the quality of the energy used and the greenhouse gas emissions resulting from the life cycle production. However, by focusing on a literature review of the energy balance studies, the recent report still concentrates on a narrow aspect of the biofuels production system. These conclusions overshadow several important characteristics of the system.

The primary themes from this thesis: uncertainty analysis, multi-objective optimization, and assessment of emerging technologies, are important in the development of a biofuels production system and must be integrated into the current net energy debate to achieve a more comprehensive assessment. The rest of the this chapter deals with the impact of uncertainty in the system, while the next two chapters integrate the multi-objective analysis and optimization of the emerging cellulosic ethanol technology.

5.4.1 Uncertainty in the system

Farrell (2006) acknowledges the variability in the underlying data, and alludes to a sensitivity analysis in the supporting material where a histogram of corn yield by county for the state of Iowa is given. However, the estimates used in the report are still point estimates collected from the other reports, and any analysis of the impacts of the uncertainty in this data is missing. This factor is evident in the difference between the Ethanol Today and the CO2 Intensive cases in Farrell (2006), Berkeley A and Berkeley B, respectively, in Figure 5.1. The authors mistakenly suggest the significant decrease in the net energy ratio (from 1.25 to 1.0) is due to using coal rather than natural gas in the ethanol process rather than the more energy intensive agriculture practices in Nebraska as compared to most other states and from the energy required for transporting the corn a further distance.

This is just one example of the importance of the variability in the system. Moving to step 3 in the methodology, the LCA calculation can be performed again while propagating the uncertainty throughout the process. The results are shown in Figure 5.11 for the inputs to ethanol production, while the uncertain inputs to corn production were shown in Chapter 4 in Figure 4.23. These graphs enable a better understanding of which inputs have the greatest variability leading to potential changes in the overall metrics which are used to rate the "goodness" of the process.

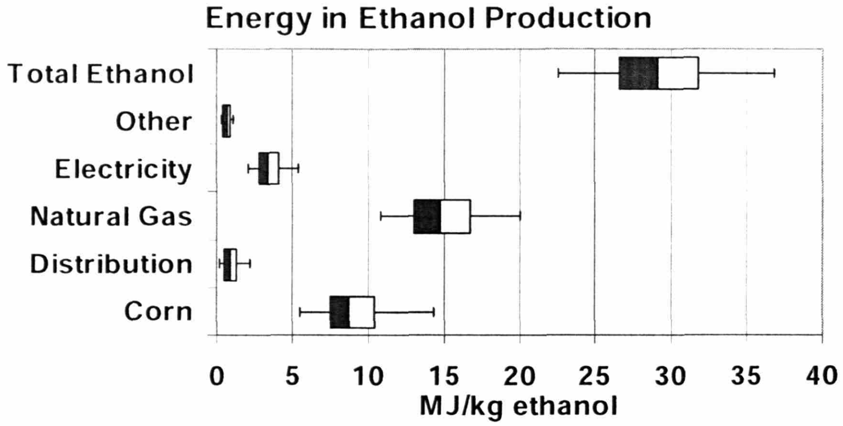

Figure 5.11 Life cycle energy utilization for ethanol production with uncertainty

Figure 5.12 applies these uncertain results to the comparison of the previous energy balance studies.

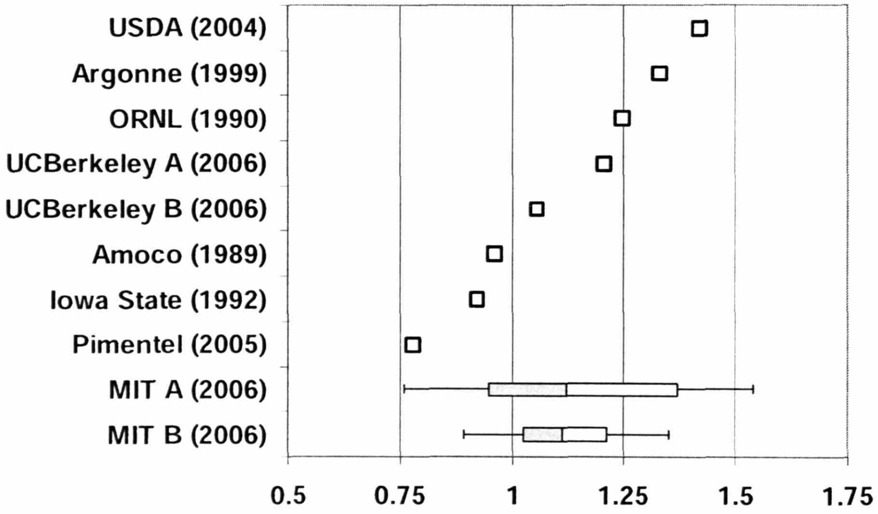

Figure 5.12 Overall energy balance with uncertainty

Note that the difference between MIT A and MIT B is that MIT A defines the allocation procedure as a variable, where the Monte Carlo simulation randomly picks one of three alternatives 1) allocate all of the impacts to ethanol production, 2) allocate the impacts to ethanol and DDGS based on their energy content, and 3) allocate based on system expansion where the DDGS is used as a replacement for soybean meal. MIT B narrows this distribution by using solely the system expansion model. An important conclusion is that this decision process significantly impacts the result.

Starting with MIT A, the study shows the range of net energy values for ethanol production considering the uncertainty in the data as compared to results from the previous studies. It is important to note that the MIT result presented from this work is NOT a collation of the results of the previous studies. Instead, the probability distribution represents the estimated net energy calculated from an LCA calculation with uncertainty using independent data. Note that some of the other studies use subsets of this data. The conclusion from the fact that the independent distribution encompasses all other data points is that the other studies are not necessarily wrong, they have just chosen data at the extremes of some of the input distributions. Additionally, the choices for allocation procedure shift the individual results one way or the other. Step 4, sensitivity analysis, will help associate the critical uncertainties with the end result.

We also look at the impact of equivalent system boundaries and consistent treatment of the coproduct credit but using the data from the previous studies (modifying where needed to incorporate all processes or to change the byproduct credit to system expansion). This analysis is shown in Figure 5.13 and demonstrates the importance of using consistent assumptions when making comparisons between systems.

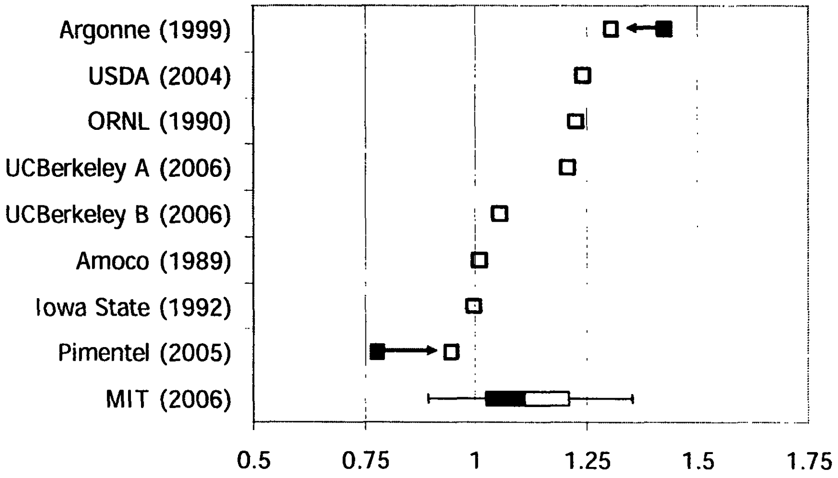

Figure 5.13 Net energy ratio with equivalent boundaries and coproduct credit

5.4.2 Sensitivity analysis

The expected value for the analysis from this work is in between the two cases from the Farrell report. However, it is important to see how the simple variability in the system validates most of the other values as well. Figures 4.23 and 5.11 broke down the overall energy utilization for ethanol production and corn production, respectively; however, a rank correlation sensitivity analysis of the Monte Carlo simulation of the life cycle assessment provides the user a mathematical tool for identifying the uncertain inputs which contribute most to the variance in the final value. The methodology for this is described in Section 4.5.4. For ethanol production, these critical inputs are shown in Table 5.5. These are the parameters whose variance need to be limited to better isolate the variance in the output of the model. Note that the absolute values of the rank correlation do not suggest a specific contribution to variance, they just rank relative influences. The list was truncated at parameters with a rank correlation higher than 0.10.

Critical Parameter	**Rank Correlation**
byproduct allocation choice	0.80
energy for distillation/drying of DDGS	0.69
corn yield	0.33
irrigation in corn production	0.25
electricity in ethanol production	0.23
nitrogen application rate	0.16
diesel usage for corn production	0.14
transportation of corn	0.12

Table 5.5 Parameters contributing most to overall variance

The next step in the methodology for applying uncertainty to LCA as depicted in Figure 4.27 is improving the variance in these uncertain parameters to reduce the variance in the end result. This next section describes how this can be accomplished.

5.4.3 Bayesian updating

One disadvantage of the uncertainty ranges is the appearance of vagueness in the results. While this is a more accurate depiction of the situation, it causes difficulties for decision makers who have to use the information. A Bayesian approach can be used to provide more refined results. Starting with the original data set for corn production from the USDA ERS, the most uncertain parameters can be updated with data for a specific case. The same is true for ethanol production inputs. The prior probability distributions which comprise the whole industry, can be update for specific cases. Analyzing the uncertain parameters, it is clear that the significant variability results from two primary themes – 1) efficiency of the ethanol production process and 2) the farming location. The allocation procedure has the biggest contribution, but choosing a single one, system expansion, removes this uncertainty.

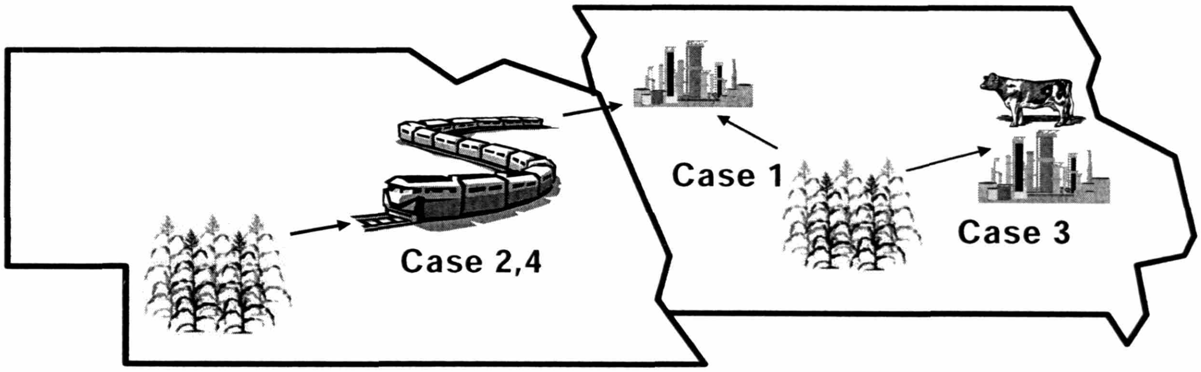

Figure 5.14 Cartoon description of case studies

Four cases studies are provided here with more specific information on location and ethanol processing: 1) High efficiency ethanol production in Iowa using local corn, 2) high efficiency ethanol production in Iowa using local corn co-sited with a cattle feedlot, 3) high efficiency ethanol production in Iowa using corn shipped from Nebraska, and 4) low efficiency ethanol production in Iowa using corn shipped from Nebraska. These four cases will show the effect of the agricultural production inputs between two different states and the difference between high and low efficiency facilities. Additionally, the co-siting of a feedlot means that the byproduct animal feed doesn't have to be dried before shipment, giving an example of the differences in production practices.

For each of these case studies the above critical parameters will be updated with more appropriate data for the specific case. All other uncertain parameters will remain unchanged. The methodology for this Bayesian updating is described in Section 4.5.4. Table 5.6 below gives the likelihood functions which will be applied to the priors resulting in new parameter distributions for these updates. For corn production, input statistics for each state from 2001 where used. For ethanol production, an energy efficiency in the 50-95th percentile was picked for the high efficiency case, while the 5-50th was selected for low efficiency, with a reduction in energy use for DDGS drying for the co-sited facility based on an Aspen simulation of the dry mill process. Because the feedlot is next to the facility, the animal feed can be used immediately rather than being dried for shipment and storage.

Corn Production			Iowa		Nebraska	
Inputs	Units	Distribution	mean/min	stdev/max	mean/min	stdev/max
Diesel	MJ/acre	lognormal	6.4	0.06	7.4	0.19
Gasoline	MJ/acre	lognormal	5.0	0.06	5.5	0.10
LPG	MJ/acre	lognormal	6.6	0.10	6.0	0.32
Electricity	MJ/acre	lognormal	4.1	0.38	6.3	0.25
Natural gas	MJ/acre	lognormal			7.0	0.50
N fertilizer	kg/acre	normal	57.5	2.28	61.4	4.62
Outputs						
Corn	kg/acre	normal	4073	358.54	3611	403.17

Ethanol Production			High Eff		Low Eff		Co-siting	
Inputs	Units	Distribution	min	max	min	max	min	max
Electricity	MJ/kg	Uniform	1.0	1.3	1.3	1.5	1.0	1.3
Natural Gas	MJ/kg	Uniform	12.0	13.5	13.5	13.5	8.0	10.0

Table 5.6 Updated inputs for corn and ethanol production

For each of these inputs, the new distributions are treated as likelihoods. The Bayesian theorem is then used, as in Chapter 4, to combine the prior distributions with the likelihoods to form a posterior distribution. Figure 5.15 gives an example of the posterior distribution calculation for corn yield using the updated data from Iowa.

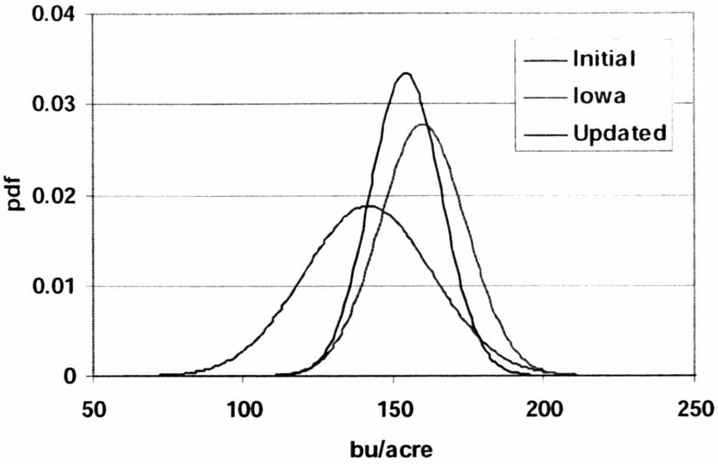

Figure 5.15 Calculation of posterior distribution for corn yield

5.4.4 Results and conclusions of uncertainty analysis

Figure 5.16 displays the comparisons between the studies after the Bayesian updating. As can be seen, the uncertainty is considerably reduced in the overall net energy with a definite differentiation even under uncertainty between the four cases. The difference between cases 1 and 3 shows the heavy influence on the corn production location. While corn production efficiency has significant impacts on overall energy production, case 2 verses 4 proves that the efficiency of the ethanol process is just as critical. While corn production choices affect the net energy, the manufacturing facility still contributes most to overall requirements, providing form the most opportunity for energy reductions from process integrations and new technologies.

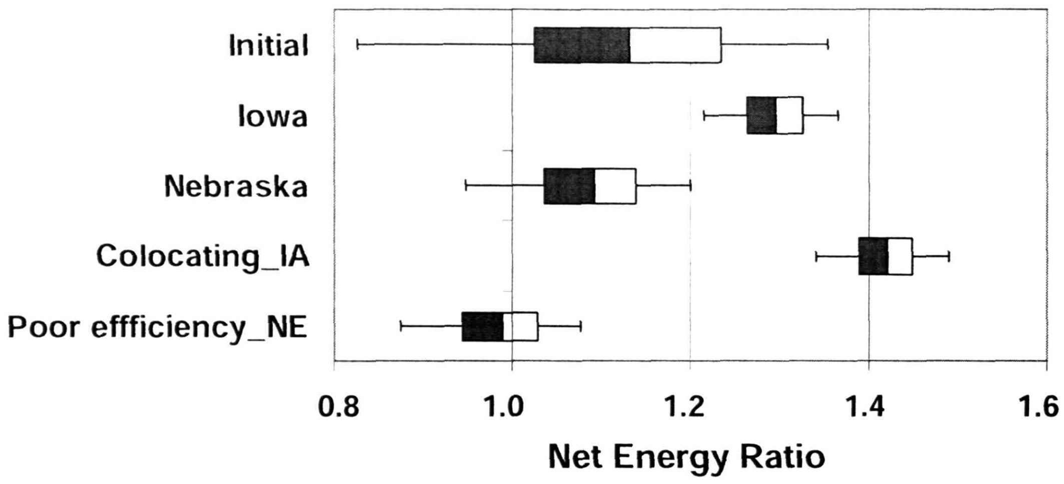

Figure 5.16 Comparison of net energy ratios of case studies

Comparing the net energy values from these four cases allows the variance in the system to be isolated so that the critical parameters impacting the energy balance can be better understood. As has been shown, the initial range with all uncertainty included spans the previous energy balance studies, while the new cases show how the variation can be isolated. For example, cases 1 and 2 in this study are similar to the Ethanol Today and CO2 Intensive cases in Farrell (2006), but the methodology from this study goes a step deeper and shows why those cases are different, namely that different corn production locations along with the additional energy for transporting the corn are the primary differences, not the use of coal as an energy source in ethanol production.

This may become a critical point as corn production expands to meet the growing demand of ethanol production. While the energy efficiency of corn production in optimal locations is high, as corn production moves into less fertile, drier regions, the lower energy efficiency may lead to lower overall energy balances for ethanol production. For example, Figure 5.17 shows the energy intensity of corn production in states which are not in the top 8 corn producers, but are the next highest producing states. As can be seen, the energy efficiency of these states are all higher than the national average, and are much higher in the instances of Kansas and Texas, where ethanol production using these values has a net energy balance moving towards zero. Moreover, the case of Iowa (continuous corn) suggests that production practices moving from a corn-soybean rotation to continuous corn also adversely affects the net energy balance.

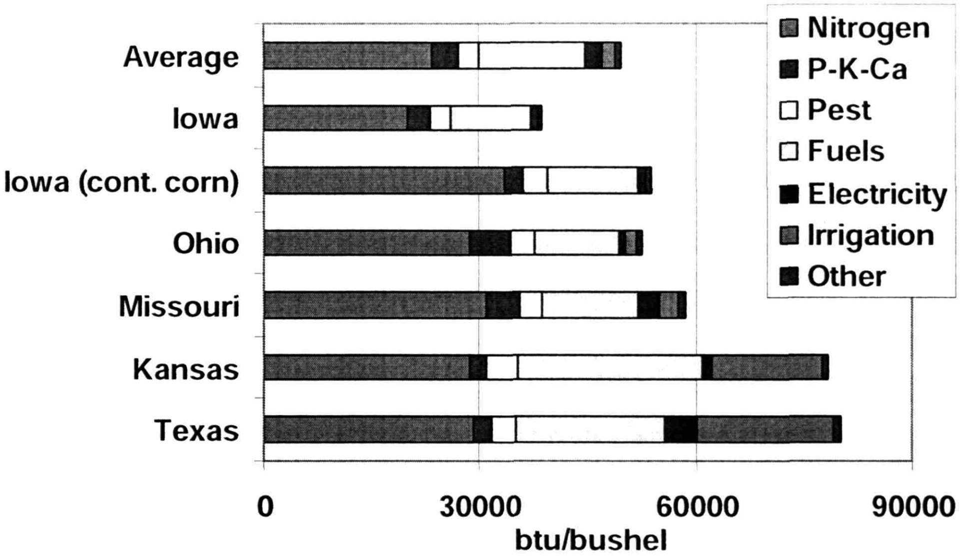

Figure 5.17 Life cycle energy consumption for states with less corn production

The conclusion from this analysis is that the net energy from ethanol production is heavily influenced by parameters such as where the corn is produced, how far it has to be transported, and the efficiency of the ethanol manufacturing facility. This is increasingly important to recognize as ethanol production is expanding and as corn production may expand to meet the increasing demand. Any energy policy focused on ethanol production should take these into consideration when providing incentives to producers. For example, subsidies provided for ethanol could use a tiered system where the energy efficiency of that ethanol production is taken into consideration. Moreover, even this analysis of the uncertainty does not provide a comprehensive view of the corn grain ethanol system. This same methodology can be applied to other metrics in the assessment of ethanol production. The next Chapter extends the analysis from a single metric analysis to one with multiple objectives, including economics and greenhouse gas emissions.

Chapter 6 Multi-objective analysis

This chapter attempts to bridge the energy balance calculations of the previous chapter with other environmental and economic considerations to achieve a more complete analysis of the corn grain ethanol system. Next generation feedstocks, processes, and products will most likely have similarities with this infrastructure and will be addressed starting in the next chapter. To fully understand the economic, environmental, and social implications of corn ethanol, one must investigate these along the entire supply chain, addressing factors such as agricultural practices, food production, distribution infrastructure, competing products, subsidies, etc. Each of these factors are related to multi-objective decisions which need to be made by farmers, processors, and policy makers.

This work focuses on a simplified methodology used to approach the multiple facets of the corn ethanol system, including the energy balance, but also including other environmental and economic objectives. As the energy efficiency debate highlights, one must consider all of the upstream processes as well as the conversion process itself, e.g., distillation, corn production, nitrogen fertilizer production, etc. However, this needs to be expanded to look at the other objectives along the supply chain to have a fuller understanding of the corn ethanol production system and all its impacts. As a demonstration of multiple objective analysis, this thesis chapter combines energy efficiency with greenhouse gas emissions and economics, as those are the critical considerations for new energy projects.

6.1 Economics overview.

Ethanol is a commodity product, and its selling price is dependent on factors such as supply, demand, and policy incentives. This section will briefly describe the details of these external factors; however, because the focus of this thesis is technology assessment instead of economics, the models described here will be based more on simple statistics and engineering economics rather than detailed macroeconomics. Therefore, most of the focus will be on production cost. Within a commodity market, small improvements in these costs can have significant impacts on an industry's profits. The economic considerations of ethanol production are summarized in this section. Later in the chapter, a more detailed analysis will give a baseline for those costs with an explanation of the variance for the most critical cost factors along with suggestions for maximizing efficiency and minimizing the variance will be given.

6.1.1 Demand

Ethanol has been used as a fuel throughout the industrialization of the 20th century. In fact, the fuel envisioned by Henry Ford for utilization in the first automobiles was ethanol. The rise of the petroleum industry quickly led to lower cost gasoline and diesel being the primary fuels used for transportation; however, examples of ethanol use can still be found throughout the last century, specifically at times of petroleum shortages as in World Wars I and II (RFA, 2006). The most recent buildup of ethanol production started during the oil embargoes of the 1970s. Currently, ethanol is primarily used as an additive with a 10% blend in gasoline, with 99% of ethanol in 2002 being of this form (Yacobucci, 2006). In some locations, it is possible to find blends with 85% ethanol. This is most popular in Midwestern states where corn is predominantly grown.

While use as a primary fuel has historically been a source of demand for ethanol, the most significant increase in ethanol demand has come from its use as a fuel additive. Ethanol serves as an oxygenate to prevent air pollution from carbon monoxide and ozone and as an octane booster replacing lead for the prevention of engine knock. The Clean Air Act Amendments of 1990 set a federal mandate for oxygen content in fuels in ozone non-attainment regions (mostly urban areas) (Yacobucci, 2006). Ethanol competes with methyl tert butyl ether (MTBE), which is produced from natural gas and petrochemicals, as an oxygenate. However, MTBE has recently been banned in a number of states due to concerns regarding its contamination of groundwater, and ethanol demand has subsequently risen. More recently, the 2005 U.S. Energy Bill mandates a capacity of 7.5 billion gallons of biomass based ethanol and biodiesel by 2012. Additionally, an amendment to the bill to spare oil companies from MTBE liability was removed, and blenders are moving away from using the additive. (Fialka, 2006) All of these factors have been instrumental in the growth of the ethanol industry from a capacity of 1.5

billion gallons in 2000 to the current situation where the combined installed (4.5B gal) and under construction (1.5B gal) capacity is greater than 6 billion gallons (RFA, 2006).

The price of ethanol has traditionally tracked the price of MTBE at a premium over gasoline because of its use as an additive. In 2005, though, as the prices of gasoline and natural gas were rising due to the increase in the crude oil market, the price of ethanol actually crossed under that of gasoline. Figure 6.1 shows the historical fuel prices. The deviation from the typical price relationship was a sign of two possible characteristics in the ethanol market. First, the capacity of ethanol was larger than what was required to fulfill the oxygenate demand, leading to a potential oversupply. Second, a larger market for using ethanol as a primary fuel competing directly with gasoline had emerged. To compete in this climate, ethanol will have to economically compete with gasoline on a energetic equivalent basis. As gasoline is more energy intensive, the price of ethanol must be lower to compete. The pricing relationship has shifted back as ethanol is now trading again at a higher price than gasoline do to the further phaseout of MTBE, but assuming that ethanol will always float at a premium above gasoline is no longer a valid assumption.

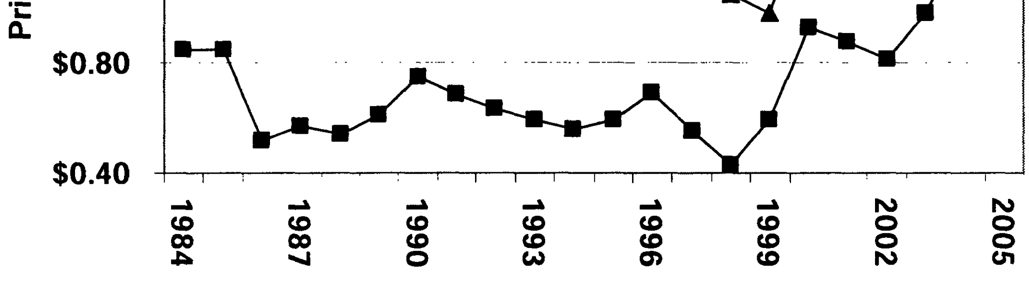

Figure 6.1 Historical ethanol and gasoline spot prices

6.1.1.1 Petroleum economics

Because of the potential phenomenon of ethanol competing directly with current fuels, it is important to have a basic understanding of the economics of gasoline production. Using a simple statistical analysis of recent gas prices, Figure 6.2 shows the cost breakdown of gasoline at the pump by crude price, refining, marketing and distribution, and taxes. The graphs display data selected from the Energy Information Agency website (EIA, 2006). The data is presented in percentiles to see the ranges. Except for crude oil, the ranges of the other components has maintained consistency over the past decade. There are slight increases in refining every once in a while, such as the cost of refining in late 2005 due to the damage and market constraints caused by Hurricane Katrina, but those are exceptions.

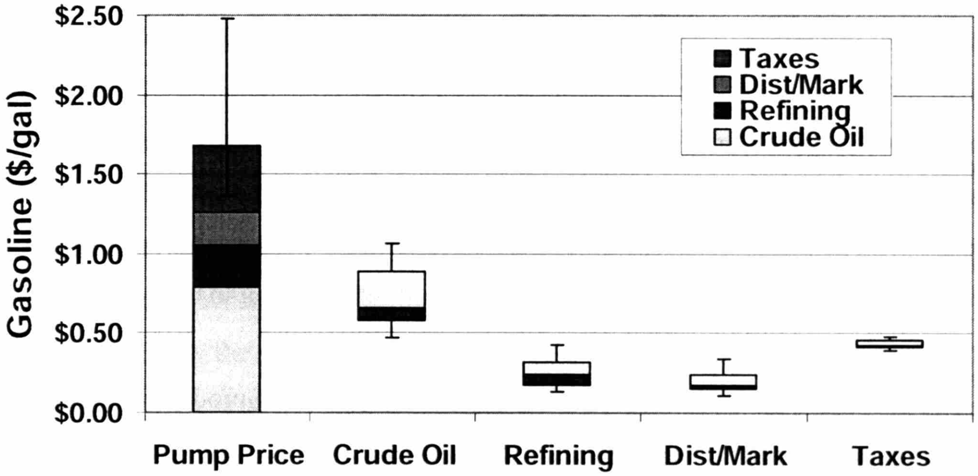

Figure 6.2 Gasoline price breakdown (EIA, 2006)

Unfortunately, the price of crude oil is difficult to predict. High petroleum prices have driven research and development in alternative fuels in the past, but as soon as the oil price returns to lower levels, the other options tend to disappear. However, the dynamics of petroleum prices are currently more driven by worldwide demand than price shocks. While a number of acute fears exist – the Katrina recovery, the Iraq war, the Iran nuclear concern among them, the primary cost driver is continually increasing demand, especially in quickly expanding countries such as China. So for comparisons throughout this chapter, gasoline options will be provided at different crude oil prices.

6.1.2 Supply

The ethanol produced in the U.S. uses corn as its primary feedstock. A number of other grains, including sorghum, barley, and wheat, can also be used, but corn accounts for approximately 95% of the total output (RFA, 2006). The two main processes for ethanol production are wet milling and dry milling. Wet mills are similar to oil refineries in that they have multiple products in addition to ethanol, such as corn gluten, oil, etc. Dry mills also have a co-product in distillers dried grain (DDGS), an animal feed, but that is the only product other than ethanol. Older facilities are chiefly wet mills, but these processes are much more capital intensive. Therefore, most of the recent corn ethanol facilities built have been dry mills. Because of that reason, the production costs for this assessment will use the dry mill technology as the basis. Details of the breakdown of these costs are shown later. For now, note that the primary cost factor for ethanol production is the price of corn, with natural gas, capital costs, and operations and maintenance being the other factors. The production of ethanol is compared to gasoline in some of the following figures. Note that the comparison is based on the rack price of gasoline which only includes the price of crude oil and refining, leaving out the distribution, marketing, and taxes.

Figure 6.3 shows the production cost of gasoline versus the production cost of ethanol at various conditions on a tax and subsidy free basis. Notice that the two axis are on different $/gal scales, with the appropriate ratio so that the production costs are equivalent on a energy basis. This conversion is made simply by keeping the gasoline costs equivalent while multiplying the ethanol costs by 1.5 to make up for the difference in energy content. The gasoline cases are listed by the price of crude oil while the ethanol cases are listed by the price of corn and natural gas. The ethanol case with $2/bushel corn and $8/MMBtu natural gas represents the typical current operation. As can be seen, ethanol production is equivalent to gasoline at about $55/bbl with current conditions. This conclusion by itself is significant in the policy discussion as it suggests that ethanol may be competitive with gasoline as a transportation fuel without subsidies and without mandates for oxygenates or renewable fuels. However, it is critical to look at the variance in these costs, just as the uncertainty in the energy balance calculation was important.

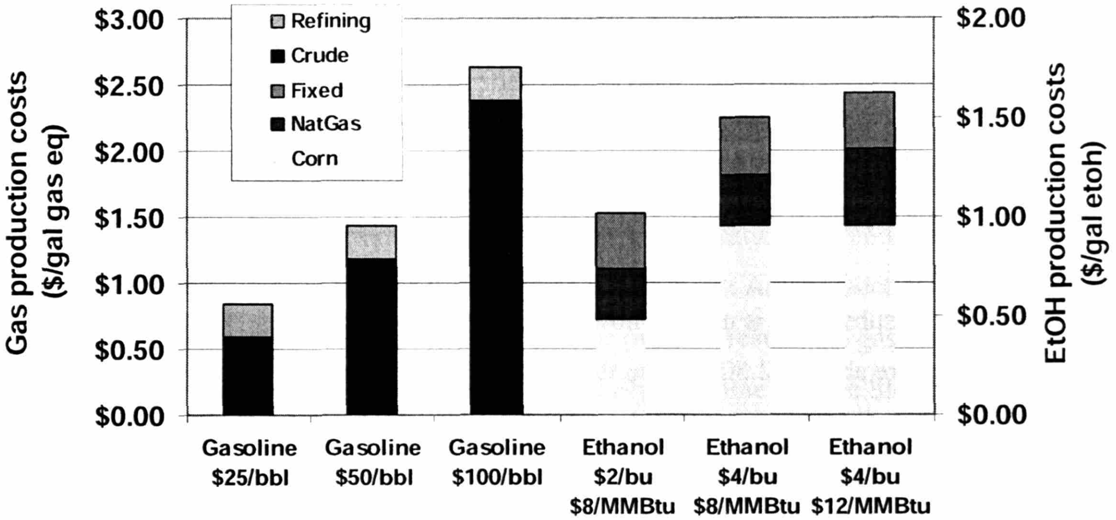

Figure 6.3 Economic breakdown of corn grain ethanol versus gasoline production

Because of the ethanol industry's current dependence on corn, the future price of corn grain is very important, and very uncertain. The price often depends on weather and other factors affecting the growing season. In good years, corn is abundant and the price drops. Years of draught or flooding tend to tighten the market and the price rises. Regardless, the U.S government provides significant subsidies to corn farmers based on production levels. The consequence of this is that farmers react to low prices by producing even more. The subsidies have the effect of keeping the price of corn artificially low. This practice actually helps ethanol producers, but it may change soon as the World Trade Organization has ruled in favor of developing countries against the United States for subsidies it provides to cotton growers (lawsuits against corn and other commodity subsidies are expected to follow). Additionally the U.S and E.U. have begun negotiations to look at their respective subsidy programs as a response. The result is that the future of corn prices is uncertain. It is difficult to predict what will happen if the subsidy programs are modified or even removed. Part of this assessment is investigating the impact in the raw material prices, such as corn, natural gas, and petroleum, and a detailed analysis of these is presented below.

6.1.3 Policy Incentives

A controversial subject regarding ethanol economics are the policy incentives which have been implemented to spur the production of ethanol. A number of states provide extra subsidies for ethanol producers, but the primary federal incentive is a $0.51/gal exemption from the federal excise tax for fuel blenders who mix 10% ethanol into gasoline. This results in an implicit subsidy, driving up the ethanol price by an equivalent amount.

Without the subsidy, it is unclear how the industry would perform. Considering that current prices are above $2.50/gal and that a typical assumption for production costs is about $1.20/gal, it doesn't appear that the subsidy is the sole driver for the industries existence. Still, the policy is criticized as a corporate subsidy by many and it eliminates funding from the Highway Trust Fund (Yacobucci, 2006). Advocates of ethanol suggest the policy is important for the development of a domestic, renewable transportation fuel, and that its primary purpose is to help build infrastructure to a point where the subsidy is no longer needed. The detailed cost analysis below touches more on the subsidy debate.

6.2 Local environmental impacts

The impact of corn grain ethanol production on greenhouse gas emissions is important to understand for policy decisions, and this is described in detail in section 6.4. However, ethanol use in combustion engines also has considerable impacts on local air emissions which is discussed here. Ethanol is used in transportation fuels as an oxygenate, an octane booster, and a fuel itself. As was stated in the demand section, the vast majority of ethanol currently blended into gasoline is to increase its oxygen content to lower emissions of carbon monoxide and ozone precursors as stipulated by the Clean Air Act Amendments of 1990 (Yacobucci, 2006). Ethanol and methyl tert butyl ether (MTBE), the other substantially used oxygenate, have led to considerable improvements in the levels of the above mentioned emissions when blended into gasoline. However, a comprehensive assessment must look at other impacts associated with the use of different transportation fuels. A number of studies have investigated the environmental performance of different gasoline blends, and this section will highlight a handful of the findings from these reports. Following the review are brief results from the life cycle assessment performed in this work. This section is more for informational purposes as the results are not included in the detailed multi-objective analysis.

To fully understand the effects of ethanol versus other transportation fuels, a description of the options will be described briefly here. The first, conventional gasoline assumes the basic refining of petroleum. Reformulated gasoline (RFG) involves another level of processing in the refinery. Most often, the additional processing includes the addition of hydrogen to upgrade the hydrocarbons with unsaturated bonds. RFG doesn't necessarily have oxygen added; however, the Clean Air Act Amendment mandates that certain areas have oxygen added to the RFG. The primary results are gasoline blended with small percentages of ethanol or MTBE. Finally, gasoline may be blended with larger amounts of ethanol, with the mixture being anywhere from almost pure gasoline to almost pure ethanol.

6.2.1 Literature review

The researchers who investigate the environmental impacts of these fuels look at the emissions from the fuel utilization, at the air quality impacts of the emissions, and at the human health impacts of the air quality. Because finding conclusions becomes exceedingly difficult from the beginning to the end of that list, simplified experiments and models are used to extrapolate the results. Often the conclusions are very uncertain and can be inconsistent. General trends and important conclusions will be described below.

Reports show that RFG can actually meet the environmental constraints on CO and VOCs, although the oxygenated fuels tend to perform slightly better. Additionally, the RFG tends to have lower NOx emissions (ozone is an air quality problem formed from VOCs and NOx), but the overall impact on ozone formation tends to be similar for the different fuels. Another area where the oxygenated fuels tend to perform better measurably is in the emission of carcinogenic compounds such as benzene.

When comparing ethanol to MTBE as additives, two primary factors favor MTBE. First, ethanol blended fuels tend to have higher emissions of formaldehyde and acetaldehyde. Second, at low ethanol blends, the vapor pressure of the gasoline tends to be higher so that the evaporative emissions from the filling station are often substantially higher. For the first issue, the catalytic converter on a vehicle could be tuned for the ethanol blended fuel. For the second issue, the vapor pressure problem decreases for higher blends of ethanol so a solution could be to have a higher ethanol percentage.

MTBE has actually been banned in 20 states because it tends to degrade slowly, and leaky gas tanks have allowed the compound to infiltrate groundwater systems throughout the United States. While claims of its carcinogenicity may be exaggerated, MTBE has a very strong odor, and for aesthetic reasons, many public water providers don't want it in their system. Ethanol actually degrades incredibly fast, which has its own problems in that microbes attack it faster within a gasoline spill, rather than focusing on more toxic compounds such as benzene.

The performance of engines using the different fuels is an important factor in not only emission control, but in determining the efficiency, such as mileage, of the different fuels. This also will have a significant impact in the next section on life cycle energy utilization and greenhouse gas emissions. The primary factor in engine performance is the energy content of the fuel. Because a gallon of ethanol has roughly 2/3 the energy as a gallon of gasoline, it will take one and a half times as much ethanol to drive the same distance using gasoline. This assumption is based on using pure fuels. That ratio varies linearly with different levels of ethanol blending. More difficult to predict is how the ethanol blend will affect the actual performance. For example, ethanol is used as an octane booster to limit an engine's tendency to knock, or to prevent early ignition. Additionally, ethanol is a homogenous fuel as opposed to gasoline which is a mixture of many different kinds of hydrocarbons. Therefore, it may be easier to tune an engine specifically for ethanol versus an engine which uses a mixed fuel.

Many of these local pollution issues are not completely well understood. However, the overall conclusions are that reformulated gasoline with or without oxygenates can have high environmental performance in a tuned engine. Some might claim that the oxygenate requirement is unnecessary, but it probably doesn't make the performance worse and in many cases actually improves it. Comparing oxygenates solely based on performance would probably slightly favor MTBE over ethanol, but because of its odor and fear of toxicity, and now the removal of liability protection for refiners, MTBE appears to be headed to a complete phaseout. Ethanol may not be as good an oxygenate, but ethanol blends still perform higher than conventional gasoline. Finally, ethanol provides the capability for use at a higher percentage blend, which is thought to lead to further improvement.

6.2.2 LCA of local air pollution

In addition to energy utilization, the environmental life cycle assessment calculation can be used to look at other environmental impacts. As was described in Chapter 4, acidification, ozone depletion, smog, and human toxicity are all impacts which can be assessed. The life cycle assessment with uncertainty performed in Chapter 5 also included the calculation of these other impact categories. Figure 6.4 presented the results of these impacts before any sensitivity analysis or distribution updating is performed.

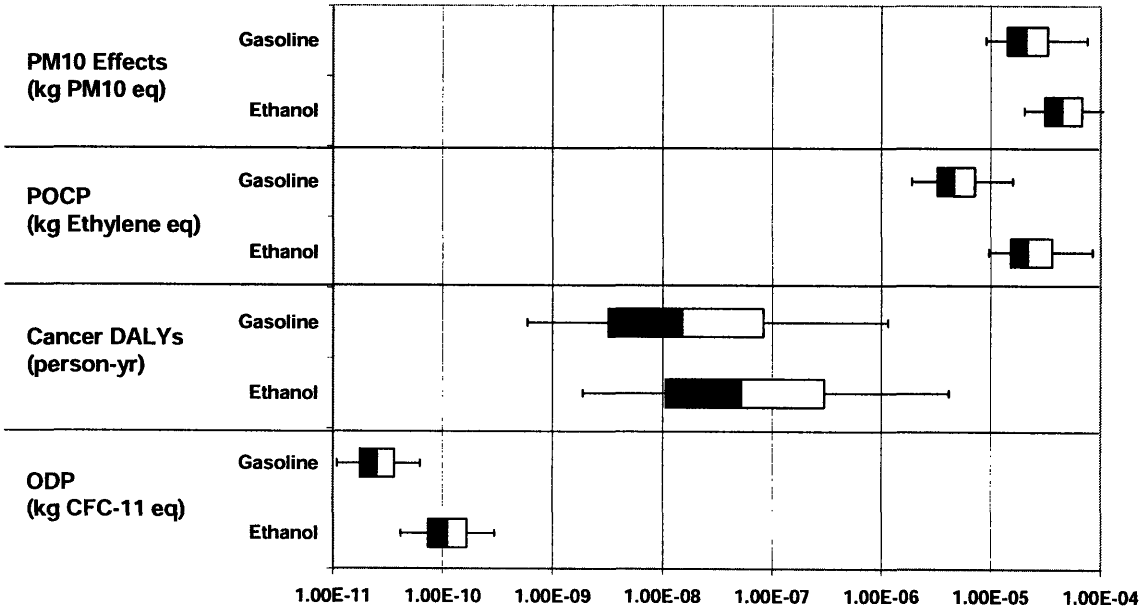

Figure 6.4 Other environmental impacts

As can be seen, most of these other categories favor gasoline production. This is primarily driven by the number of combustion processes required for ethanol production versus gasoline production. Understanding the tradeoff between the improved global warming potential and resource depletion versus the decreased environmental performance in the other impacts still needs to be understood. For now, the assumption is that these local air impacts occur in primarily rural regions with low population density and the relative improvement at the tailpipe justifies these additional pollutants. Because of this assumption, further investigation to lower the output variance is not performed.

6.3 Detailed economic assessment with uncertainty

Figure 6.3 presented a quick overview of the production costs of corn grain ethanol, but this section will probe the question with further detail. The goal is to present an overview of the economics of ethanol production, while also looking at the variability in the costs and the impacts of government incentives. The methodology for the economic assessment will be similar to the energy balance assessment in Chapters 4 and 5. While the production economics of every input in the life cycle will not be addressed, the economic cost of corn production will be analyzed in significant detail.

The primary methodology will be to develop simple economic models for the ethanol production and upstream corn production, and to perform Monte Carlo simulations on those models. For ethanol production, the simplified economic model will be based on a hybridization of the Aspen model describe in Chapter 5 and the input-output model developed for the life cycle assessment. For corn production, the simplified model will be based on a USDA data which describes the production costs for corn farmers. Details follow in the next two sections.

6.3.1 Ethanol production

The economic analysis of corn grain ethanol production will use the total annualized cost approach as defined in Chapter 3. Starting with the detailed Aspen model, the production cost can be calculated with the following equation

$$\begin{aligned} TAC = \sum F_{prod} P_{prod} - \sum F_{raw\,mat} P_{raw\,mat} - \sum F_{util} P_{util} \\ - \sum OC_{fix} - AF \times \sum CC_{equip} \end{aligned} \qquad (6.1)$$

where F_i – flow rates per gallon of ethanol produced, P_i – prices, OC_{fix} – fixed operating costs for labor, maintenance, overhead, taxes, etc. per gallon of ethanol produced, CC_{equip}

– installed capital equipment costs, AF – annualization factor. The annualization factor is further defined as

$$AF = \frac{i(1+i)^N}{(1+i)^N + 1} \times \sum C_{TCI} \tag{6.2}$$

where i – interest rate considering debt/equity ratio, N – lifetime of plant in years, C_{TCI} – total capital cost factors for site, contingency and startup.

The F_i are determined from the material and energy balance calculations in the Aspen simulation, while the CC_{equip} are determined by using the material and energy flows for equipment sizing, followed by the use of equipments costing estimations from textbooks such as Peters (2002) or programs such as Capcost (Turton, 2003). The appendix gives more details on the Aspen simulation and equipment costing. These calculations represent an optimized ethanol production cost, as the efficiency of an actual facility will probably be lower than the simulation version.

Another shortcoming is that they fail to show the uncertainty in the production costs. To rectify this, Monte Carlo simulations can be performed on the Aspen simulation; however, this procedure proves very time intensive as each flowsheet run can take up to a couple of minutes. For this simple analysis, that level of detail is not required, and a simple economic model can be developed using the basic results from the Aspen simulation while varying the critical inputs using the distributions formed in the previous chapter for the input-output analysis.

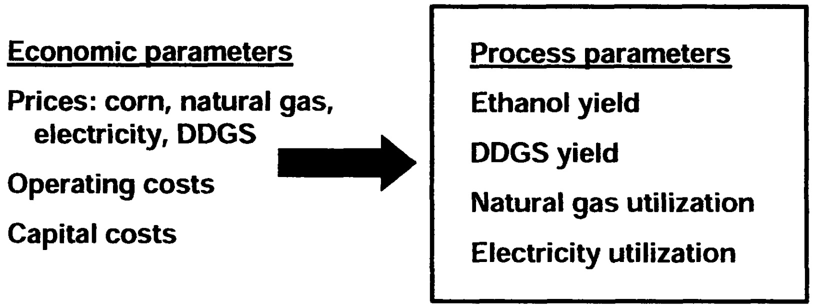

Figure 6.5 Uncertain inputs for simplified economic model of ethanol production

The simplified model is represented in Figure 6.5 where the both the process and economic parameters are represented by random variables. Equation 6.1 is still used for the calculation of total cost of production. The distributions for the prices are taken from analyses of data from USDA and EIA using equations 5.3 – 5.6 to define the standard parameters. The distributions for the other operating and capital costs are taken from sensitivity analyses of the Aspen simulation where the significant inputs are varied and a uniform distribution between the lower and upper constraints are used. Finally, the distributions for the process parameters are the same as was used for the LCA calculation in Chapter 5. Table 6.1 lists the distributions which are used for the Monte Carlo simulation.

Parameters	Units	Distribution	Mean ln(x)	Stdev ln(x)
Yield	kg etoh/kg corn	lognormal	-1.24	0.03
Natural Gas	MJ/kg	lognormal	2.60	0.10
Electricity	MJ/kg	lognormal	0.27	0.19
DDGS	kg ddgs/kg etoh	lognormal	-0.003	0.11
Prices				
Corn	$/kg	lognormal	-2.47	0.15
Natural Gas	$/MJ	lognormal	-5.13	0.23
Electricity	$/MJ	lognormal	-4.34	0.08
DDGS	$/kg	Correlated with corn, $=20+34*P_{corn}+N(0,10)$		
Costs			Min	Max
Other Raw Materials, Utilities	$/gal	uniform	0.10	0.14
Labor, Supplies, Overheads	$/gal	uniform	0.12	0.18
Total Capital Investment	$/gal	uniform	0.125	0.25

Table 6.1 Inputs for simplified model

Performing the Monte Carlo simulation results in an economic cost assessment with the uncertainty of each of the inputs displayed, similar to the energy balance calculations of the previous chapter. The results for the simulation are shown in Figure 6.6. Additionally, the black dots for each input represent the specific costs from the detailed, optimized simulation with a corn cost of $2/bushel and a natural gas cost of $8/MMBtu.

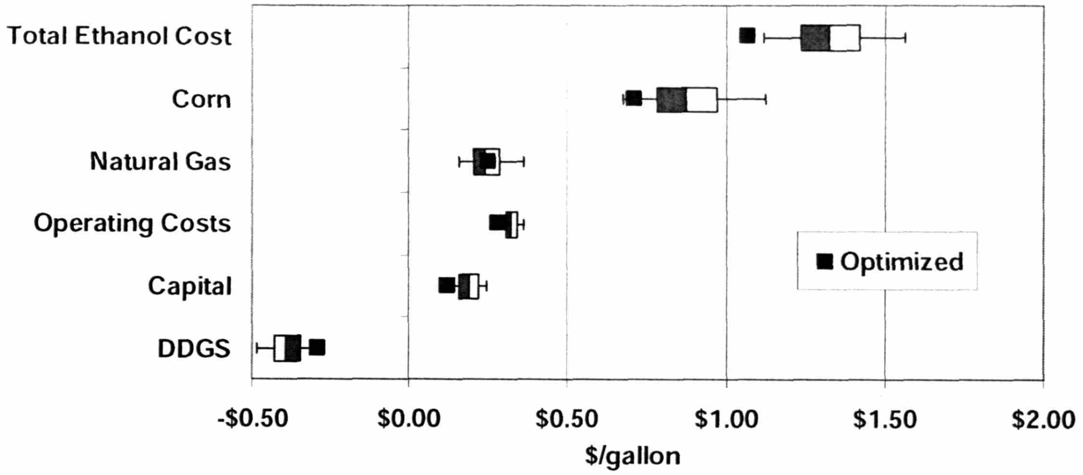

Figure 6.6 Uncertainty in the production cost of ethanol from corn grain

Performing a sensitivity analysis on the input parameters results in rank correlation coefficients with the importance of the uncertainty in the corn and natural gas prices and total capital investment greater than the process yields as is shown in Table 6.2. This highlights the importance of the commodity costs, especially corn for ethanol production. Additionally, the significance of the DDGS price suggests that producers should be concerned about the potential for a saturation of the market as the ethanol industry continues to expand.

Critical Parameter	**Rank Correlation**
Corn price	0.70
Natural gas price	0.38
Total Capital Investment	0.27
DDGS yield	0.24
Ethanol yield	0.22
Natural gas usage	0.17

Table 6.2 Sensitivity analysis of Monte Carlo simulation of simplified model

6.3.2 Corn production

The sensitivity analysis above shows the critical influence of corn grain on ethanol production. Therefore, it is also important to analyze the production costs of this feedstock, as its inexpensive cost is critical for the continued growth of the ethanol industry. The methodology used here will be similar to that used for the development of the input-output model for corn production in Chapter 5. Once again, data is available from the USDA. In this case, a survey called the Agricultural Resource Management Survey is performed by the agency for specific crops every year. The survey tallies the costs associated with all of the inputs to corn farming for farmers across the country.

As was the case in the nitrogen application study in Section 5.3.1, the data from multiple locations and years is collected over the last five years using equations 5.3 – 5.6. The results are shown in Figure 6.7. Perhaps, the most interesting aspect of this chart is the comparison between product price and product cost. As the top two entries demonstrate, typical corn production actually costs more than the economic value of selling the corn grain to market, with a high probability. Investigating further, the difference between cost and price ranges from \$0.15 - \$0.75 per bushel of corn, with an average value of \$0.35/bu. This coincides with the average farm subsidy for corn production over the last 10 years. Thus, the \$4 billion in subsidies to farmers is used to make up for the economic loss which corn production entails for all but the biggest and most efficient producers. This subsidy effectively dampens the corn grain price by allowing for producers to sell the grain at that loss. As was shown in the ethanol economics assessment, this lowered corn grain cost, actually helps ethanol producers, but what would happen if the subsidy were to be removed?

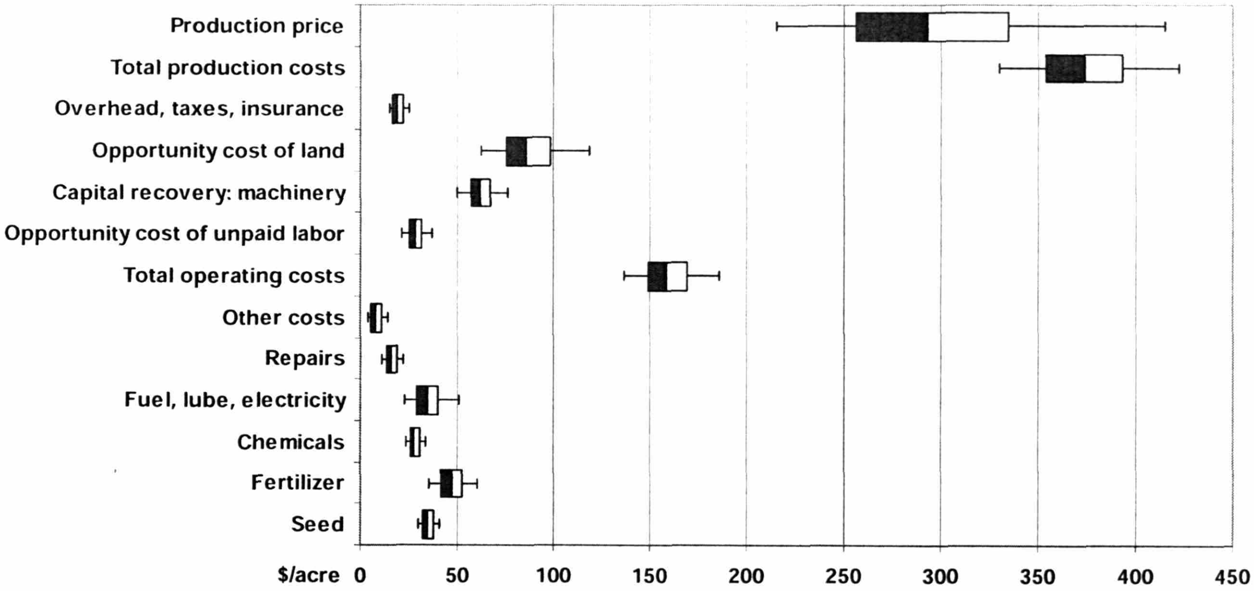

Figure 6.7 Corn production economics

The next step in the analysis is to apply this actual cost of production to the overall ethanol supply chain to determine the ethanol production cost without the corn subsidy. Returning to the simplified model described above, the corn price distribution must be modified to take into consideration the actual cost. This is accomplished by using a distribution derived from the results shown in Figure 6.7 for corn production. Additionally, a transportation input is added to account for the cost of hauling the corn from an intermediated storage sight to the ethanol facility. The parameters for these new inputs into the model are – corn production cost ~LogN(-2.2, 0.14) $/kg and transportation cost ~U(0.05, 0.20) $/kg.

Repeating the Monte Carlo simulation results in Figure 6.8. As can be seen, the adjusted corn cost is shifted by about $0.35, or the effective change from the corn subsidy. The impact on the cost of ethanol production is about $0.25 per gallon. This analysis demonstrates how ethanol production is positively impacted by not only the federal excise tax break, but also by the domestic agricultural subsidies program.

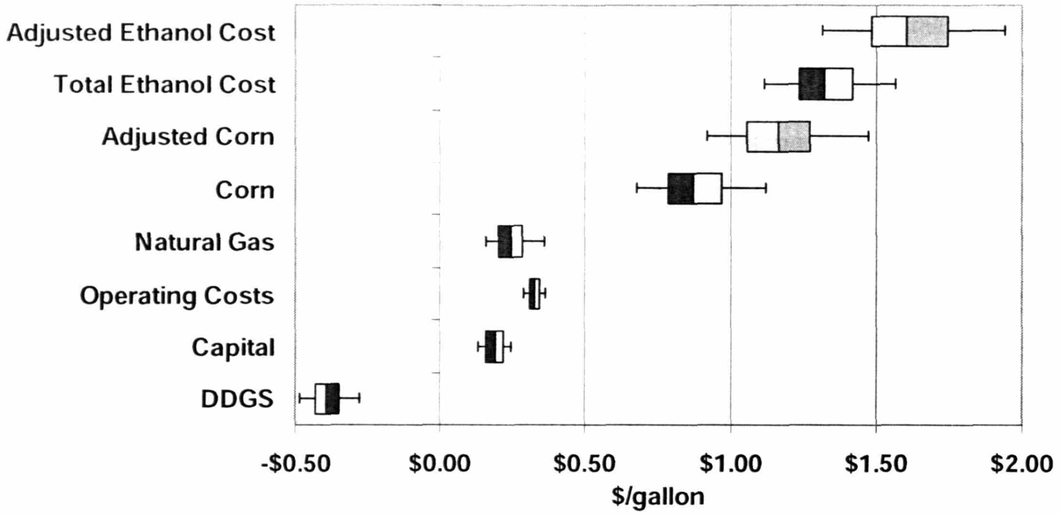

Figure 6.8 Ethanol production costs adjusted for the true cost of corn

6.4 Detailed global warming potential with uncertainty

Along with energy efficiency and the economics of ethanol production, the third primary objective in the multi-objective analysis is the impact of ethanol on global warming. As described in Chapter 2, fuels derived from biomass are considered carbon neutral as the CO_2 which is emitted during their utilization was originally absorbed from the atmosphere during the photosynthetic growth stage of the plant. Thus, ethanol form corn grain is theoretically carbon neutral. However, it is critical to take into consideration the CO_2 which was emitted during other stages of the ethanol supply chain. This section describes the results of the LCA calculation to find the overall abatement of greenhouse gas emissions provided by the replacement of fossil based transportation fuels with ethanol.

The calculation of the global warming potential of the ethanol fuel cycle has already been performed in the life cycle assessment in Chapters 4 and 5. While those chapters focused primarily on the overall energy throughput in the system, extending the calculation with equation 4.9 simply requires several additional sheets in the EnvEvalTool and the inventory emissions data. This data is already in the database for the upstream subsystems and is straightforward for the corn and ethanol production systems as well. The one exception is N2O emissions from the volatilization of ammonia fertilizer. Also note that the CO_2 emissions from the fermentation process and from the combustion of ethanol are not included as they are considered to be negated by the carbon uptake in plant growth. This issue was touched upon in the sensitivity analysis section of Chapter 4.

Once all of the emissions are inventoried, they are summed using equation 6.2.

$$GWP = \sum H_i e_i \qquad (6.2)$$

where e_i is the total emissions for material i and H_i is the relative radiative forcing of material i, with CO_2 as the basis. This calculation is performed for both the ethanol and gasoline supply chains. Additionally, this calculation is performed using a Monte Carlo simulation to integrate uncertainty, and for the four case studies presented at the end of Chapter 5. The results for the deterministic case are given in Figure 4.9. Notice this significant impact of the nitrous oxide emissions.

The results for the integration of uncertainty are given in Figure 4.24. A primary conclusion form this figure is that the reduction in greenhouse gas emissions is relative small, ranging from 0 to 35%. Assuming the expected value of an abatement of 0.1 kg CO2 eq/mile driven, achieving a 1 GtC/y abatement using ethanol would require replacing 30 billion barrels per year of petroleum, approximately the current global consumption.

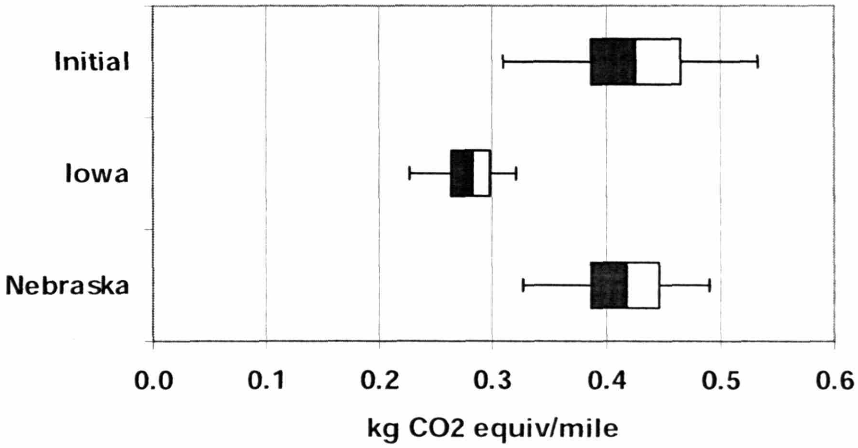

Figure 6.9 Greenhouse gas emissions for ethanol using corn from two different states

The case study differences show that the greenhouse gas emissions similarly dependent on the same factors which impacted the energy balance as can be seen in Figure 6.9.

6.5 Multi-objective analysis

The concept of multiple objective analysis is introduced in Chapter 3. The primary theme is that choosing between alternatives becomes challenging when more than one metric is used to rank the choices. While the option of weighting the multiple objectives to arrive at a single one simplifies the decision process, it eliminates the information provided by the original metrics. The solution used in this thesis is to present all of the objectives at once using a Pareto optimum scheme letting the decision maker choose between the alternatives while fully understanding the potential tradeoffs. Further, as will be shown in Chapter 7, this Pareto framework allows for the searching of the potential technology advancement space for improvements which will benefit all of the multiple objectives.

This section provides an introduction to that by combining the results from the energy balance, economics, and greenhouse gas analyses to show where the required tradeoffs will be. Because it is difficult to visually display more than two dimensions, two graphs will be shown side by side to view the comparisons.

6.5.1 Conclusions of corn grain ethanol assessment

The cases presented in Figure 6.10 comprise two gasoline case with petroleum at $25/bbl and $75/barrel, real cost ethanol which is based on the total life cycle cost not including subsidies as described above, the Iowa case study form above, the optimized case study, and a case with all of the subsidies included. As can be seen from part A of the figure, real cost ethanol is comparable economically at over $80 petroleum, while optimized ethanol is closer to $60/bbl oil, but once again, that is considerably dependent on corn and natural gas prices. Note that the ethanol production cost is shown on a gallon of gasoline equivalent basis, which amounts to 1.5 gallons ethanol.

Displaying the net energy ratios can be somewhat confusing as the numbers mean two different things between gasoline and ethanol. For gasoline, the life cycle efficiency is about 85%, meaning that 15% of the heat value of the fuel is used in the upstream exploration, production, transport, and refining. For ethanol, the 1.5 energy ratio does not mean that ethanol is 150% efficient, it simply means that most of the energy required for conversion is implicitly solar. However, as part B shows, these energy ratios correlate well with the greenhouse gas emissions so they are somewhat useful.

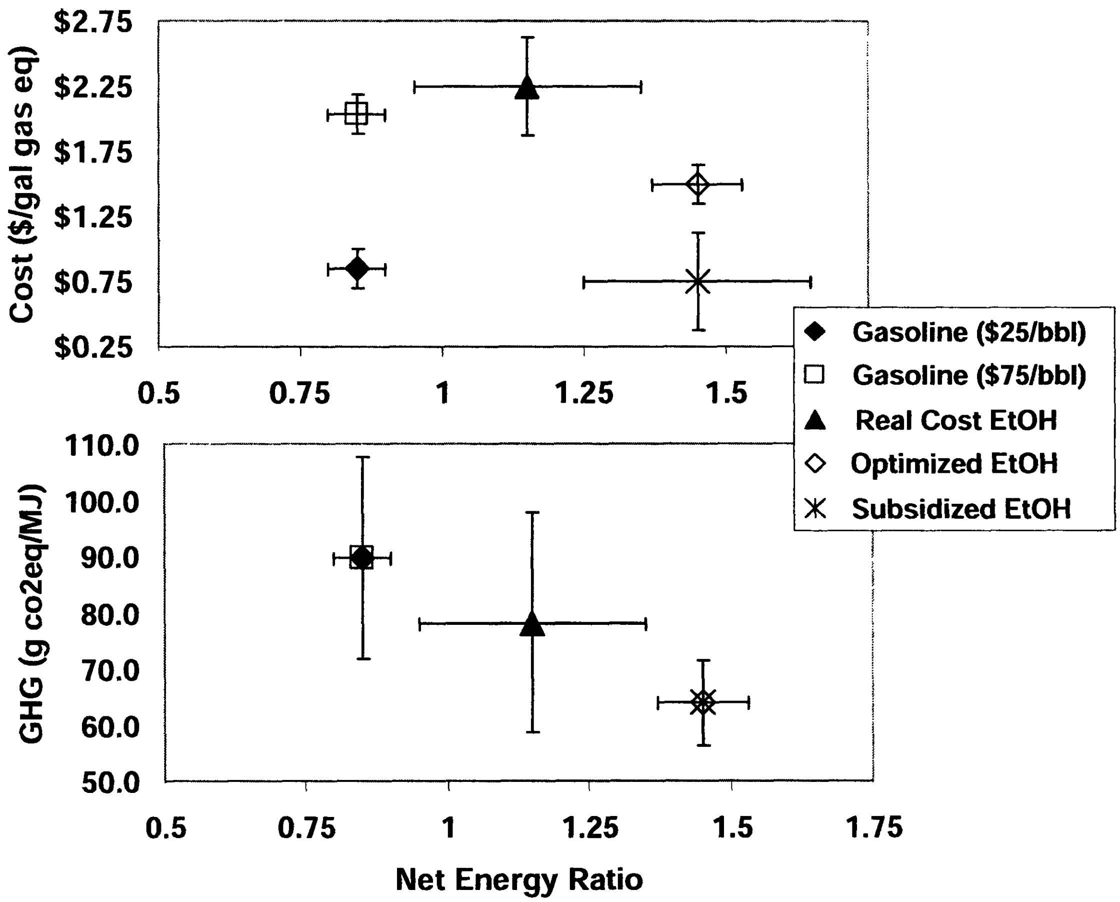

Figure 6.10 Multiple objective analysis of corn grain ethanol versus gasoline

A couple of other conclusions can be taken from this analysis. First, if corn grain ethanol were used to replace 10% of the petroleum consumed in the U.S. (an equivalent amount to 75% of Middle East oil imports), the input requirements based on the life cycle calculation in Chapter 4 would result in an increase in U.S. natural gas consumption of 14%. Moreover, the land requirement would double the current corn acreage in the country. Finally, keeping the current subsidy levels, the combined farm and ethanol subsidies would approach \$35 billion annually. The second point is to look at the greenhouse gas abatement. If the ethanol subsidy is justified as a carbon tax, the equivalent cost of reducing 0.1 kg CO_2 eq/MJ is >\$1000/tonne C, considerably higher than what is expected to be the levels of eventual carbon taxes.

A significant conclusion from the analysis is that the subsidy for ethanol, \$0.51/gallon, probably does not make sense from a greenhouse gas abatement point of view, or from an energy production point of view.

6.6 Initial improvement option – bioethanol

Another conclusion from the above multi-objective analysis is that a feedstock other than corn grain will be required for large scale ethanol production. Cellulosic biomass, which is a more abundant and less energy intense resource, will be the likely choice (Walsh, 2003; Mielenz, 2001; Berndes, 2001; Lynd, 1998; Lynd, 1991). A number of possible lignocellulosic materials are being investigated for feasible ethanol production, with the current focus being primarily on corn stover, the residue of corn grain production, and switchgrass, a perennial grass which grows natively throughout the U.S (Spatari, 2005; Sheehan, 2003). To understand the implications of using a non-corn feedstock, economic and environmental analyses similar to those form the earlier chapters must be performed on the corn stover and switchgrass derived ethanol.

A difficulty associated with performing the economic and life cycle environmental analyses of a cellulosic ethanol production process is that currently no commercialized facilities exist. While the cellulosic material is less expensive and more abundant, the cost associated with converting the biomass into ethanol is expected to be considerably higher than the traditional corn grain ethanol process, and so any transition in the industry is still in the preliminary development stage. A number of pilot plants have been operated and lab studies performed (Schell, 2004; McMillan, 2001.), so estimations of the technical feasibility and process economics are available. However, the significant amounts of operating data which were used in the previous case studies are not available for this process, and the resulting analyses are much more uncertain. Additionally, the expected lignocellulosic feedstocks are not fully integrated into the agricultural infrastructure, so models describing the costs of production and transport are equally uncertain.

The goal of this section is to present a base case for the current status of lignocellulosic ethanol. As will be shown, the current production technology is not quite competitive with corn grain ethanol on an economic basis despite the apparently considerable benefits with net energy production and greenhouse gas emissions. The next chapter will describe the development of a biomass energy model, which is modified from earlier chapters to investigate the economic and environmental performance of using multiple feedstocks for ethanol production. Using a decomposition of the overall network model, more detailed models which describe the specifics of the feedstock production and ethanol conversion processes will be assessed to determine a pathway for enabling the economic feasibility of the process..

6.6.1 System model development

This next case study will investigate the economic and environmental performance of a facility which converts this corn stover into ethanol. A number of researchers have studied aspects of the economic and environmental performance of this system (Spatari, 2005; Sheehan, 2003; English, 2004; Gallagher, 2003; Thorsell, 2004). This work adds to the previous studies by incorporating the concepts from previous chapters: uncertainty and multi-objective analysis. While the analysis maintains a life cycle perspective where the objectives of the entire supply chain are assessed, a key tool in the analysis is the development of a simplified process flowsheet for ethanol conversion. This Aspen Plus flowsheet can be easily modified to handle changes in the technical specifications of the process and links to spreadsheets which calculate the economic performance parameters and the life cycle environmental impacts for the process. The value of the simplified flowsheet is demonstrated in the next chapter as a number of assessments for specific technology advancements within the life cycle of the process are performed. The current analysis provides a base case performance estimate for a facility using current technology if it were built today.

The process flow of the overall system remains unchanged from the original corn grain ethanol analysis with three primary processes: feedstock collection, transport of the feedstock to the conversion facility, and ethanol production. However, the models developed for the corn grain case study are modified significantly for the corn stover production process to account for the differences in corn stover versus corn grain collection along with the processing difference. These model modifications are described in this section with explanations of the tools used for both economic and environmental considerations.

6.6.2 Corn stover collection

While cellulosic ethanol can be produced from any lignocellulosic biomass, corn stover is considered the most likely initial feedstock because of its current availability. American farmers grow 80 million acres of corn every year, harvesting over 10 billion bushels (NASS, 2006). While the corn kernels are harvested, the corn stover, the lignocellulosic material consisting of the stalks, leaves, and cobs, is left on the field. The biomass ratio of corn grain to corn stover is typically 1:1 on a dry basis. Therefore, overall biomass production of amounts to 266 million tons annually.

The stover is not solely a waste material as it has nutrient value and helps control erosion on the corn acreage. Any removal of the material must be constrained by erosion regulations and be followed by replacement of lost nutrients. A stover collection scheme must consider the economic impacts associated with not only the harvest but also the nutrient replacement, and the environmental impacts of the fuel inputs for collection and consequences of the soil carbon balance. With these economic and environmental considerations, the potential cellulosic biomass available from corn stover ranges from estimates of 60-120 million tons annually (ORNL, 2005; Kadam, 2003). Currently, though, corn stover is not harvested on a large scale. The typical practice for corn grain harvest is to chop the stover as the grain is being collected and deposit it back onto the field. This material is then tilled into the soil in preparation for the next season's crop. Using machinery available today, it is possible to envision a corn stover collection infrastructure, but it would not be optimized.

As with other lignocellulosic material, the corn stover comprises primarily cellulose, hemicellulose, and lignin, although a small amount of other components are also found. Table 2.1 gave an average breakdown of the composition. The hexoses and pentoses in the cellulose and hemicellulose polymers, respectively, are the important sugars for fermentation into ethanol. The primary components are tightly interconnected in the plant cell wall, and releasing the sugars involves the initial breaking apart of the cellulose and hemicellulose followed by the hydrolysis of the polymers. This initial degradation can be achieved by any number of pretreatment and hydrolysis processes, and they are considerably more complex than the liquefaction and saccharification in the typical corn grain dry mill ethanol process. By contrast, the fermentation and downstream ethanol purification are basically the same for both processes, except for the treatment of coproducts where the remaining lignin and other solids from the stover are combusted for process heat and power. More details related to the conversion process are given below.

Input-output information for corn stover collection is difficult to find because of the lack of large scale collection projects. Parameters such as fuel and machinery required, or the amount of additional fertilizer required to replace what is removed can be estimated with simple models developed from the various published reports which have predicted inputs and costs and from interviews with individuals who have performed small scale collection studies. These studies are based on varying levels of details, from one which tracks the performance of an actual farmer cooperative which collected corn stover over a couple of years for use as a building material (Glassner, 1999), to another which is solely based on theoretical calculations of the equipment, fuel, and labor necessary for each of the individual field events in the collection process (Sokhansanj, 2002; Perlack, 2003). Other studies investigate the performance of modified machinery for collection of the corn stover in field trials (Shinners, 2003). The combination of these reports leads to the development of a model with varying levels of detail and high uncertainty.

Unfortunately, the environmental exchanges are even more difficult than estimating emission factors as the impacts involve loss of soil due to erosion which affects long term growth or loss of soil organic compound which may have a significant impact on global warming. Other potential impacts resulting from corn stover removal are changes in pests and pesticide requirement. A number of studies have been performed and several other authors attempt to access the quality and quantity of the impacts of large scale corn stover removal. This previously reported research is used as the basis for the system representation (Nelson, 2002; Hanegraaf, 1998).

The simplest approach to modeling the collection system is to use a basic input-output model. Similarly to the corn production model, the inputs and outputs will be provided on a per acre basis. The variables for the most simple level of detail are given in the appendices for the analysis in chapter 7.. From these inputs, the economic costs and the LCA environmental impacts associated with the removal of stover and replacement of nutrients are estimated. The previous studies tend to underestimate the overall cost (Glass, 2006) so a premium is added. Because the corn grain has been harvested for other purposes, all inputs for the original corn stover production are allocated to the grain, but this modeling decision is assessed in the case studies. The long term impacts on soil carbon levels and future yields are not included in the analysis.

6.6.3 Conversion process

The corn stover is delivered to a processing facility where the material is degraded into sugars and then fermented into ethanol. The lignocellulosic feedstock is initially treated with dilute sulfuric acid and high temperature steam in the pretreatment and hydrolysis stage (Wyman, 2005) These initial reactions break apart the cellulose-hemicellulose-lignin matrix into a hemicellulose hydrolyzate along with the remaining cellulose and lignin. Because step is performed at extreme conditions, the metallurgical requirements for the reactor led to exorbitant costs (Aden, 2002). The hydrolyzate stream is filtered of the solids and treated in a detoxification step where lime is added to neutralize the remaining acid with gypsum as the waste product. The liquid stream is then recombined with the solids from pretreatment and pumped to the saccharification reactor where enzymes are added. These enzymes hydrolyze the cellulose into its component glucose sugars. The saccharification is performed in cascading tanks and is followed by fermentation tanks, where both the glucose and the pentose sugars from the hemicellulose are converted to ethanol (Aden, 2002). The ethanol is purified using a series of distillation columns to separate out the solids and break the azeotrope in the ethanol/water mixture. The final drying of the ethanol is performed using a molecular sieve. Solids from the initial distillation are separated and dried using a centrifuge and evaporators before being combusted for steam production and power generation for the processing facility. Excess electricity is sold to the grid as a co-product (Aden, 2002).

The conversion process can have several variations. The most typical difference is in the pretreatment and hydrolysis processes (Wyman, 2005). While the base case process here relies on dilute acid pretreatment followed by enzymatic hydrolysis, a number of other technologies are being investigated. Examples of other processes are concentrated acid hydrolysis, hot water pretreatment, and ammonia explosion pretreatment. The process of breaking open the biomass to liberate the sugars is difficult and as will be seen in the economic assessment, the extreme conditions lead to high processing costs, so developing a process which more closely follows the dry mill liquefaction process is important.

6.6.4 Base case results

Figure 6.11 adds the initial case for bioethanol from corn stover to the multi-attribute analysis. As can be seen, the net energy ratio and greenhouse gas abatement is significantly improved over even he optimized ethanol case. However, the initial economic cost assessment shows that to be economically competitive, petroleum would have to be over $120/bbl. While that price may not seem completely unrealistic in these days of high energy prices, for this technology to become commercialized, significant technology advancement must be made.

Chapter 7 moves in the direction to those technology advances by looking at potential alternatives throughout the supply chain and determining which improvements will have the biggest impact for the multiple objectives.

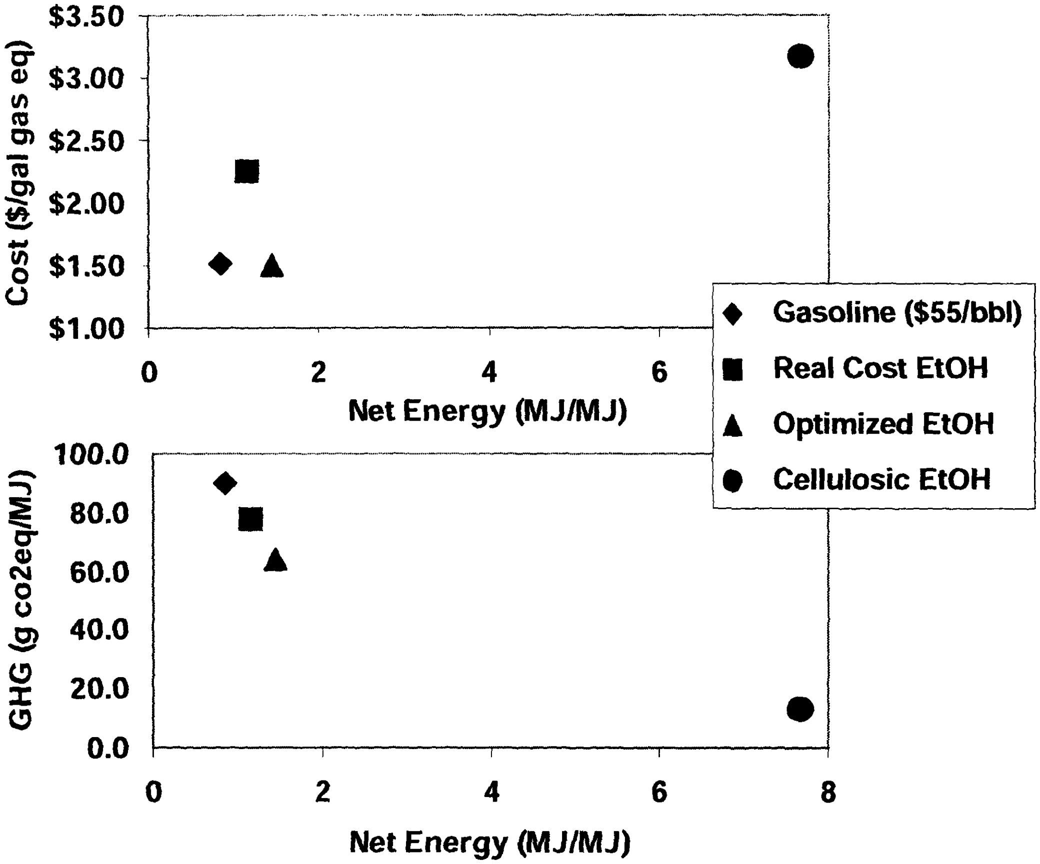

Figure 6.11 Multi-objective assessment of base case corn stover ethanol production

Chapter 7 Hierarchical network optimization for resource allocation

The previous chapter focused on a multi-objective analysis of the corn grain ethanol process. Significant conclusions from the analysis were that the ecological and social performance of the system do not justify the considerable subsidy awarded to buyers of the ethanol and that the pace of expansion in the industry is not feasible because of land, natural gas, and cost constraints. However, the initial assessment of lignocellulosic ethanol suggests that while this biomass is a more plentiful resource with positive impacts on the net energy balance and greenhouse gas abatement, the high economic cost associated with producing the ethanol is prohibitive. Because of these conclusions, the next step in the overall technology assessment methodology is to explore emerging technology options for improving the potential performance of lignocellulosic ethanol production within an agricultural system. This step will be demonstrated in this chapter using a framework of network optimization followed by subsequent hierarchical decompositions to more detailed models. This chapter will start with an overall model describing agricultural production of multiple products and the conversion processes or market options which are available for those crops. The chapter will conclude with a detailed analysis of the process for converting lignocellulosic material to ethanol, with a focus on the parameters in the fermentation step.

The development of the multi-objective network optimization framework has two objectives. The first is to simply model the performance of a hypothetical system where agricultural products are used for both traditional purposes, but also energy production. Understanding the different tradeoffs which lead to using one crop over another or producing an industrial product versus and agricultural one are important from both a business and policy point of view. Second, once the system has been defined, the optimization algorithm can be used as a scoping tool for investigating the impact of various technology advancements. In this sense, the network optimization can be used for resource allocation, comparing alternative technologies to determine which has the greater impact on the economic and environmental performance of the system.

7.1 Development of overall network model for biomass energy

This last step of the technology assessment methodology will be built by integrating two significant tools for evaluation described in Chapters 3 and 4: mathematical programming for optimal design and life cycle assessment for environmental performance analysis. Typically, mathematical programming is used for supply chain or process design optimization using a single economic indicator such as net present value as the objective function, but as described earlier, the LCA addition will integrate a multi-objective component. While LCA does not provide the capability to analyze the economic and environmental tradeoffs between processes and products in the design stage, the network framework, along with decision analysis, can compliment LCA to lessen these disadvantages by allowing its use as a design tool in addition to an environmental assessment. The methodology proposed here uses linear programming and hierarchical decision analysis tools to make use of comparisons where multiple feedstocks, processes, and products are feasible.

Expansion of the system boundaries to a life cycle framework is required to adequately investigate the multi-scale, multidimensional factors involved in assessing biomass energy. A traditional, inside the battery limits approach to process design is not sufficient as it ignores the impacts of the upstream corn production and distribution and downstream product utilization. Additionally, rather than focusing solely on corn ethanol production, an expansion of the possible feedstocks and products is included to determine the best alternative for allocation of available resources.

- Identify economic, environmental, social objectives
- Identify potential feedstocks and products
- Utilize hierarchical decomposition to develop process and life cycle models
- Optimize the system performance
- Identify critical elements of solution using a value of improvement framework
- Successively refine level of detail

The approach taken for managing the large systems in this problem is an iterative, hierarchical multi-objective analysis. A combination of simple models are used to initially represent the system. The parameters and decision variables which are shown to be important in this initial analysis are studied with increased levels of detail. Further decompositions are implemented to achieve appropriate levels of detail. The above bullet points provide an outline for the problem formulation.

7.1.1 Systems boundaries and objectives

As is the prevailing theme in the thesis, rather than limit the design decisions to the biomass conversion facility as in traditional process design, the decision maker should start out by looking at the life cycle of the process, as suggested in Figure 7.1.

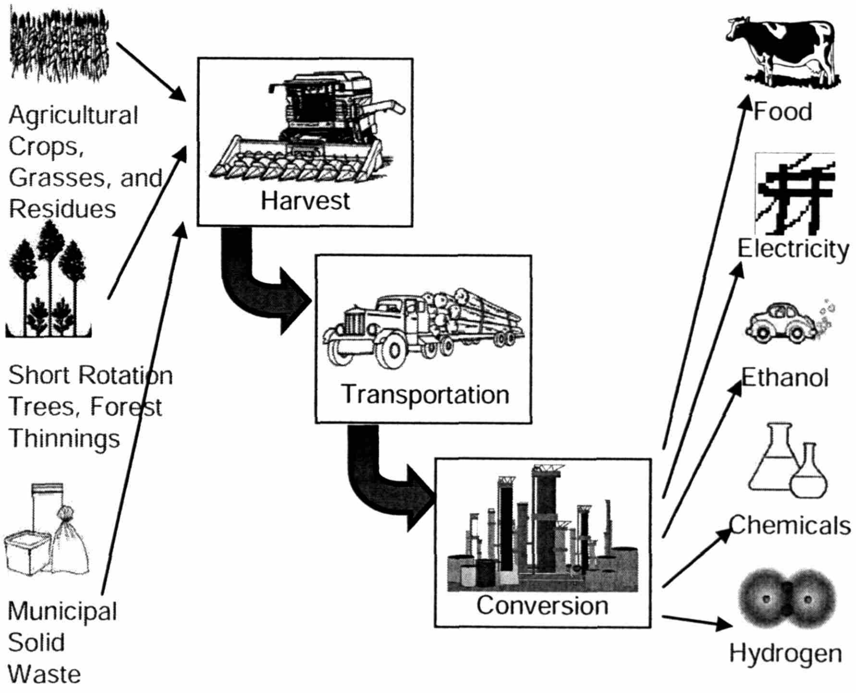

Figure 7.1 Life cycle view of the problem statement

A traditional hierarchical approach can be used to determine initial estimates for material, energy, and economic inputs and outputs for each of the subsystems. With a basic understanding of the subsystems, prior knowledge can be used to develop simple process models for agricultural production and chemical processes. Utilizing these existing models will not give precise values for the economic, material, and energy flows, but using estimations of prior distributions for the possible values will allow a comparison of the relative impacts of each of the subsystems. With knowledge of the relative impacts, the pertinent subsystems can be decomposed to a finer model to determine more accurate values for the key parameters. In the instance of this thesis, the performance of the subsystems is defined using the results from the initial case studies found in Chapters 4-6. Following are quick descriptions of the systems in question. More detailed descriptions and analyses can be found in the previous chapters.

The primary case study for the chapter will be framed from the point of view of a hypothetical farmer's cooperative in Iowa which is involved in agricultural production and is using the crops for downstream processing or commodity sales. Therefore, the first objective is economic profit. However, as agriculture is increasingly becoming looked upon for energy development, the cooperative is also looking at options which maximize greenhouse gas abatement in case future policies are enacted which favor this. Other social and environmental metrics could be applied within the general framework; however, the model development below is limited to the economic and greenhouse gas abatement flows.

7.1.2 Feedstock production

The overall project will consider two crops in rotation – corn and soybeans. Both the crops can be sold to the agricultural commodity market. However, the corn grain can also be utilized as a feedstock for the cooperative's corn grain ethanol facility. In addition to the corn grain, the cooperative has the option of collecting the corn stover for ethanol production in a second ethanol facility, this one for lignocellulosic feedstocks. More details related to the feedstocks for ethanol production can be found in Chapter 2. Finally, while total acreage is fixed, the amount of land used for each crop is variable, and economic or environmental performance may shift the rotation to more of one crop then the other. While many other agricultural crops and ethanol feedstocks can be potentially integrated into the network, just two are selected to keep the framework simple while showing the importance of integrating multiple options. A schematic of the feedstock production is given in Figure 7.2. In the improvement assessment section, the impact of adding an energy crop feedstock, switchgrass, will be investigated.

Detailed models for the economic and environmental performance of corn production and corn stover collection were developed in the previous chapter. The economic and environmental costs for soybean production are from (ERS, 2006). The resulting parameters for cost and energy utilization are used as the inputs into this system and are shown in Table D.1 of the Appendices.

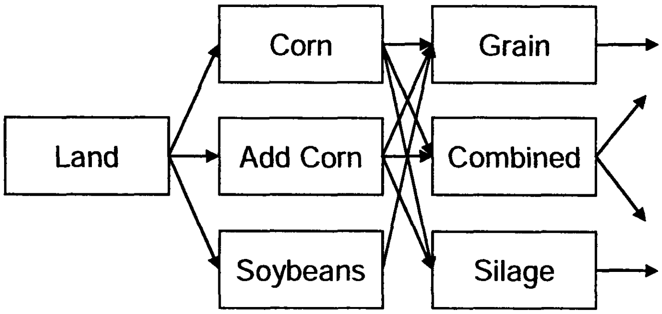

Figure 7.2 Feedstock production decisions

7.1.3 Biomass transportation

The transportation of biomass from the field to the processing facility is a critical step. The cost involves all of the infrastructure for short and long range transportation including truck, rail, and barge. Moreover, because biomass collection is typically performed at certain times of the year, e.g., corn harvest, significant analysis of the required storage facilities needs to be included. Researchers have performed analyses including detailed transshipment programs to demonstrate the complicated nature of this aspect of the process (Graham, 2000; McLaughlin, 2002; Sokhansanj, 2004).

This level of detail is not included in the present analysis, as it represents an hypothetical biomass energy system, not a specific one where this optimization would be critical for economic and environmental performance. Instead, the economic and energy costs of transporting the material over assumed distances using the available transportation modes will be calculated. This information is widely available for the corn grain transportation sector, as the infrastructure for that industry is well developed.

The data is less available for corn stover transportation because of the lack of an industrial use. Unfortunately, the distribution of this material is more problematic as its low density leads to higher shipment costs. For large scale truck hauling, the density of the stover is limited by volume rather than weight. This is even more problematic on rail and barge as these two modes have even higher weight limits, but limited cubic capacity. Because of this transportation problem, analyses of lignocellulosic biomass conversion often include limited feedstock availability. Figure 7.3 shows a simple schematic of the network program for transportation. In the figure, Staging represents the costs associated with storage and loading prior to distribution to the market or the conversion facility. Pre-processing will be discussed in the resource allocation section.

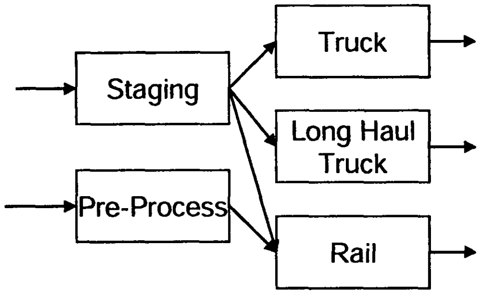

Figure 7.3 Biomass transportation schematic

Table D.1 shows the parameters for the different transportation modes and feedstocks in the appendices. In the improvement section which follows, the impact of increasing the density of the stover, and thus making its transportation cost less, is investigated.

7.1.4 Conversion processes

The potential products are limited as were the feedstocks for simplicity. Two primary processes are investigated: using corn grain for the production of ethanol and DDGS and corn stover for the production of ethanol and power. Additionally, corn grain can be sold at market prices, and the corn stover can be left on the field. It is assumed that the farmer's cooperative owns the processing facilities.

Both conversion processes were introduced in Chapter 2. Details of the corn grain ethanol production, using dry mill technology, is described in more detail in Chapter 4. A brief process description of the corn stover process was given at the end of Chapter 6. A more rigorous explanation of the model development for the material and energy balance, economic costs, and environmental impact calculations is given in the improvement analysis section of this chapter. For the initial network optimization model, simple inputs, outputs, and economic and environmental costs are derived once again from the previous case studies. Figure 7.4 represents the decisions for the production options and Table D.1 gives these conversion process parameters.

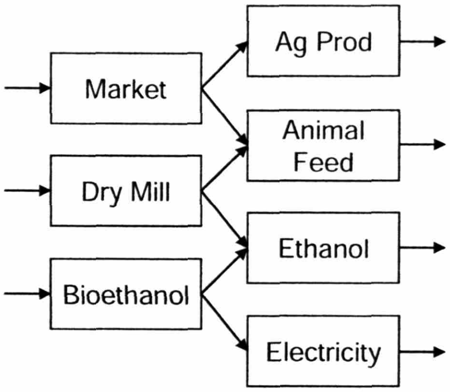

Figure 7.4 Biomass utilization schematic

7.2 Mathematical representation

A network flow is used to describe the overall system as each of the above blocks can be regarded as an input-output model where the arrows represent material fluxes from one box to the next. Associated with each of the material fluxes are flows of money and environmental metrics. The coefficients which determine these parameters such as conversion, cost, energy requirements, etc. are given in the tables above and have been assumed from previous studies, literature, models, etc. This representation is very typical for a network program.

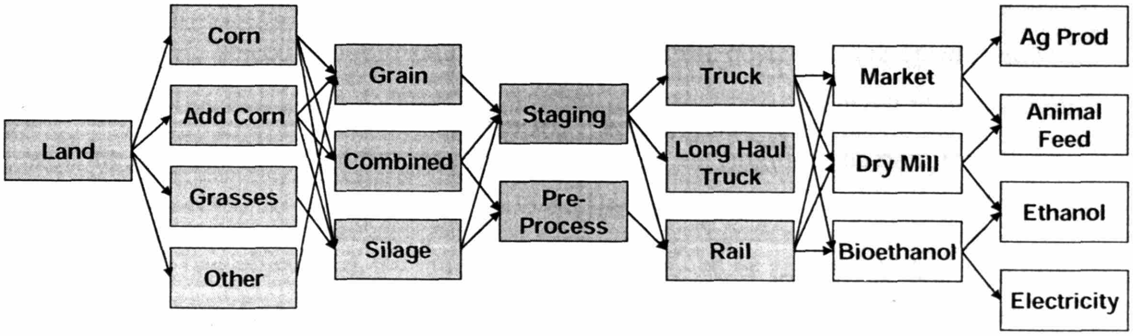

Figure 7.5 Overall system network

This initial hypothetical model is not very detailed, and the results of any specific optimization aren't necessarily applicable to every situation. However, by starting with a low level of detail over the large system, the initial goal is to determine the relative magnitudes of impacts between the different technologies. These relative impacts will be found using an optimization method which will give sensitivity results such as shadow prices and reduced costs, and the input-output models can be decomposed to look at the subsystems in more detail.

For a demonstration of how the model will work, a mathematical derivation has been performed using the above network flow. With corn and corn stover being the available feedstocks, the options how to harvest and in which facility to process the feedstock. Each process has an operating cost, environmental cost, and a revenue from the product. The equations show how the decision problem can be mathematically formulated.

7.2.1 Problem Definition

$$\max Econ = \sum_{l} P_l z_l - \sum_{i}\sum_{k} C_{ik} y_{ik} - \sum_{i}\sum_{j} C_{ij} x_{ij}$$

$$\max Env = \sum_{i}\sum_{j}\sum_{k}\sum_{l} EC_{l,ijk} z_{l,ijk}$$

such that

$$\sum_{k} y_{ik} \le \sum_{j} x_{ij} \quad \text{for all } i$$

$$\frac{x_{ij}}{Y_i} \le AH_{ij} \quad \text{for all } i, j$$

$$\sum_{j} AH_{ij} \le AA_i \quad \text{for all } i$$

$$D_l \le z_l \quad \text{for all } l$$

$$z_l \le \sum_{i}\sum_{k} Y_{ikl} y_{ik} \quad \text{for all } l$$

$$0 \le x_{ij}, y_{ik}, z_l \quad \text{for all } i, j, k, l$$

The indexes, model parameters, and decision variables are defined below.

Variable Sets	Label
Feedstocks – CG (corn grain), CS (corn stover), SW (switchgrass)	i
Removal schemes – GC (grain), BL (bales), CH (combined)	j
Processes – DM (dry mill), BM (biomass mill), MK (market)	k
Products – ET (ethanol), P (power), AF (feed), AG (ag products)	l
Parameters	
Product demand	PD_l
Acres available	AA
Yield or conversion	Y_i
Production cost	$C_{i,k}$
Environmental costs	$EC_{i,k}$
Product price	P_l
Decision variables	
Acres harvested with each scheme	$AH_{i,j}$
Mass of each residue removed using each scheme	$x_{i,j}$
Mass of each feedstock converted through each process	$y_{i,k}$
Production of each product	z_l

Table 7.1 Parameters and variables for network optimization

7.3 Base case analysis

The network optimization is solved within Matlab, with the code given in the Appendices. As described in Chapter 3, the ε-constraint method will be used to solve the optimization. This procedure transforms the original multi-objective optimization into a series of single objective optimizations. First, each of the objectives are optimized with the second objective ignored. Then, each of the objectives are optimized multiple times, with the second objective defined as a constraint of ε, varying from its minimum to its maximum.

With two objectives, the optimization problem can be solved multiple times for each objective to find a dominance frontier which can be plotted as a Pareto optimum curve. Figure 7.6shows such a plot with the associated material fluxes and how their relative magnitude are changed for different optimizations. Note that the parameters in this example are certain, i.e., the prior distributions have not integrated into the calculation.

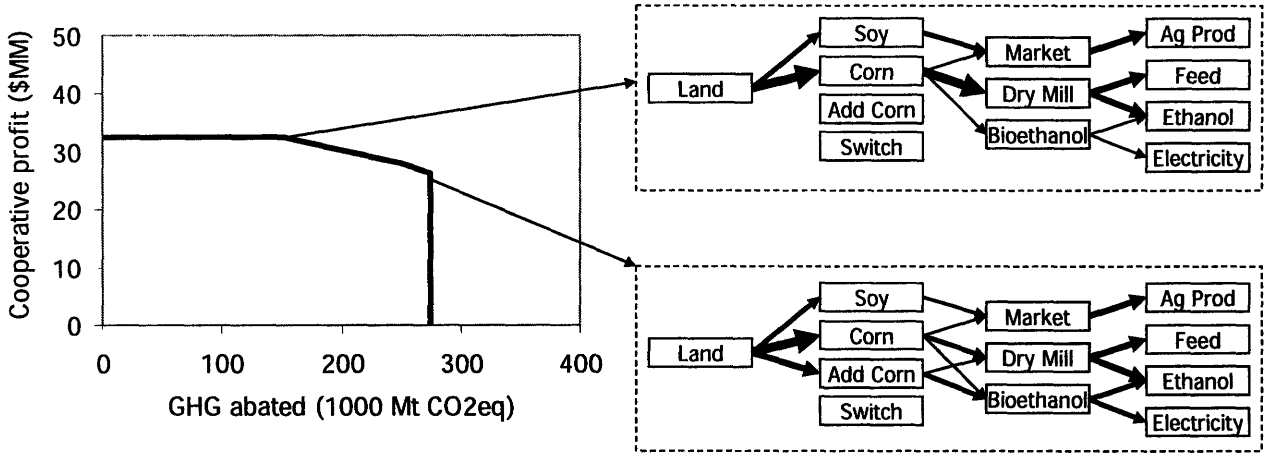

Figure 7.6 Pareto frontier for network optimization with associated material fluxes

7.3.1 Food vs. Fuel

This initial optimization presents a base case optimization for the process, but the results also demonstrate an interesting characteristic of the industry of converting agricultural crops into fuels: the influence of having the food market as a competitor for corn grain. With the current prices and constraints, this hypothetical farm cooperative would be inclined to produce as much ethanol as possible, as the price of ethanol is so high Because this is a simple local optimization, rather than a regional or economy scale equilibrium model, the supply, demand, and prices are constant rather than variables. However, the optimization can be performed multiple times at different price levels to see how the decision variables change. As an example where only the economic objective is optimized, we can see how changes in the crop and ethanol commodity prices effect two decision variables, 1) percentage of land planted to corn and 2) percentage of corn harvested converted into ethanol. The results of these optimizations are shown in Figure 7.7. More general conclusion about the overall cannot be made because of the limited scope of the model, but this can be extended to that scale as described in Chapter 9.

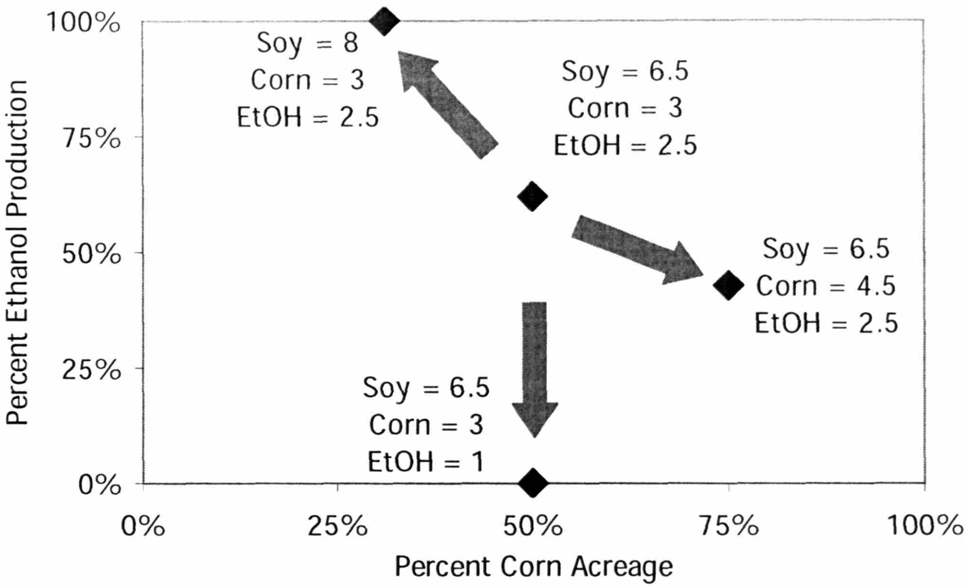

Figure 7.7 Impacts of price changes on the decision variables

7.4 Hierarchical decomposition

The next step is to find the technology advancements which provide the highest probability for improved performance within the system. However, for the process to be meaningful, it must be much more rigorous than simply listing off the options. This section will provide a systematic framework for comparing different technology alternatives with multiple objectives to determine how best to allocate resources for future research and development. A theoretical case study will be used with a large research and development organization investigating a number of promising technologies for a biomass energy system. The case study will be based loosely on the National Bioenergy Center within the U.S. Department of Energy (DOE). The NBC has published a roadmap of the potential technology advancements that should be prioritized over the next ten years along with the budget for those research projects (DOE, 2005). Table 7.2 lists several of these goals which will be the focus of this analysis. Moreover, as a rough metric for research and development priority, the DOE budget broken down by technology focus is given. Using the proposed methodology from this thesis, the technology alternatives from Table 7.2 will be examined to determine which ones provide the potential for the greatest performance increase. This analysis becomes a systematic framework for developing priorities for resource allocation in research and development.

Technology goals – 2010		
Feedstock		
	Crop development	
		Genetic yield/composition improvement
	Logistics	
		Reduce harvest, storage, transport costs
Conversion		
	Pretreatment	
		Lower materials requirements
	Fermentation	
		Increased xylose conversion
		Increased ethanol concentration
		Decreased fermentation time
	Coproducts	
		FT fuels from lignin

Table 7.2 NBC Bioethanol Technology Goals

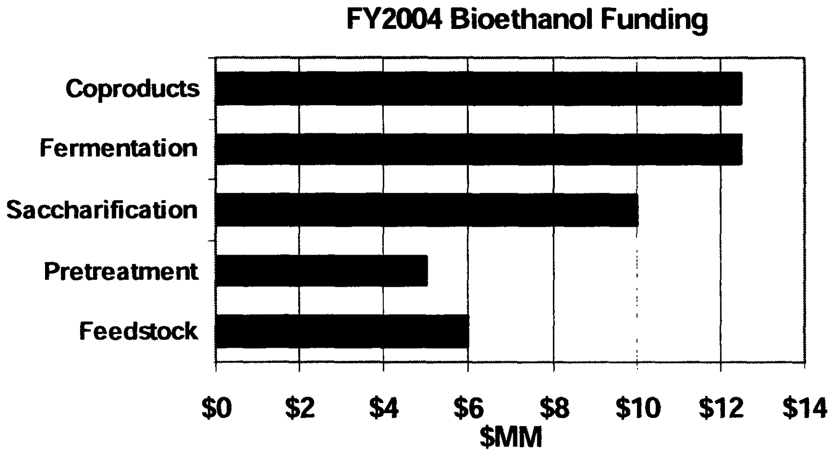

Figure 7.8 FY2004 DOE research and development budget for bioethanol

7.4.1 Resource allocation application for emerging technologies

As stated in the previous chapter, research and development is ongoing in many of the processes considered vital for commercialization of a biomass to energy industry.

Unfortunately, the funds available for this research is limited. Therefore, it is essential to have an understanding of which of the potential improvements in the processes will have the most significant effect on the overall system. This information will give policy and decision makers an idea which areas to allocate the limited funds. For each of the process improvement which are to be compared, estimates are needed for the potential improvement and the cost of the research which is required for the process development. Using this information, the value of the research can be determined by modifying the base case network optimization to include the improvements. A new Pareto surface is formed showing the relative improvement in each of the objectives. The goal is to find the research option with maximizes the differenced in the various objectives from the base case.

This methodology has two significant weaknesses. First, the simple nature of the analysis means that the conclusions are highly dependent on the constraints in the specific hypothetical system. The analysis of an another specific system or the overall economy will potentially lead to different results. However, this is a simple demonstration and the more detailed analysis is left for future work. Second, this analysis focuses on the value of improvement from the development of these R&D projects. They are ranked by the potential outcomes from their realization. Missing from the analysis is the estimations of the costs of these projects. For example, the analysis concludes that advancements in the feedstock collection and distribution step are just as important, if not more so, than improvements in the inhibition of yeasts by fermentation projects. A disadvantage of this conclusion is that the relative costs of the projects are not addressed. It is possible for a technology improvement to be slightly better than a comparable one while, being much more expensive. In this case, a decision maker would have to integrate the multiple objectives of research cost and technology opportunity. This addition of cost of improvement analysis is also left for future work.

7.4.2 Comparisons between different advancements

The initial comparison will show the impacts of technology advancements for various modifications to the feedstock development, collection, and distribution steps, first for corn stover, but then investigating switchgrass, as compared to a 20% decrease in the combined operating and capital costs associated with lignocellulosic ethanol production. A description of how that initial decrease could be achieved follows in the next section on conversion process improvements. The impact of the conversion cost improvement is given in Figure 7.9.

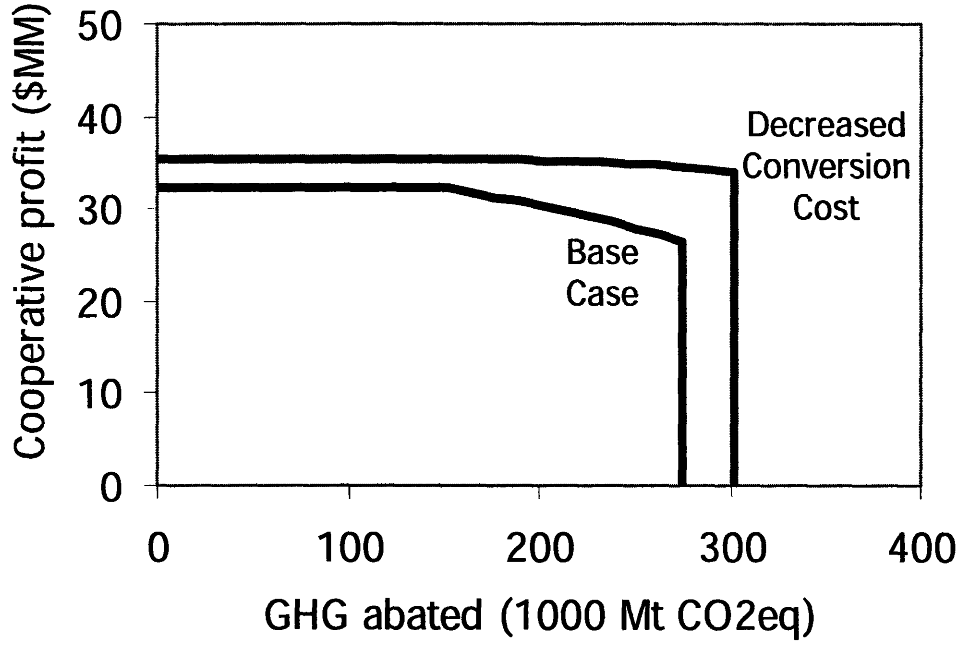

Figure 7.9 Improvement resulting from a decrease in the bioethanol conversion cost

7.4.3 Feedstock Improvements

The next several sections will describe three potential improvements or modifications to the feedstock delivery system – 1) modification in the feedstock collection system 2) an increase in the density of corn stover to that of corn grain, 3) a subsequent increase in the size of a bioethanol facility, and 4) the incorporation of switchgrass as an energy crop. Each of these are compared to the initial technology advance described above for a relative comparison.

7.4.3.1 Improvements to Corn Stover Collection

Several processes are being investigated for a corn stover collection system (Sokhansanj, 2002). The most readily available option is to utilize machinery typically used for baling and transporting hay. After combining the field to collect the corn grain, the farmer would follow with another one or two passes to wrap the leftover stover into bales which are then hauled off the field to a storage area. This is the option used for the base case analysis. A second option is to chop the remaining stover with a forage harvester and transport the material using wagons to a storage facility. Finally, an intriguing option is to modify the grain harvester so that the two streams, grain and stover, are collected simultaneously. Each of these collection processes is expected to be optimized as more stover is collected for downstream conversion, and a number of researchers are working on improvements in machinery and operations.

Enabling the collection of stover will have a considerable impact on the cost of the feedstock. The farmer will still have to be reimbursed for the nutrient loss plus profit, but the additional costs could be significantly lower. Assuming a 33% decrease in the collection costs from an integration of the harvest process results in Figure 7.10.

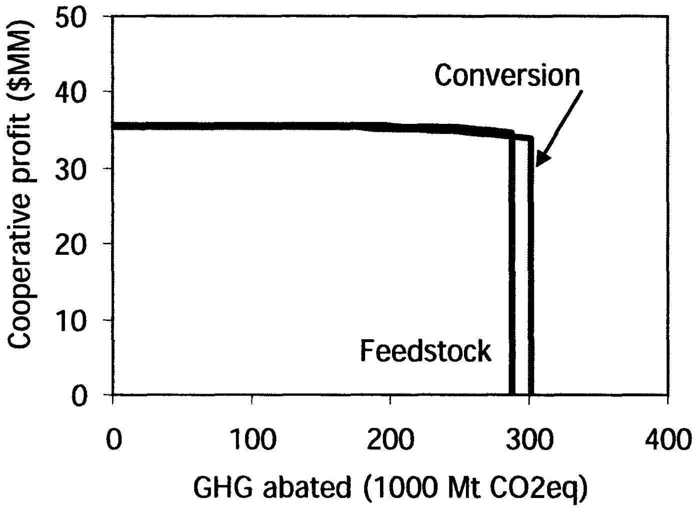

Figure 7.10 System Improvement with reduced corn stover collection costs

As can be seen the economic improvement between the decreased conversion and collection costs are the same. The environmental improvement is not as significant because of the decrease in the distillation requirements of the conversion improvement, but the two technology modifications are close to equivalent.

7.4.3.2 Corn Stover Densification

A critical difference between corn grain and corn stover is its density. While corn kernels have a dry bulk density of close to 0.8 kg/l, corn stover is much lower, less than 0.2 kg/l. The primary ramification of this is a considerable increase in the transportation cost. Most importantly, the low density results in rail distribution not being cost effective. While corn grain can utilize this mode (with an associated cost of $0.02/ton-mile), corn stover is limited to shorter haul trucking (with an associated cost of $0.25/ton-mile). Because of this, every 40 miles of hauling costs an addition $10/ton.

Using the improvement assessment methodology, the impact on the system assuming a decrease in the transportation cost for corn stover to the equivalent of corn grain is investigated (Sokhansanj, 2004). The actual parameter changes are shown in Table D.1. The results of the optimization assuming this modification are shown in Figure 7.11

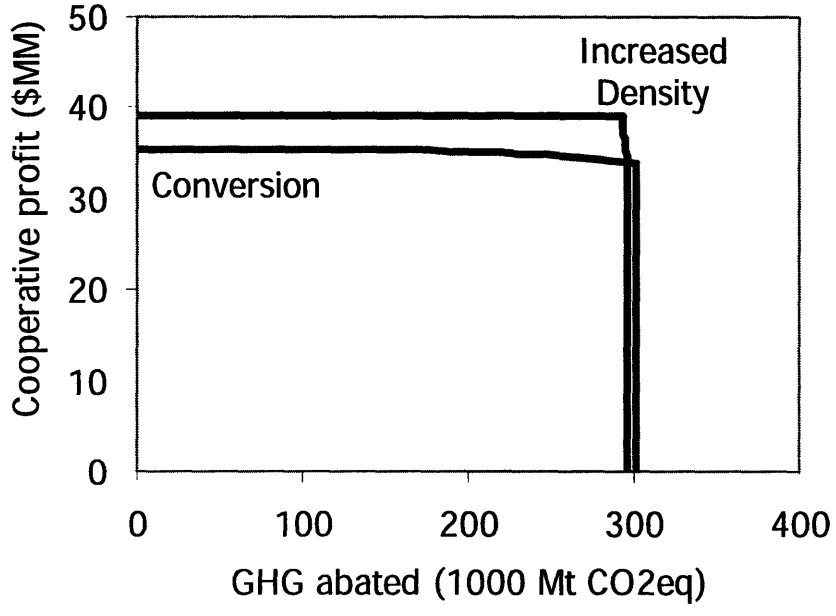

Figure 7.11 System improvement form the increase in corn stover density

As can be seen, the improvement in the economic performance is greater for technology advancement related to the feedstock distribution compared to the conversion cost decrease. This improvement is even more pronounced when investigating the increase in facility capacity size.

7.4.3.3 Increase in Facility Capacity

The typical capacity of corn grain ethanol facilities is about 50 million gallons per year. This is reasonably small on the scale of fuel production as the average refinery in the United States has a capacity of 100,000 bbl/day, about 30 times larger. The size of ethanol facilities are kept smaller because there are not significant economies of scale in dry mill production. Additionally, the lower capital cost allows for farmer cooperatives to be owners. Lignocellulosic ethanol facilities may be a different story. As was shown in the previous chapter, the production cost of these have a much more significant capital component. However, the size is typically limited by the available feedstock. If a distribution network where developed from an increase in the density of this material, though, the ability to use much larger facilities may arise.

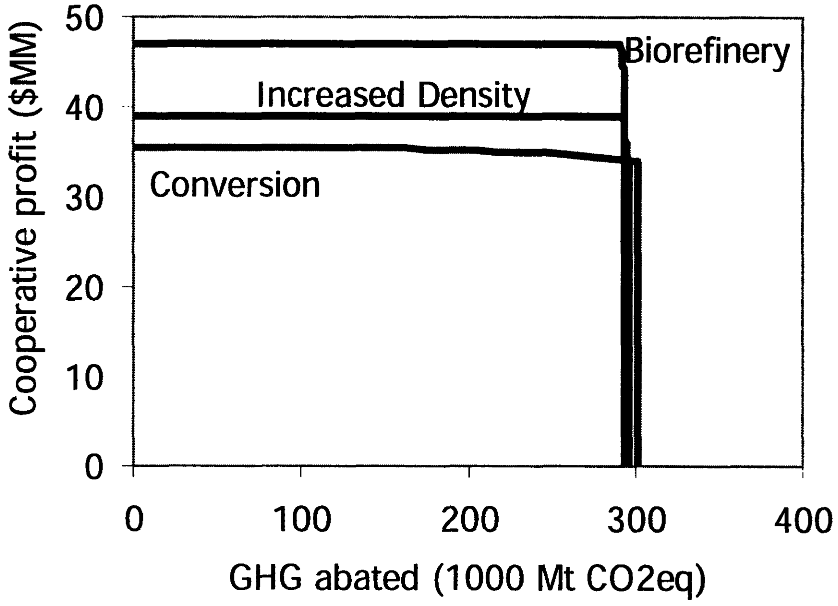

Figure 7.12 System improvement form the increase in facility capacity

This case study builds off the previous one by investigating the impact of building a large scale production facility, 300 MM gallons per year. This is still significantly lower than the average petroleum refinery, but it is about the same scale as a corn grain ethanol facility being proposed by Archer Daniels Midland. Once again, the parameter changes are shown in the appendix. The results of adding this capability into the system is shown in Figure 7.12. As can be seen, the overall increase in the economic metric is considerable compared to the reduction in conversion cost.

7.4.3.4 Integration of Switchgrass

The final feedstock development case study investigates the impact on the system of enabling the economic production of switchgrass for ethanol production. (Brown, 2000; Vogel, 2002; McLaughlin, 2005) As was described in Chapter 2, the utilization of energy crops such as switchgrass may be critical for large scale ethanol production. However, the utilization of such a technology has been limited by the large economic cost of building the infrastructure. For this case, we simply assume that technology has been developed for the cost to no longer be prohibitive. The resulting impact on the system is shown in Figure 7.13.

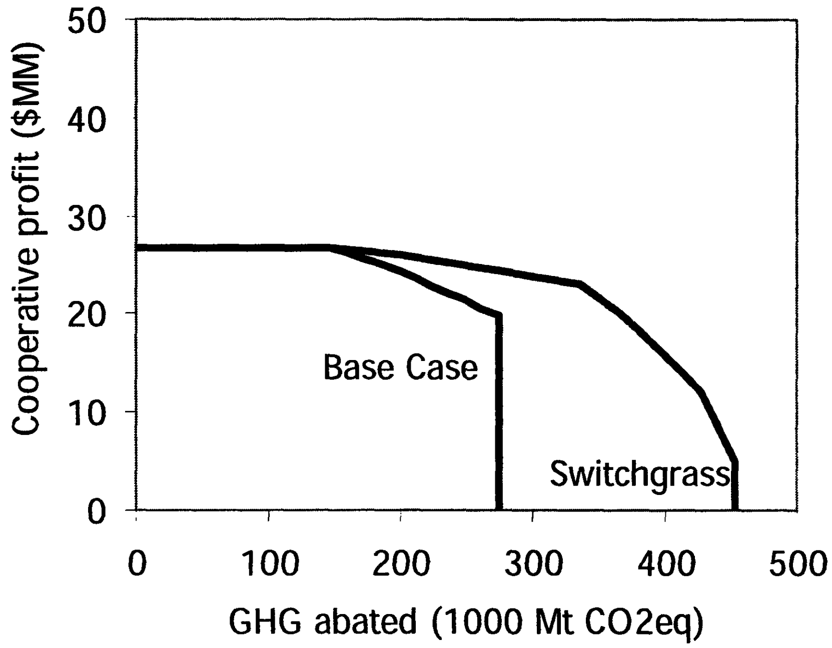

Figure 7.13 System improvement from the incorporation of switchgrass

As is demonstrated, the incorporation of this feedstock considerable increases the environmental potential demonstrated in the Pareto curve, but it doesn't contribute to the economic profit. What this is suggesting is that while the integration of switchgrass is allowing increased greenhouse gas abatement from the production of lignocellulosic ethanol, the overall economic performance is being limited as the switchgrass is simply replacing a more profitable crop be it corn or soybeans.

This is an important result from an energy policy stand point. Energy crops such as switchgrass are viewed as positively because of their quick growth and supposed inexpensiveness. However, the land switchgrass is grown on will have other potential uses, and providing the optimal economic benefit will be important. In some case that may require the implementation of incentives focused on improved greenhouse gas abatement versus economic performance.

The comparison between the improved feedstock density cases and the lower cost conversion case highlights the importance of the distribution infrastructure. As described in Chapter 2, a wealth of lignocellulosic residues and wastes are available for ethanol conversion. However, a limiting step is the ability to actually collect the material and transport it to a conversion facility. Until this is possible in a cost-effective manor, cellulosic ethanol will not be utilized on a large scale. In the last case study, it was even demonstrated that the development of a less disperse energy crop feedstock doesn't necessarily impact the economic costs.

7.5 Hierarchical Decomposition

This section demonstrates the next step in the resource allocation methodology – decomposing the overall model to component subsystems to investigate how modifications to parameters from the more detailed models impact the overall performance as shown in Figure 7.14. Despite having just shown that the upstream feedstock collection and distribution may be more important, as chemical engineers, we are more adept at focusing on the process conversion aspects and that is the focus here. To look at the impacts of these detailed parameters, we will focus on the Aspen process simulation developed for the lignocellulosic process.

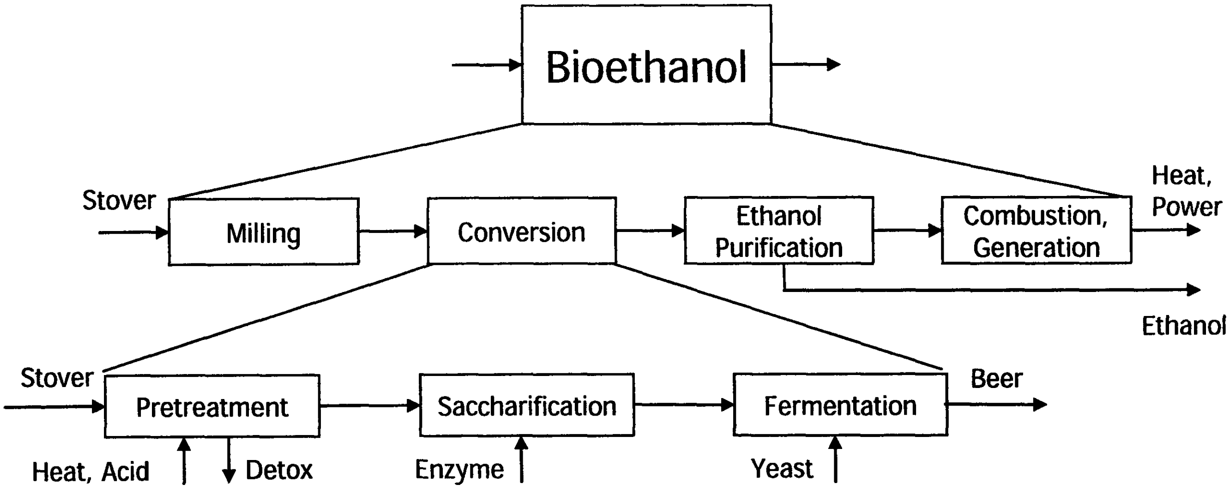

Figure 7.14 Hierarchical decomposition of the bioethanol process

7.5.1 Simplified ASPEN Plus Process Model

The National Renewable Energy Laboratory has developed an Aspen Plus process simulation model which depicts the material and energy balances for a facility which converts corn stover into ethanol. Additionally, the same researchers have developed a detailed economic costing model to determine the capital, operating, and overall production costs of such a facility. The process model and techno-economic analysis is described in Aden (2002). Both the process and economic models are very detailed with the simulation including such details as utilities and wastewater treatment while the economic analysis includes a comprehensive assessment of even the smallest equipment costs. While this level of detail is required for the process design and optimization of a facility which is intended for construction, the analysis in this work is focused more on identify the uncertain parameters and specific technological advancements which could contribute most to the overall improvement in economic and environmental performance. Therefore, a simplified model was developed for this technology assessment project. A quick description is given here while a detailed discussion of the model development is given in the appendices.

Using the process description and the original simulation, a new simulation was developed with only the most critical reactors, heat exchangers, and separation equipment being modeled. Some of the sub-processes were simplified by being modeled as single blocks while some of the extraneous components were combined. The utilities were eliminated from the process except for their calculation for power and heat requirements. The phase equilibrium and component properties from the original NREL simulation were used. The new simulation was developed using the basic material and energy balances from the process description. Control blocks were installed to keep the process models consistent. The number of Aspen parameters were considerably reduced while the overall material and energy balances of the two models remain similar.

The second step of the modification was the development of a new economic costing model to link to the new simulation. While the original costing model provided a very detailed estimate of the overall production costs, the modified version was a considerable simplification. By performing an analysis of the NREL model, it was determined that the capital costs of the major pieces of equipment (>$100,000 installed cost) which were included in the modified model accumulated to ~95% of the overall capital cost. Using this estimate, the capital costs of the modified simulation were estimated using various costing methods (Capcost (Turton, 2003), Peters (2002)) and multiplying that by 1.05 to make up for the detailed equipment left out. Consistency checks were performed against the original cost model with the overall difference being <2%.

The simplified model results in quicker calculations of the overall material and energy balances and ethanol production costs. The advantage of this is the ease in assessing various changes in the performance parameters, whether that be changes in conversions, concentrations, or process conditions. The use of the model is described in the next section. The details of the process and economic model are found in the Appendix.

The NREL simulation describes the production costs associated with a design case for a facility assumed to be operational in 2010. While most of the equipment costs and operational parameters are based on the current technological status, some of the specifications associated with the design assume technology advancements before that date. One of the most critical assumptions is that the five carbon sugars in the feedstock will be converted at a high yield to ethanol. While this has been demonstrated by various research groups, large scale conversion at the required processing conditions has not been demonstrated. Therefore, the base case chosen for this analysis assumes a much lower five carbon sugar conversion, while the improvement in this processing parameter will be considered as one of the case studies. Additionally, more realistic costs for delivered corn stover and purchased enzymes were given. The result is a base case production cost of $1.67 per gallon of ethanol, which is more realistic for the current state of the technology than the $1.07 per gallon cited in the NREL report. However, the goal of assessing the following case studies with the simplified model is to highlight the technology advancements which would be most critical to reducing the production costs to make it competitive and even cheaper than corn grain ethanol.

7.5.2 Resource allocation for cellulosic ethanol

Once the base case has been developed, the Aspen simulation can be used to investigate the relative value of different technology improvements. The specific technology advancements listed are derived from the DOE Biomass Roadmap described above, and are considered achievable in the near future. For the specific process, these improvements consist of: increasing the ethanol fermentation concentration to 30%, decreasing the production costs of enzymes by 50%, lowering the severity of the pretreatment process by 50%, and enabling the production of high value coproducts, such as Fischer-Tropsch liquids.

As was demonstrated in the overall system above, potential feedstock cost reductions are still the most important improvements, and a significant focus should be on feedstock and logistics development. However, as a demonstration of the hierarchical decomposition framework, this next section will focus on process improvements, starting with an analysis of improvements to the fermentation subprocess.

7.5.3 Fermentation Model

The next level of decomposition investigates further details of the fermentation process. While the previous section highlighted that other processes may deserve more attention, fermentation receives most of the research as the incorporation of metabolic engineering tools are easiest here. The fermentation model will still remain simple. Rather than developing a kinetic model of ethanol production through fermentation, we will focus on the specific output parameters from a more detailed investigation.

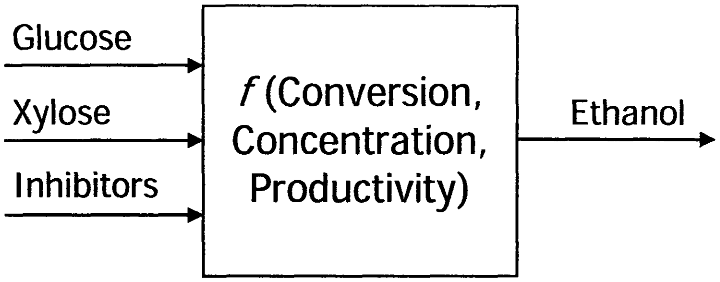

Figure 7.15 Important parameters for fermentation processes

As Figure 7.15 demonstrates, ethanol production will be described as a function of sugar conversion, productivity, and concentration. Each of these parameters are defined within the case study, but the next several charts show the relative decreases in ethanol production costs when improvements in these parameters are applied to the simplified process and economic models.

7.5.3.1 Fermentation Parameter Sensitivities

The Aspen process and associated cost model was simulated using a range of improvements for the three parameters described above. The results are shown in the following graphs, Figure 7.16 - Figure 7.18. At first glance, the increase in ethanol tolerance seems to have the largest impact primarily because of the reduction in separation costs for both capital and energy in the downstream distillation steps; however, it is important to note that the overall ethanol concentration in the fermentation reactor is set not only by the ethanol tolerance of the fermentation organism, but also by the maximum solids content in the upstream processing. Because the cellulose is not soluble before being hydrolyzed to the component glucose sugars, there is a requirement for more water upstream. This leads to a limit in the potential improvement of the concentration to less than a 10% reduction in the ethanol production cost as is shown in Figure 7.16.

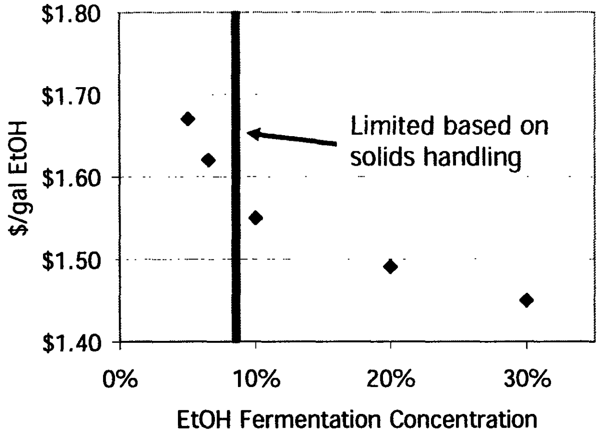

Figure 7.16 Impact of improved ethanol tolerance on ethanol production cost

The xylose conversion parameter is probably the most critical as it directly relates to the amount of ethanol produced per ton of biomass. This is slightly moderated by a decrease in the downstream heat and power byproduct production. However, even considering an improvement to complete conversion of all of the sugars in the process, the overall improvement in costs is only slightly higher than 10%.

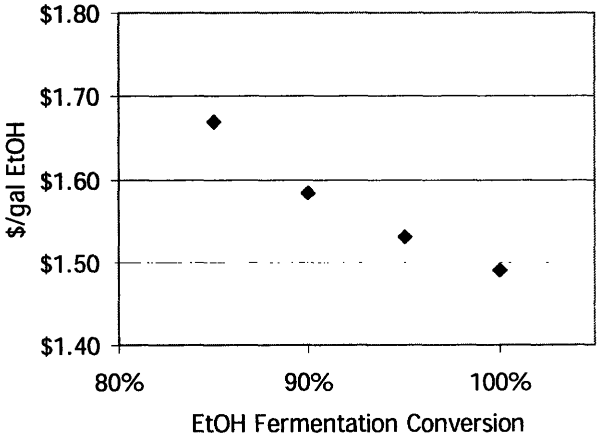

Figure 7.17 Impact of improved sugar conversion on ethanol production cost

Finally, as can be seen in Figure 7.18, the production cost is not very sensitive to ethanol productivity as even a five fold increase only improves the cost by a couple of percentage points. This is because the most significant impact of productivity is on the fermentation reactor capital costs. Considering this cost is small relative to other capital in the process, significantly decreasing this cost will not have a huge impact.

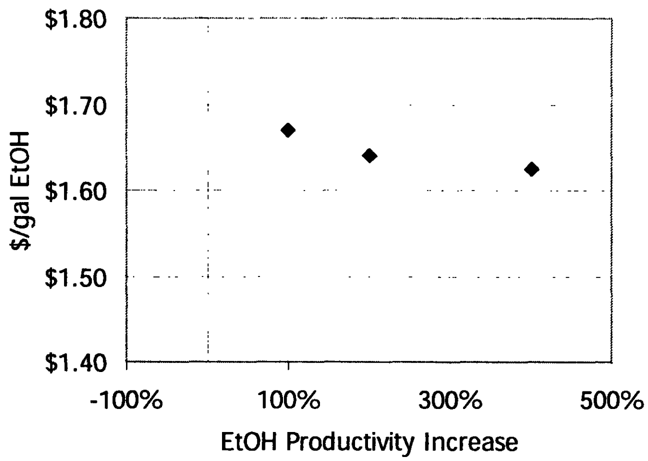

Figure 7.18 Impact of improved fermentation productivity on production cost

Based on this initial assessment, a group focusing on optimized fermentation should focus on conversion > concentration > productivity. As a reminder, this assessment doesn't include the costs associated with the research and development required for making these improvement so an inclusion of the cost of improvement might impact the priority levels.

7.5.4 Pretreatment vs. Fermentation

Returning to the conversion decomposition from Figure 7.14, we can repeat the above analysis, but for the pretreatment section instead and compare the relative improvements between the two processes. The pretreatment section in the base case has significant capital and operating costs associated with the extreme materials of construction associated with the severe temperatures and pH. Additionally, the detoxification subsystem adds capital and operating expenses in addition to the acid, lime, and waste costs. Once again, a detailed kinetic model is not developed, but the costs of pretreatment can be shown as a function of the process severity and conversion of the hemicellulose into the component sugars. Process severity is a proxy describing the relative change from the base case cost, to the cost of the saccharification and fermentation reactors.

Figure 7.19 depicts a comparison between technology advancements in the pretreatment step versus the fermentation step. The actual comparisons are for pretreatment severity reduction and ethanol tolerance as an assumption of conversion improvement to 95% is made in both cases. Once again, the fermentation advancement appears to be more worthwhile, but considering the solids limitation this isn't the case and resources should be focused on pretreatment. Moreover, the pretreatment improvements could also enable further improvement in the fermentation stage by earlier conversion of the cellulose into soluble sugars and by eliminating fermentation inhibitors.

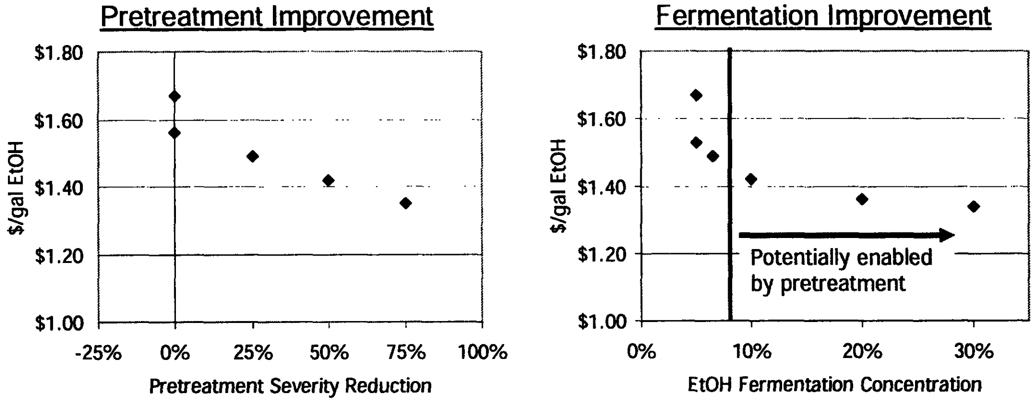

Figure 7.19 Cost improvements for pretreatment and fermentation advancements

7.5.5 Coproduct Integration with Fischer-Tropsch Liquids

The final case study is an assessment of the incorporation of gasification and Fischer-Tropsch technology into the process as a method of increasing the value of the lignin residue which is combusted in the base case. Gasification and FT have been used in the production of synthetic fuels from coal (Dry, 2002) and have been explored for the conversion of biomass (DOE, 2001). In this process, the lignin would be gasified in a partial oxidation reaction with pure oxygen. The resulting syngas is primarily hydrogen and carbon monoxide. Following a shift reaction, the syngas is converted into hydrocarbon chains in a Fischer-Tropsch reaction before being upgraded into high quality diesel. The process material and energy balance and economic cost model is based on a similar assessment of coal to liquids, which is presented in the appendices. A schematic showing how the process fits into the overall conversion is given in Figure 7.20.

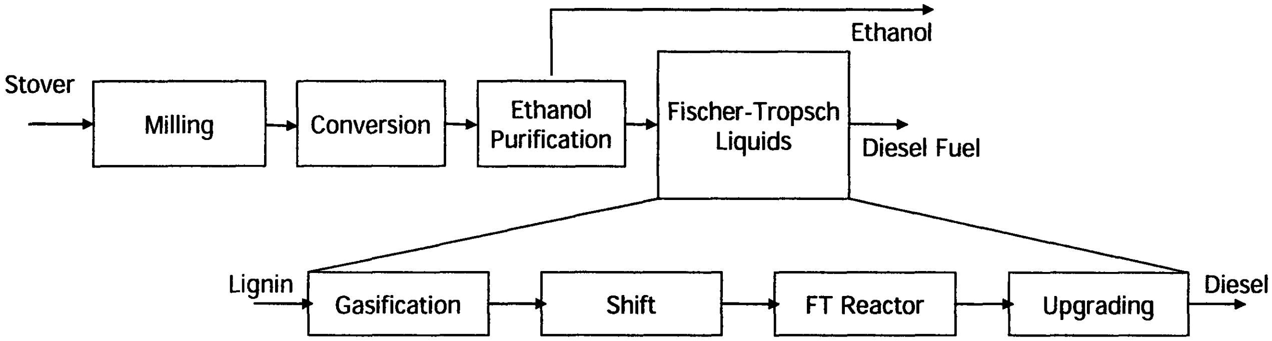

Figure 7.20 Conversion decomposition to Fischer-Tropsch process

An initial cost assessment shows the ethanol production cost actually increases with the incorporation of this process as it is even more capital intensive than the combustor and turbogenerator. Therefore, Figure 7.21 shows the relative cost comparisons as the size of the facility is expanded to take advantage of the increased economies of scale. At capacities larger than 100 MM gallons per year, the introduction of the FT process becomes feasible. (Although, this is a best case scenario as the economics are based on $70/bbl diesel and the overall process is based on the efficiency of a coal facility whereas the wet lignin will more than likely not be as efficient).

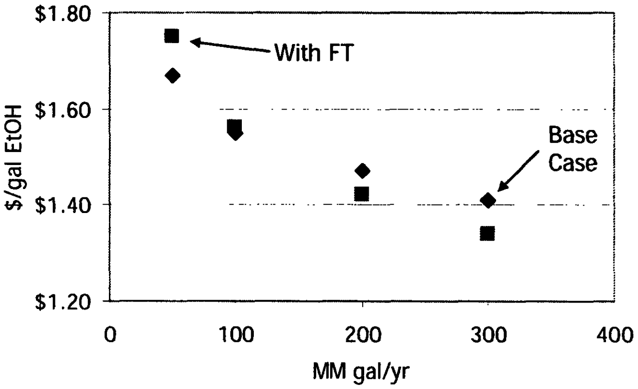

Figure 7.21 Impact of FT at increasing capacities

But as described above, this capacity is infeasible with the current inability to distribute the corn stover without significantly high transportation costs. Additionally, the premium over the non-FT facility is only about 5%. Therefore, the incorporation of FT technology into the process provides the ability to convert the residue into a higher value product at higher efficiencies, but probably will not occur until the stover to ethanol industry has been commercialized and matured.

While all of the above figures show that the returns from the technology advancements are limited and that a combination of different advances will be required for large scale implementation, the overall methodology allows an industrial decision maker to look at research and development alternatives along the overall supply chain to determine which provide the possibility for the largest impact. Subsequently, the subsystem processes can be decomposed to finer levels of detail to see how improvements in parameters at the microscale can affect the system performance.

7.5.6 Research and Development Priority

The technology assessments in this chapter have demonstrated a systematic comparison between different alternatives. Looking at the improvements from each of the advancements enables a comparison of the different options, as is shown in Figure 7.22. Using this framework, we have provided a methodology for systematically determining the priority for how resources can be allocated within a research and development program.

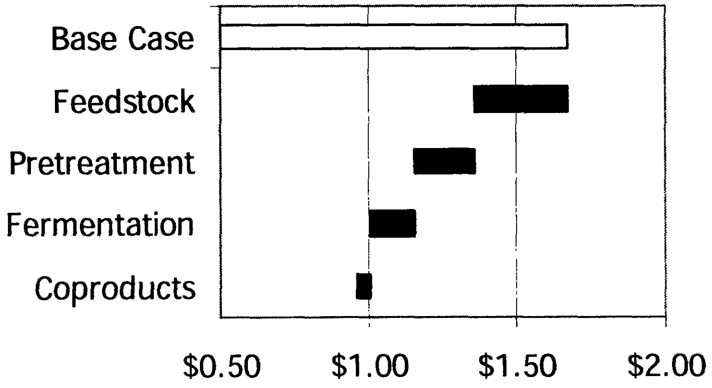

Figure 7.22 Relative improvements of different technology options

An important point to make is that current optimized ethanol production cost $1.00 per gallon, so barring a doubling of corn prices or a energy policy which designates subsidies based on energy efficiency or greenhouse gas abatement, significant advancements in multiple areas will be required for cellulosic ethanol to be competitive. However, the methodology still demonstrates how to determine which technology alternatives should be the focus with limited resources available.

Interestingly, this priority list can be compared to the original research and development budget from Figure 7.8. Comparing that to Figure 7.22, it appears that DOE dollars are focused on the wrong areas. Figure 7.8 shows that the largest targets of funding are the fermentation process and coproducts development, while the work here highlights the importance of the feedstock development and pretreatment processes.

7.6 Conclusion

This chapter has demonstrated how a multiobjective, hierarchical network optimization can be used to compare the potential impact of emerging technologies along the supply chain of a product or process. This is especially useful from a resources allocation perspective for a research and development organization.

For the development of cellulosic ethanol from agricultural crops, this methodology has been used to demonstrate that feedstock development, distribution logistics, and the pretreatment process provide the greatest potential for improved economic and environmental performance.

Chapter 8 Conclusions

The discussion of the primary findings from this thesis will be divided into two parts. The first will focus on the conclusions from the methodology development, while the second will target what was learned from the case studies themselves.

8.1 Methodology implications for traditional process design

8.1.1 Expansion of system boundaries

The bioenergy case study is a perfect one to show the necessity of investigating the entire supply chain when performing a technology assessment. For the case of using corn stover as a feedstock, the economic and environmental (greenhouse gas emissions) impacts of the upstream process were critical to the performance of the overall system. Any group proposing the construction of a lignocellulosic ethanol facility will face an important hurdle when it comes to scheduling the logistics of feedstock delivery. While this fact may not be quite as critical for every production process, it cannot be overlooked.

This extension of system boundaries has become more relevant in determining environmental performance as life cycle assessment is becoming an important tool for assessing products and processes; however, the concept of investigating impacts of those products and processes from resource extraction to utilization and disposal must also be integrated into other business and policy decisions. Explicitly considering the economic, environmental, and social performance of each step along the supply chain is especially important for identifying bottlenecks, or technology advancements which could provide the best improvements. As another example, the analysis of the production costs of corn in this thesis allows the reader to understand the potential impacts on ethanol costs resulting form the removal of agricultural subsidies.

8.1.2 Incorporation of multiple objectives

The recognition that the intense industrialization of the global economy has resulted in numerous environmental problems suggests that future decisions regarding industrial development must explicitly consider how new technologies will affect the environment. For energy development, the growing consensus around global warming and the continued concern about air quality from criteria pollutants means that industrial decision makers need to be ahead of government regulators when designing new processes. This is especially critical as social responsibility has become an important characteristic for potential investors who want to see companies with environmental performance records beyond that of simply meeting government regulations.

Beyond simply including economic and environmental objectives, the bioenergy case study also shows the importance of social and political considerations such as rural development and energy security. While this thesis is engineering focused and didn't concentrate much detail on these objectives, industrial and policy makers must consider how technologies will impact the overall welfare of groups in the rural economy. Moreover, geopolitical concerns relating to from where the U.S. derives its energy are important for policy makers because of the economic and security implications of relying on less stable regions for that energy.

Incorporating multiple objectives requires a methodology for addressing the potential tradeoffs which occur. In this work, the use of Pareto frontiers which describe operating points where no objective can be improved without another being decreased. While this process leads to uncertainty as to which process along the Pareto frontier is best, it allows the decision maker to fully recognize what tradeoffs are being made. For example, the analysis of bioethanol explicitly shows the tradeoff between increased economic cost versus the increased energy efficiency. Policy makers need to assess the tradeoff when determining what, if any, incentive should be applied to encourage the development of the bioethanol process.

8.1.3 Explicit consideration of uncertainty

Traditional process design and technology assessment has occurred using deterministic parameters. Uncertainty is typically not included because it adds mathematical difficulty to the analysis and ends with results that may be difficult to interpret because of the vagueness of probability distributions. A decision maker prefers a single economic point to use in comparing competing processes. Unfortunately, this deterministic approach misses out on the complexity of the decision process and may result in a less than optimal answer. The corn grain ethanol energy balance paper by Farrell (2006) shows how a lack of understanding of the uncertainty in a system may given skewed conclusions. Specifically, they present two case studies with different technology alternatives for ethanol production resulting in different energy efficiencies. This thesis shows that the difference in efficiency is actually resulting from different corn production practices in Iowa versus Nebraska and increased requirements for corn distribution rather than the difference in ethanol processing.

While uncertainty may be difficult to manage, the tools utilized in this thesis demonstrate that it is both possible and important to explicitly consider that uncertainty and variability. A multiple step process consisting of: 1) development of prior distributions for parameters, 2) propagation of the uncertainty using Monte Carlo simulation, 3) sensitivity analysis of the parameters contributing most to output variance, and 4) updating of the critical distributions using Bayesian concepts, is demonstrated to show how the most critical uncertainties can be isolated.

8.1.4 Managing uncertainty in life cycle assessment

One of the primary shortcomings in the development of environmental life cycle assessment methodology is determining how to handle uncertainty. The inventory stage of LCA can be very time consuming because of the large amount of data which must be accumulated to describe the inputs and outputs for all of the process and products. Moreover, these models attempt to describe systems which in reality are incredibly variable from process to process or from region to region. One specific example is the production of nitrogen fertilizer. As was described in the case study, ammonia is typically the key building block for the fertilizer; however, it can be applied in a number of different forms, urea and ammonium nitrate being a couple examples. Each of the forms has different processing requirements. Additionally, the efficiency of nitrogen production is very non-uniform, often depending on the age of the manufacturing facility. The LCA inventory development stage must be modified to explicitly include these uncertainties. The impact assessment stage is also uncertain as the impact categories are simply weighted functions of the individual emissions to formulate a proxy measure of environmental impact for such indices as global warming potential, acidification, or human toxicity. As Cano-Ruiz (2000) shows, expert models may have significantly different weighting systems.

This thesis work shows how applying the above four steps to LCA allows for uncertainty propagation and management. Other researchers have applied Monte Carlo simulation to LCA, but the vagueness of the output distributions makes comparisons between alternatives difficult. The demonstration of the sensitivity analysis and subsequent updating shows the narrowing of those output distributions. Moreover, the application of Bayesian methods enables the use of generic inventories with built in prior distributions for the upstream processes. The implication is that the inventories which are developed for commercial LCA applications can be expanded to use probability distributions rather than deterministic numbers. The user will then have the ability to find the most critical parameters and update those distributions with data more appropriate for the specific alternatives. The case studies to compare greenhouse gas emissions for different ethanol production processes and gasoline production demonstrates the use of the Bayesian updating in LCA.

8.1.5 Network optimization of bioenergy systems

The use of mathematical programming is a prolific field in chemical engineering process design. Rigorous tools have been developed to optimize the complicated, nonlinear systems implicit in chemical processes. However, even the more simple algorithm of linear programming can be very powerful in helping decision makers with process design. Guinard (2001) demonstrates how network programming can be utilized in existing manufacturing facilities to determine how best to retrofit the plant for optimized performance. The work in this thesis expands that concept with the multi-objective, life cycle approach. In this case the network optimization is used to describe the bioenergy system from the agricultural production state to the energy conversion stage. The tool shows how envisioning the performance of a theoretical system can help identify the bottlenecks. Using sensitivity analyses, the shadow prices and reduced costs can be used to determine which parameters in the bioenergy system can be improved to provide the largest improvement for both economic and environmental objectives. As described in the case studies, the network describing the bioenergy system was optimized multiple times, first using a base case, and then following with examples of modifications due to technology advancements. Potential modifications had initially been identified by the most promising parameters in the sensitivity analysis.

8.2 Bioenergy conclusions

8.2.1 Corn grain ethanol energy balance

The controversy over whether it requires more energy to make ethanol using corn grain than is contained in the ethanol itself has existed for over three decades (Ladisch, 1979). As was reported in the case studies, many other research groups have performed the calculation and have achieved differing results. For this work, we developed independent models which described the inputs into and outputs from the corn dry mill process and all upstream processes. Moreover, using the methodology described in the thesis, each of these input and outputs were represented by probability distributions. Applying the LCA calculation to the inventory resulted in a range of net energy production from –9 to +10 MJ/l ethanol, with an expected value of +2 MJ/l. Note that this also includes different methods for allocating energy to the co-product DDGS, or animal feed. This range actually encompasses all of the major studies which had previously been performed. The primary conclusion from this initial result is that the different studies aren't necessarily using bad data, or bad allocation methods, they may simply be choosing the most extreme data or methods.

The next step of the methodology requires a sensitivity analysis of the LCA calculation and this results in the identification of the following parameters as the biggest contributor to the overall variance: allocation decision, drying of DDGS, distillation reboiler steam, corn yield, irrigation requirements, nitrogen fertilizer usage, corn production fuel use, and corn distribution. Updating the distributions for each of these parameters for two specific case studies – corn production location: Iowa or Nebraska, and ethanol production efficiency: low or high, with the system expansion allocation procedure results in considerably decreased variances. For high efficiency ethanol from corn produced in Iowa, the net energy ranges from +4.5 to +7 with an expected value or 6 MJ/l. For low efficiency ethanol from corn produced in Nebraska, then transported to Iowa, the net energy ranges from -2.5 to +1.5 with an expected value or -1 MJ/l. Other variations result in different values. Therefore, assessing the overall ethanol production in the U.S., the net energy production is probably positive, but only slightly. Using the +2 MJ/l expected value, this translates to a production excess of 10%. Moreover, the variance in that net energy production is heavily dependent on not only the efficiency of the conversion facility, but also the corn production practices and the distances required for transporting the corn.

8.2.2 Economics, area, and greenhouse gas emissions for corn ethanol

The energy balance issue is an important discussion, but perhaps more critical to the growth of the ethanol industry is its continued economic performance, and in the future, its ability to reduce carbon emissions. The economics of ethanol production is another controversial topic. The fact that gasoline blenders who buy the fuel are given a \$0.51 excise tax incentive also incites critics. This incentive is on top of the benefit ethanol producers gain by buying a raw material, corn, which already has price suppression because of the agricultural subsidies provided by the government to farmers. By investigating the supply chain economics, this work elucidates some of the economic impacts of these subsidies.

The excise tax incentive doesn't affect the marginal production cost of ethanol so much as it inflates the selling price. Ethanol is primarily used as an oxygenate additive for gasoline, so it is sold at a premium. However, because the energy content of ethanol is 2/3 that of gasoline, the volumetric price of ethanol would be expected to be lower. The subsidy effectively bumps that price up \$0.51, allowing ethanol to float on the price of oil. Therefore, a simple assumption for the real price of ethanol is its price minus the subsidy. Using the production costs analyzed in the case studies, an optimized ethanol facility with average corn and natural gas prices from the last five years would produce ethanol at \$1.00/gallon ethanol. This is comparable to gasoline from \$55/barrel oil on an unsubsidized, energy equivalent basis. With the subsidy, the average 2006 price of ethanol is \$2.25, and optimized producers are returning significant profit. At current high energy prices, these producers would still have a margin even without the incentive. Even, the average producer, which operates closer to \$1.50/gallon in production costs, would be close to profitable without the subsidy.

Moving upstream, an analysis of corn production costs shows that the majority of farmers grow corn at an economic loss, with this being made up by government subsidies ranging from \$0.25-0.75 per bushel. Looking simply at production costs, a farmers' cooperative which grows corn and uses it in its own ethanol manufacturing facility would have an effective increase of \$0.15-0.30 per gallon without the agricultural subsidies. Combing the subsidies, the effective oil equivalence of the average ethanol producer in the U.S. is \$95/barrel.

As business and government moves closer to a regime of taxes for carbon dioxide, fuels which have lower greenhouse gases will have an additional premium. Using the life cycle calculation, corn grain ethanol emits –0.05 to +0.15 kg CO_2 equiv/mile less than conventional gasoline. Updating to the high efficiency, Iowa produced corn case study, this range narrows to +0.1 to +0.18 with an expected value of +0.15 kg CO_2 equiv/mile. If the excise tax incentive were applied solely as a carbon dioxide emission reduction policy, the effective price for carbon would by \$63/tonne C, considerably higher than the current European trading values below \$10/tonne C.

Finally, to replace a significant amount of petroleum usage in the U.S., large amounts of land will be required. President Bush has announced the Advanced Energy Initiative which aims to replace 75% of Middle East petroleum imports by 2025. Simply using current consumption data and ignoring the assumed growth in demand over the next two decades, this value amounts to 10% of current usage, or 2 million barrels of petroleum per day. Replacing this amount of petroleum with ethanol will require the expansion of corn production to twice the current U.S. corn acreage, and increase the U.S. natural gas consumption by 14% because of ethanol's dependence on natural gas for fertilizer production and process heat.

The primary conclusion from this multi-objective assessment is that while corn grain ethanol does have slight energy production and greenhouse gas emission reduction advantages over gasoline, the subsidies which promote its production are probably disproportionately high. A recommendation is that the policy regime be modified to a tiered incentive structure where higher efficiency producers be awarded incentives at higher rates than those with lower subsidies. The next section begins to look at how improvements in efficiency can be made.

8.2.3 Economic and environmental performance for cellulosic ethanol

The primary emerging technology for ethanol production is a shift to using lignocellulosic biomass rather than starch from corn grain. This material has the advantage of being less economic and energy intensive than corn and much more available. Using estimates of forest residues, agricultural residues, and potential energy crops, a recent study by Oak Ridge National Lab suggests the availability of 1.3 billion tons of biomass annually, an amount which could result in the production of over 100 billion gallons of ethanol, 20 times the current industry capacity. Moreover, because much of this is waste and residue, the anticipated development of dedicated energy crops consists of an area of 30 million acres, only 1/3 of current corn acreage. The disadvantages of this biomass is that it is disperse, low density, and difficult to breakdown into component sugars for fermentation.

The development of a simplified process simulation and costing model allowed for the assessment of the economic costs of lignocellulosic ethanol. Additionally, the models for feedstock collection and ethanol conversion were integrated into the environmental life cycle assessment models to explore the multi-objective performance, in this case, using corn stover, the residue left on the field after corn grain harvest, for ethanol production. Because this case is performed on non-commercialized technology, the analysis will focus on the optimized performance rather than using statistical data. The base case analysis results in much improved net energy and greenhouse gas emissions versus gasoline, +20 MJ/l ethanol, and 6 kg CO2 equiv/gal respectively. The economics show the opposite trend, though, with the production cost of corn stover ethanol at $2.10/gallon. While the environmental case for cellulosic ethanol is high, the economic performance is still too far away from potential commercialization. Further technological advances are required to meet the goal of economic competitiveness.

8.2.4 Assessment of R&D alternatives

Many researchers are working on developing improved technology along the supply chain of cellulosic ethanol production; however the R&D is marked by a lack of analysis showing how resources could best be allocated. Some of the technologies with the highest potential for improving the economic and environmental objectives receive the least attention and funding. The last step of the methodology, the network optimization of a hierarchical model with subsequent decomposition, is utilized here to elucidate the impact of individual and combinations of technology advancements. The goal is to present a coherent analysis of the spectrum of potential R&D projects with an emphasis on identifying the most critical.

With the first order assessment of the bioenergy system, the initial finding is that the costs of raw materials, the delivered corn stover and purchased enzymes, provide the highest potential for reducing overall costs, especially when compared to process optimizations. Using fiscal year 2004 National Bioenergy Center funding as the comparison, the raw material projects received only ~35% of the total $46 million funding compared to the other ~65% focused on the process development. Meanwhile, for the raw material programs, the DOE has significantly funded a couple of companies for enzyme development, but the breadth of the work has been limited. Moreover, work on feedstock development and collection logistics has been significantly under-funded at just over 10%.

The following step in the methodology is to decompose the overall network into more detailed models. For this step, the process design was scrutinized further, with the process simulation and linked costing model providing the opportunity to quickly investigate different process modifications. The three primary processing steps: pretreatment, fermentation, and purification, were assessed to determine how improvements in each of the stages would affect overall process economics. Because of its influence on overall conversion, downstream inhibitors, and capital cost, the pretreatment step revealed the largest potential cost gradient, followed by fermentation and then purification. Note that the purification process is pretty optimized, but this analysis did not address the potential for radical technology changes such as replacing distillation with a high efficiency membrane process, or replacing the by product turbogenerator with a gasification and Fischer-Tropsch synthesis section as these development seem further down the road.

Finally, a further level of decomposition was performed on the fermentation process. While the above paragraph states that the pretreatment process has more opportunities, the fact remains that it is much less understood. Therefore, using the basic parameters for fermentation, the more detailed analysis looked at improvements of production rate and product tolerance. This analysis showed that the ethanol tolerance had the larger effect than rate of production.

These conclusions are just for a handful of examples, and this methodology could be applied to a comparison of any of the processes within the bioenergy system to give industrial leaders and policy makers a framework for assessing the research and development

Chapter 9 Future Work

Both the technology assessment methodology and the details of the bioenergy case study have many opportunities for further exploration. Potential ideas for these are presented below. Once again, the first section will focus on potential future directions for methodology development, while the second will target next steps for the assessment of biomass energy.

9.1 Methodology development next steps

9.1.1 Further expansion of the network optimization problem

The linear program developed in this work is reasonably simple with a small number of parameters to describe a theoretical region. More information could be provided by expanding it to an economy wide scale. Because this system describes a complex interaction of the agricultural, transportation, and energy industries, a tool which is able to combine large scale models for each of those: POLYSIS, NEMS, and EPPA. The economy wide modeling would enable moving beyond the simple marginal analyses to which this thesis was limited. Moreover, moving from a static environment to exploring the system dynamics of potential land use changes, economic policies, etc. would be incredibly interesting.

9.1.2 Extension of tools to commercial or open source software packages

The life cycle assessment software developed by Cano-Ruiz (2000) is an excellent tool; however, but it needs to be updated with more current and extensive inventory databases. Additionally, the link to the Monte Carlo simulation software needs to be upgraded. Another option is to integrate these concepts into existing LCA and process design software packages. LCA inventories should be developed with probabilistic representations rather than deterministic values. The user should have the option to update the distributions using the Bayesian concepts suggested here.

For further academic research, using a commercialized modeling package, such as Umberto (2006) combined with recognized inventories from groups such as SimaPro

(2006) would be helpful for better translation of the ideas to industrial groups who may actually incorporate the methodology. Additionally, more sophisticated methods for the uncertainty propagation, such as using WinBUGS (2006) for Monte Carlo simulations and optimizations would be helpful

9.1.3 Expand objectives beyond economics, energy balance, and air pollution

The effect of land use changes, soil carbon, water requirements, and increased agricultural intensity was not explored extensively in this work. Each of these, and other considerations, may lead to important insights regarding the large scale production of bioenergy. Stakeholder considerations also should be explored in further detail. The case study of how a farmers' cooperative integrates economic, environmental, and social consideration into their individual and group decision making would be fascinating. However, the stakeholder theory should not be limited to the farmers themselves. The utility functions of other individuals in the communities, environmental groups, etc., should also be included.

9.2 Bioenergy case study next steps

9.2.1 Inclusion of more feedstocks, processes, products

The work in this thesis focuses on the biological conversion of corn grain and stover into ethanol with corresponding coproducts. This is just a small example of all of the potential biomass, conversion processes, and end products. For example, in the ORNL report estimating that 1.3 billion tons of biomass is potentially available annually, corn stover comprises less than 10%. Other feedstocks such as energy crops, forest residues, and urban wastes make up the remainder. While the commercialization of an agricultural residue based cellulose ethanol manufacturing facility will promote the expansion to other feedstocks, detailed optimizations of the performance of those changes will be required.

Moreover, biological conversion is only a subset of the possible processes. Many research groups are looking at thermochemical conversion, a specific example being the gasification of the biomass with downstream power generation or Fischer-Tropsch synthesis. While the fermentation process is the basis for the majority of bioenergy projects currently, the advancement of the thermochemical process could have a significant impact. In fact, an integration of the biological and thermochemical processes may be a route for optimized utilization of all of the biomass components.

Finally, the tradeoffs between producing biomass for energy versus food was briefly touched on in this work, but as bioenergy products become more expansive, an understanding of the economic, environmental, and social implications will become more important. Additionally, other potential plant-based products, such as hydrogen or plastics will factor into these decisions. A next step would be to expand the network optimization problem presented here to include many more feedstocks, processes, and products.

9.2.2 Explicit study of the short and long term impacts of soil carbon

The removal of agricultural residues for industrial products is a concern for some soil scientists because the residue contains nutrients, controls erosion, and has a considerable impact on the soil carbon content. Each of these factors has environmental concerns from greenhouse gas emissions to impacts on subsequent years' yields. In this work, a constraint on the residue removal per acre was used; however, this may not be the most appropriate approach as an optimization would treat different soil types and regions differently.

Potential future work is the integration of a soil model which describes the geochemical cycles and the impacts of agricultural residue removal or energy crop production. This is a critical step in understanding the long term viability of a large scale bioenergy production system.

9.2.3 Interaction of overall model with groups investigating molecular biology

The final model decomposition in the improvement assessment chapter focused on a couple of the parameters describing the kinetics of the fermentation process. The final model was very simple, but the possibility of integrating a more detailed model is intriguing. A number of groups are working on metabolic engineering for the improvement of the fermentation microbes and process. Interdisciplinary collaborations integrating the large scale economic and environmental models with the very detailed metabolic engineering models would be useful in identifying which specific conditions and parameters provide the best potential for overall improvement. Moreover, this potential collaboration could be applied to groups working on the details of other steps in the conversion process or even upstream feedstock development and transportation logistics.

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Appendix A Process design for ethanol production from corn stover

The economic and environmental analyses presented in Chapters 4-7 are based on a process which converts corn stover into ethanol. An Aspen Plus process simulation and associated economic cost model was used for the calculations. The actual process flowsheet is based on a design described by the National Renewable Energy Lab (Aden; 2002).

For those reports, researchers built an Aspen Plus process simulation which describes the material and energy balances for a corn stover to ethanol facility. This simulation is linked to a detailed costing model which estimates the capital costs of each of the significant pieces of equipment and the subsequent overall capital and operating costs. The methodology used by the NREL group is similar to what is described in the section on chemical process design in Chapter 3.

For the methodology proposed in this thesis, a less detailed process and economic model was required to investigate the different technology alternatives. For example, the original NREL simulation contains 144 unit operations, 668 material, heat, and work streams, 57 components, and 70 control blocks, whereas the simplified simulation provided here contains 40 unit operations, 75 streams, 20 components, and 12 control blocks. The following appendices describe the details of the process simulation which was used for this thesis.

The base case follows the same basis as the NREL simulation – conversion of corn stover into ethanol with five basic steps: 1) dilute acid pretreatment of the biomass to break apart the lignocellulosic, 2)enzymatic hydrolysis to degrade the cellulose into its component sugars, 3) fermentation to ethanol, 4) distillation for ethanol purification, and 5) combustion of residues for heat and power. The initial size of the facility is initially the same – 2000 tons per day of corn stover, 70 million gallons per year of ethanol to check the material and energy balances and economic costs for consistency, but the base case size will be lower, 50 million gallons per year, for comparison with the USDA dry mill case presented in Chapter 3. The components for the simulation are given in Table

A.1. The physical property database and the user-defined components used are from the original NREL simulation and are described in their reports.

A brief process description was given in Chapter 7. Here we give a more detailed description of the models used to describe each of the subsystems. For a more detailed description of the overall process, see the original NREL reports. An explanation of the economic model for the process follows. Subsystems such as feedstock handling, utilities, etc., are not modeled but are included in the economic analysis.

Component ID	Type	Component name	Formula
GLUCOSE	CONV		
CELLULOS	SOLID		
XYLOSE	CONV		
XYLAN	SOLID		
LIGNIN	SOLID		
SOLSLDS	CONV		
GYPSUM	SOLID		
ACETATE	SOLID		
C5SOLID	SOLID		
C6SOLID	SOLID		
CAH2O2	SOLID	CALCIUM-HYDROXIDE	CA(OH)2
ASH	SOLID	CALCIUM-OXIDE	CAO
ETHANOL	CONV	ETHANOL	C2H6O-2
H2O	CONV	WATER	H2O
FURFURAL	CONV	FURFURAL	C5H4O2
HMF	CONV	FURFURAL	C5H4O2
H2SO4	CONV	SULFURIC-ACID	H2SO4
CO2	CONV	CARBON-DIOXIDE	CO2
LACID	CONV	LACTIC-ACID	C3H6O3-D1
AACID	CONV	ACETIC-ACID	C2H4O2-1

Table A.1 Aspen components

A.1 Dilute acid pretreatment

The pretreatment reactor is modeled using a heat exchanger and a stoichiometric reactor as shown in Figure A.1. The corn stover inlet stream defined in Table A.2 is combined with process condensate (the concentration of which is based on the outlet of the evaporators from the combustor section; a full material and energy balance is given in Table A.7-Table A.10) and low pressure steam. The condensate is controlled by a design spec to have a flow ratio of 0.4 to the corn stover stream. The LP steam flow rate set such that the outlet temperature of the first half of the reactor set, M202LO, is 130°C. The second stage of the pretreatment reactor is modeled by M202HI. The outlet of the heat exchanger is fed to the stoichiometric reactor along with high pressure steam and an acid stream diluted by another process condensate stream. The high temperature and low pH are used to break open the lignocellulosic matrix to hydrolyze the hemicellulose and free the cellulose for downstream enzyme degradation. The steam rate is set so that the outlet temperature of the reactor is 190°C, and 12 atm while the condensate/acid streams are set such that the sulfuric acid concentration is 1.1% while the overall solids in the reactor outlet are 30%. The reactions for the pretreatment reactor are given in Table A.3. The reactor outlet is flashed to 1 atm int T203, and the vapor is used to preheat the feed to the beer column while the liquid is pumped to the detoxification stage to prepare the hydrolyzate for saccharification and fermentation.

Substream: MIXED			Substream: CISOLID	
Mass Flow kg/hr			Mass Flow kg/hr	
SOLSLDS	7505.56		CELLULOS	30833.2
H2O	14700.24		XYLAN	17499.92
Total Flow kmol/hr	1268.557		LIGNIN	14999.93
Total Flow kg/hr	22205.8		ACETATE	2499.989
Total Flow l/min	605.1948		C5SOLID	3333.319
Temperature C	45		C6SOLID	2499.989
Pressure atm	1		ASH	4166.648
Vapor Frac	0		Total Flow kmol/hr	576.0243
Liquid Frac	1		Total Flow kg/hr	75833
Solid Frac	0		Total Flow l/min	660.019
Enthalpy cal/mol	-48048.92		Temperature C	45
Enthalpy kcal/kg	-2744.904		Pressure atm	1
Enthalpy MMkcal/hr	-60.95366		Vapor Frac	0
Entropy cal/mol-K	-2.961503		Liquid Frac	0
Entropy kcal/kg-K	-0.1691826		Solid Frac	1
Density mol/cc	0.0349352		Enthalpy cal/mol	-2.39E+05
Density gm/cc	0.611533		Enthalpy kcal/kg	-1812.56
Average MW	17.50477		Enthalpy MMkcal/hr	-137.4538
Liq Vol 60F l/min	369.5553		Entropy cal/mol-K	-734.7028
Substream: $TOTAL			Entropy kcal/kg-K	-5.580772
Total Flow kg/hr	98038.8		Density mol/cc	0.0145456
Enthalpy MMkcal/hr	-198.4075		Density gm/cc	1.91492
			Average MW	131.649

Table A.2 Corn stover feed stream

Stoichiometry	Yield
H2O + CELLULOS(Cisolid) --> GLUCOSE	0.08
H2O + XYLAN(Cisolid) --> XYLOSE	0.9
XYLAN(Cisolid) --> FURFURAL + 2 H2O	0.05
C6SOLID(Cisolid) --> HMF + 2 H2O	0.05
C5SOLID(Cisolid) --> 2 H2O + FURFURAL	0.05
ACETATE(Cisolid) --> AACID	1
C5SOLID(Cisolid) + H2O --> XYLOSE	0.9
C6SOLID(Cisolid) + H2O --> GLUCOSE	0.9

Table A.3 Pretreatment reactions

The process stream is combined with another condensate stream to bring the soluble solids concentration to 10% and is subsequently cooled to 50°C in the DETOXHX. A pneumatic filter, PNUFIL is used to separate the cellulose and lignin solids from the hemicellulose hydrolyzate and liquid inhibitors formed in the pretreatment reactions. Of the soluble materials, 6.6% continues on with the solid product (except for water and ethanol, which are passed at 13% and 3%, respectively). For the insoluble biomass, 99.5% is separated into the solid product, which is pumped downstream to the saccharification reactor. The liquid product is combined with another sulfuric acid stream, with a flow rate of 0.55 the initial acid stream and a lime stream equal to the sum of the two acid streams. CONDTNR consists of the lime and sulfuric acid reacting to form gypsum which is removed in another filter, DRUMFILT, with the 99.5% of the solids, and 0.05% of the remainder being filtered out. The detoxified hydrolyzate is then pumped onto the saccharification section to be remixed with the cellulose stream.

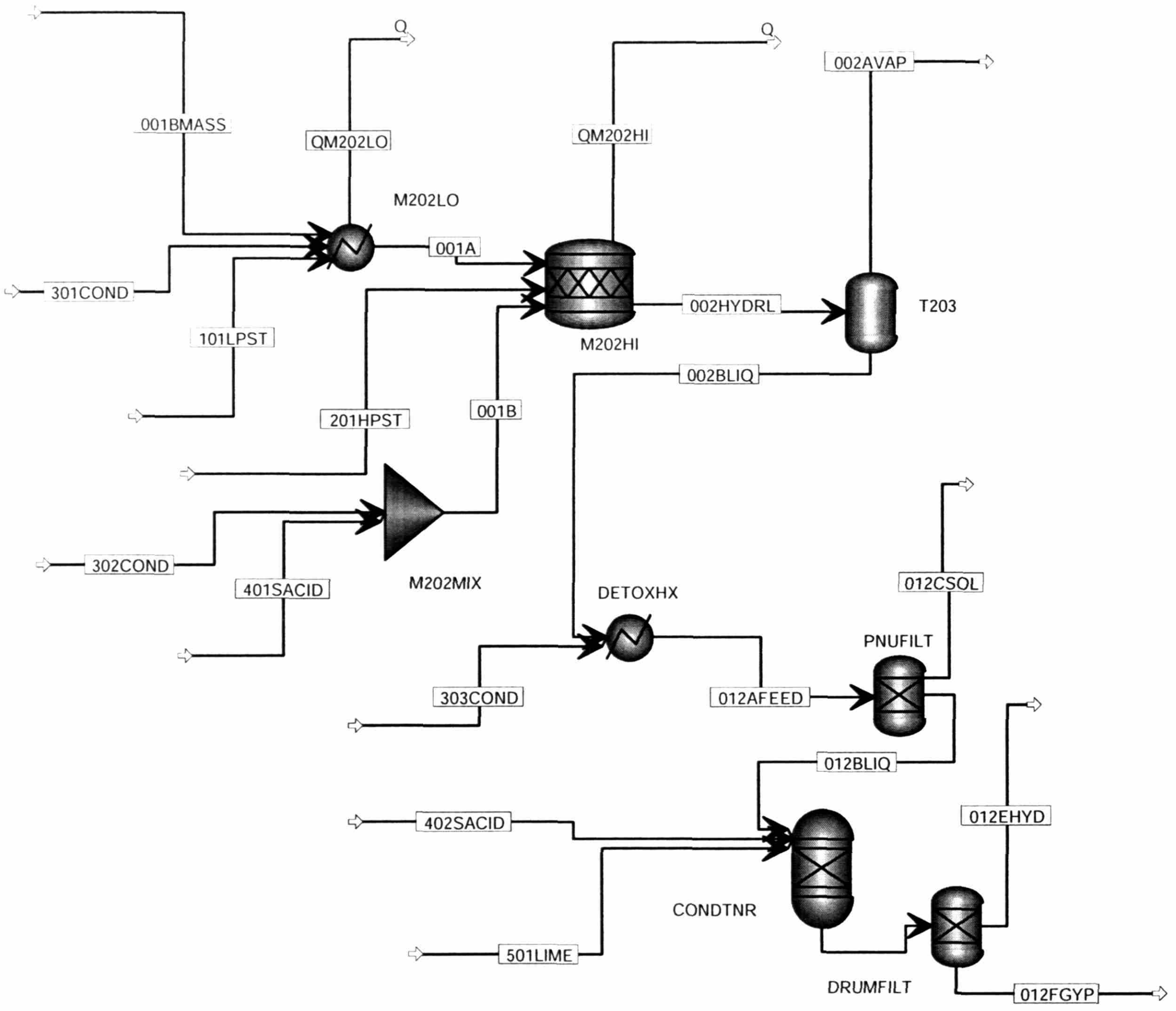


Figure A.1 Pretreatment Section

A.2 Enzymatic hydrolysis and fermentation

Figure A.2 shows the Aspen flowsheet of the saccharification and fermentation section. The cellulose and hydrolyzate streams are recombined with another process condensate stream before being heated to 65°C in HYDHEAT. The condensate stream is varied to achieve 20% total biomass (soluble and insoluble solids) in the saccharification and fermentation reactors. Enzymatic hydrolysis of the cellulose is modeled in SACCHAR using a stoichiometric reactor. In reality, purchased enzymes are added to the reactor to facilitate the hydrolysis, but these are left out of this simplified simulation. Moreover, the saccharification occurs in a series of tanks rather than a single one while the tanks are cooled by a pump around loop which circulates the slurry through heat exchangers. While these aren't modeled in the Aspen simulation, they are accounted for in the economic analysis section. Only one reaction is modeled in SACCHAR with 92% of the cellulose being converted to glucose,

$$\text{CELLULOS (CISOLID)} + \text{H2O} \rightarrow \text{GLUCOSE} \qquad \text{(A.1)}$$

Following these reactors, the saccharification slurry is cooled in SACCOOL to 41°C for conversion to ethanol in FERMENT. The reactions modeled in the stoichiometric reactor are given in Table A.4. The fermentation reaction also occurs in a series of tanks with pump-around cooling units. Additionally, the fermentation process requires a system of seed tanks where the fermenting yeasts are produced. Once again, while not modeled explicitly in Aspen, the cost of this additionally equipment and processing is included in the economic model. The fermentation reactions produce considerable carbon dioxide which is vented to the scrubber, described in the next section. Downstream of the fermentation reactors is a surge drum, FERMVENT which acts as a buffer for the distillation process while collecting recycle from the scrubber. Additionally, this flash drum serves as the modeling tool for describing the CO_2 vent from the fermentation. The liquid product from this drum is heated using the vent stream from the pretreatment section to 95°C before being pumped to the distillation section.

Stoichiometry	Yield
GLUCOSE --> 2 CO2 + 2 ETHANOL	0.9
GLUCOSE --> 3 AACID	0.03
GLUCOSE --> 2 LACID	0.03
3 XYLOSE --> 5 CO2 + 5 ETHANOL	0.8
2 XYLOSE --> 5 AACID	0.1
3 XYLOSE --> 5 LACID	0.03

Table A.4 Fermentation reactions

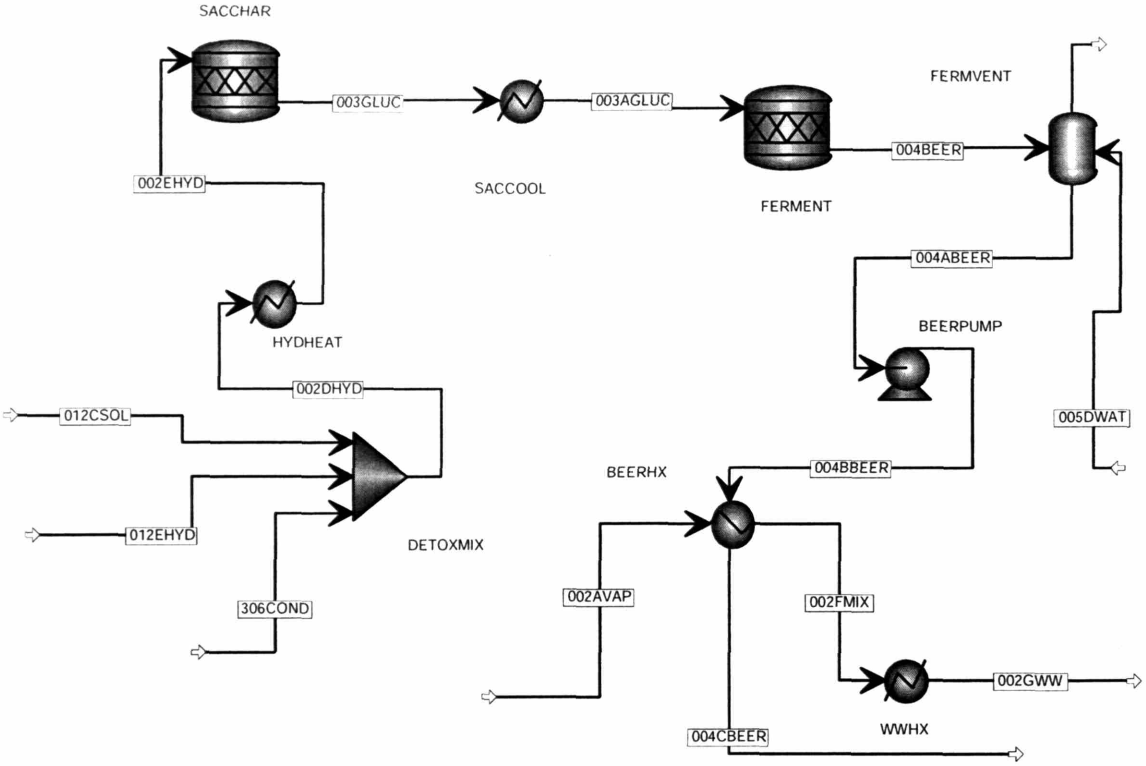


Figure A.2 Saccharification and fermentation

A.3 Ethanol purification

Figure A.3 depicts the Aspen flowsheet for the distillation section of the lignocellulosic ethanol process. The beer stream from the fermentation section is heated further to 100°C in a feed-bottoms heat exchanger, FDBOTHX, before being fed to the initial distillation tower, BEERCOL. The column separates the remaining solids out the bottom and produces a CO_2 stream out of the top and a 40% w/w ethanol stream out of stage 8. The column is modeled using the RadFrac Aspen unit operation with 32 stages with 50% efficiency (feed stage 4), a partial-vapor condenser, and a kettle reboiler. The column operates at 1.85 atm with a 0.25 atm drop down the column. The initial specifications are a distillate rate of 450 kg/hr, a reflux ratio of 3, and a sidestream of 60,000 kg/hr. For convergence, design specs are the condenser temperature, 60°C, and the ethanol mass purity in the bottoms stream, 0.0005. The varied parameters are the distillate and sidestream rates.

The vapor stream from the beer column is mixed with the vent stream from the fermentation section and sent to the SCRUBBER, where process condensate is used to scrub out the organic compounds in the CO_2 streams. The scrubber is modeled with a 4 stage RadFrac unit with no condenser and no reboiler. The vent feed is fed at the bottom while the condensate enters at the top. The design spec for the scrubber is a ratio of ethanol released to the atmosphere to dry corn stover input of 0.0000527. This is to meet permit regulations for volatile organic compounds. The process condensate stream, 304COND, is varied to achieve this specification. The bottoms stream from the scrubber returns to the fermentation surge drum from the previous section.

The bottoms from the beer column contains all of the biomass residues which cannot be converted into ethanol. This stream returns to the feed bottoms heat exchanger before being sent to the residue recovery section where it is dried before being combusted for heat and power.

The sidestream from the beer column contains the vast majority of the product ethanol. This stream is fed to the next distillation step, RECTIFY, where the column purifies the ethanol to its azeotrope at 92.5% w/w with the bottom stream being recycled to the system as process condensate. The column is modeled using the RadFrac Aspen unit operation with 60 stages with 60% efficiency (primary feed stage 44, feed from molecular sieve 22), a partial-vapor condenser, and a kettle reboiler. The column operates at 1.7 atm with a 0.25 atm drop down the column. The initial specifications are a reflux ratio of 3.2 and a boilup ratio of 0.2. For convergence, design specs are the ethanol mass purity of the vapor stream, 0.925, and the ethanol mass purity of the bottoms stream, 0.0005. The varied parameters are the reflux ratio and boilup ratio. This column is challenging to converge, and the nonideal convergence algorithm is used.

The azeotrope stream is sent to the molecular sieve unit which is modeled in this simulation with a handful of heat exchangers and a separator. The actual molsieve is based on proprietary data so this is simply an estimation of the material flows and utility requirements. The initial unit operation is a heat exchanger, MOLSHEAT, where the temperature is increased to 116°C. This is followed by the MOLSIEVE where 20% of the ethanol and 95% of the water is separated out to be returned to the rectifier. Before returning to the column, the stream is first cooled to 35°C and then heated back to 70°C while being used to cool the product ethanol stream in MOLSIVHX. The ethanol product stream is further cooled to 38°C. The final production specs of the ethanol product is shown in Table A.5.

Substream: MIXED	
Mass Flow kg/hr	
ETHANOL	24601.74
H2O	124.6679
FURFURAL	0.0611688
HMF	3.84E-06
CO2	4.04E-04
AACID	1.16E-09
Total Flow kmol/hr	540.9398
Total Flow kg/hr	24726.47
Total Flow l/min	531.5368
Temperature C	38
Pressure atm	1.7
Vapor Frac	0
Liquid Frac	1
Solid Frac	0
Enthalpy cal/mol	-65881.35
Enthalpy kcal/kg	-1441.283
Enthalpy MMkcal/hr	-35.63835
Entropy cal/mol-K	-80.72909
Entropy kcal/kg-K	-1.766106
Density mol/cc	0.0169615
Density gm/cc	7.75E-01
Average MW	45.71021
Liq Vol 60F l/min	519.8381

Table A.5 Ethanol product stream

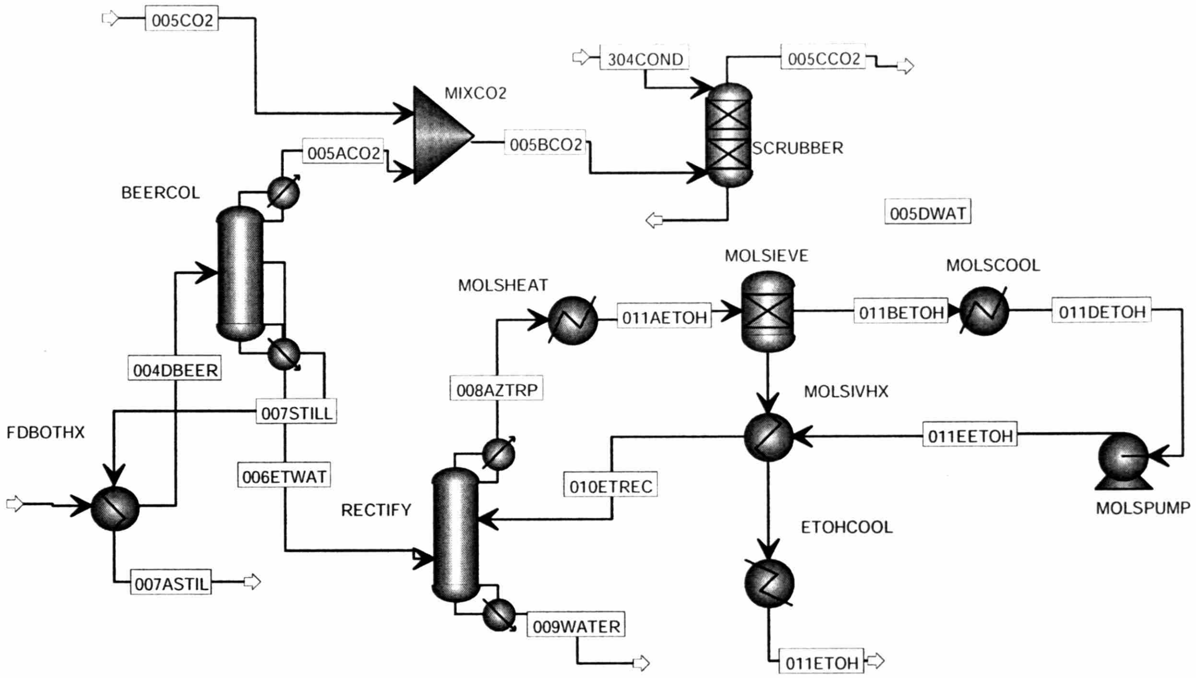


Figure A.3 Ethanol purification

A.4 Residue recovery

Figure A.4 shows the Aspen flowsheet for the evaporators section. In this subsystem, the lignin and other residues from the beer column bottoms are dried for use in the combustor and turbogenerator for heat and power production. A spreadsheet model is used for the heat and power generation and so it is not described in this section.

After the feed bottom heat exchanger, the beer column stillage is sent to the first effect of an evaporator system. This effect serves as the rectification column condenser as its heat is provided by the overhead vapors from that column plus a small amount of additional low pressure steam. This effect is modeled using a control valve, a heat exchanger, and a flash drum. The valve, EVCV1, flashes the stream to 0.60 atm. EVHEAT1 represents the overhead vapors plus LP steam. The overall heat to the exchanger is set so that the moisture content of the outlet slurry to the third effect in the evaporator is 0.6. The flash drum is used to separate the vapor, which will be used to heat the second effect of the evaporator, and the slurry, which is sent to another pneumatic filter. The filter has three output streams, a process condensate stream which consists of 23% of the soluble components and 0.5% of the insoluble solids, a solids stream which contains 98% of the insoluble solids, and a slurry with 69% of the soluble components which is used as the feed to the second effect of the evaporator.

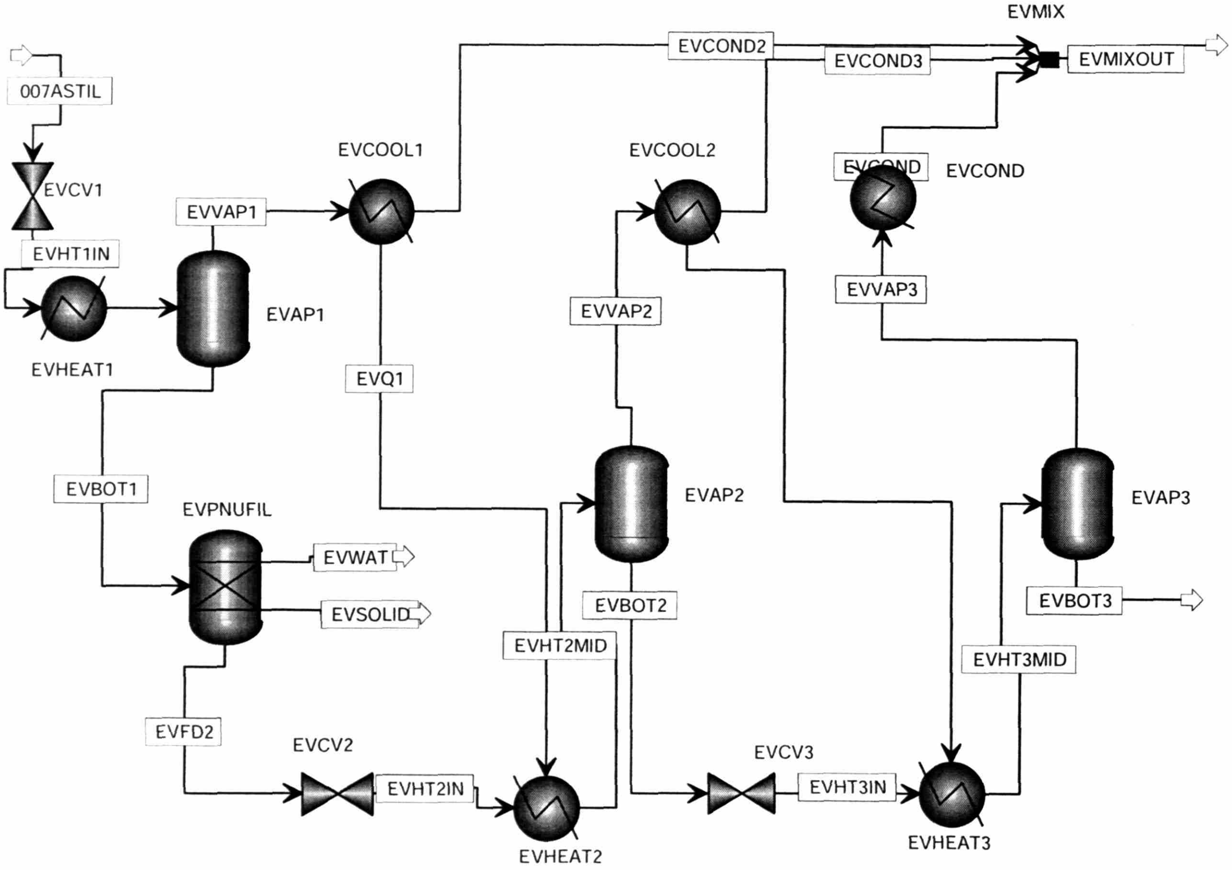


Figure A.4 Evaporators section

The second effect is modeled similarly to the first effect with a control valve, EVCV2, a heat exchanger, EVCOOL1/EVHEAT2, and a flash drum, EVAP2. The slurry from the pneumatic filter is flashed in the control valve to 0.31 atm. Then, the vapor from the first effect is condensed, EVCOOL1, and the heat generated is applied to the flashed slurry stream, EVHEAT2. The vapor and liquid from this stream is separated in the next flash drum, EVAP2, with the liquid being sent to the third effect, while the vapor provides the heat to that effect. The third effect is modeled exactly the same with the pressure being dropped down further to 0.21 atm. The condensed vapors from the three effects are used as process condensate streams, while the final slurry from the third effect is combined with the solids from the pneumatic filter for the combustor.

A.5 Economic cost model

The process simulation described above determines the material and energy balances for the corn stover to ethanol facility as shown in Table A.7 - Table A.10. Using these streams and unit operation calculations from the process simulation, economic costs can be calculated. The first step is to calculate the capital costs of the primary equipment for the process. The equipment is divided into five categories – heat exchangers, pumps, tanks, towers, and others. As the Aspen simulation is a simplified model, the economic model is simplified as well. All of the equipment from the original NREL report with capital costs over $100,000 are included in the simplified assessment and an additional 5% is added at the end to make up for the smaller pieces of equipment which is left out.

A.5.1 Heat exchangers

For each exchanger, the temperatures and heat duties from the material and energy balances are used to determine the size of exchanger required based on the following equation.

$$Area = \frac{\dot{Q}}{U\Delta T} \tag{A.2}$$

where the log mean temperature difference is used for ΔT.

$$LMTD = \frac{(T_{Hin} - T_{Cout}) - (T_{Hout} - T_{Cin})}{\ln\left(\dfrac{T_{Hin} - T_{Cout}}{T_{Hout} - T_{Cin}}\right)} \tag{A.3}$$

For utilities, Table A.6 provides the stream conditions of the steam and cooling water.

Utilities	LP Steam	MP Steam	HP Steam	CW
Inlet Temp (°C)	115	164	268	25
Outlet Temp (°C)	115	148	192.0	35
Pressure (atm)	1.7	4.4	13	

Table A.6 Utility temperatures and pressures

Once an area is defined, other parameters such as number of exchangers and spares, type of exchanger, and materials of construction are used to determine a capital cost associated with the heat exchanger. A number of equipment costing resources are available. For this work, Capcost (Turton, 2003) was chosen, although the costs from the original NREL study were used for specialized equipment, such as the evaporators. Table A.11 shows the spreadsheet used for the heat exchanger calculations.

A.5.2 Pumps

Most of the pumps in the ethanol facility were left out of the capital costing model, as they are less expensive and fall under thee $100,000 level. The only exceptions are the large slurry pumps which are used to move the biomass through the saccharification and fermentation reactors and recirculation and through the evaporator system. The parameters required from the simulation to size the pumps were volumetric flow, pressure increase, and density, while the type, number of pumps and spares, and materials of construction were once again required for the cost. The following equation was used to calculate the power required.

$$\dot{w} = \rho \dot{V} \Delta P \tag{A.4}$$

Again, Capcost was used to calculate the equipment cost of the pumps, and Table A.12 shows the calculations used for the costing.

A.5.3 Tanks

This section includes all flash drums and the saccharification and fermentation reactors. The pretreatment reactor is a specialized piece of equipment, and it is described in the section on other equipment and packages. The primary sizing parameter for the tanks is volume which is a function of volumetric flow and residence time.

$$V = \tau \dot{V} \tag{A.5}$$

The volume can further be used to determine the height and diameter of the flash drums, where the ideal length to diameter ratio is 4, and therefore the diameter can be found using

$$D = \left(\frac{V}{\pi} \right)^{1/3} \tag{A.6}$$

For equipment costing, the NREL fermentation and saccharification tanks were used as the basis for this analysis, whereas Capcost was used for the other holding tanks and flash drums. Table A.13 gives the calculations used for the costing in the base case.

A.5.4 Towers

The distillation towers are sized based on height and diameter. The heights of the towers are specified in the design, based on the standard distance between trays or the standard packed stage, plus an additional four meters for the tower heads. The diameters are more complicated and depend on the vapor flow through the tower. This information is not derived from the material and energy balances, but instead relies on the detailed vapor liquid equilibrium calculations within the unit operation. Fortunately, Aspen calculates the required diameter for each sieve tray and the maximum value is given to the user for the overall tower diameter. A typical equation for the sizing of theses diameters is as follows:

$$D = \left(\frac{4\dot{V}}{C\left(\frac{\rho_L - \rho_V}{\rho_V} \right)^{0.5} \pi \rho_V} \right)^{0.5} \tag{A.7}$$

where C is an empirical capacity factor based on flooding, surface tension, and foaming (Henley, 1981). Using the diameter, height, and materials of construction data, Capcost is used to determine an overall equipment cost. Table A.14 shows the calculations for the tower costs.

A.5.5 Other equipment costs

A number of the equipment in the process design are more unique and require specific costing. The most prominent in the overall cost is the pretreatment reactor. Because the pretreatment used in this process design is based on dilute acid, the conditions are very acidic and very high temperature. The materials of construction are therefore very severe, with Hastelloy steal being required. For this equipment, the base cost assumed in the NREL report is scaled with a factor or 0.6 from NREL based on total flow through the reactor. Other specific equipment which are costed in a similar fashion are the pneumatic filters and the molecular sieve.

Additionally, sections such as the feedstock handling and utilities are not modeled by Aspen, but need to be included in the overall process design. The capital cost for these generic sections are also based on the original NREL report. Using the overall flow rates through the system, they can be scaled up or down to determine the package cost. The total capital costs of the installed equipment for each section and for the total facility is given in Table A.16.

A.5.6 Combustor and turbogenerator

Another specific subsystem which contributes significantly to the overall installed equipment cost is the combustor and turbogenerator for converting the residue into heat and power. As was mentioned in the process description, a spreadsheet model based on an NREL design is used for the calculation of the operations of this system and the overall capital costs. The feed to the combustor is the combined solids from the evaporator filter and third effect. The biomass is used to generate superheated high pressure steam at 510°C and 86 atm. This steam is then used in a multistage turbine and generator. At each stage, power is produced, steam is withdrawn for the process and for recycle, and the pressure is knocked down for the next stage. Table A.17 shows the calculations for the steam and power flows. For each stage, the specific steam requirements for the process and for turbine recycle is given. The remaining steam for each stage is used for power generation. The values for power generated and recycle fraction at each stage are from the NREL design basis. The overall power generated is used to supply electricity to the plant which is estimated to be 0.5 kWh/kg of ethanol production. The biomass flow rate into the subprocess is used to scale for capital costs.

A.5.7 Total capital costs

Once the overall installed capital costs are determined, the other factors, such as site costs, startup costs, contingencies and fees which were described in Chapter 3 can be added. Table A.15 shows these calculations along with the percentages describing how they were arrived at. As the table shows, the overall project investment for the corn stover to ethanol facility is estimated at $199.3 million. For consistency, this value is checked against the original NREL report which. The overall project investment for their process design is $197.4 million so this economic analysis is within 1% of their analysis.

A.6 Operating costs

The material and energy balances are used to calculate the costs associated with raw materials, waste streams, and co-product credits. For fixed costs, the NREL report estimates the number of employees required for management, administration, engineers, technicians, and maintenance. Additionally, costs for overhead, maintenance, taxes, and insurance are included as percentages of other calculated values. The results of these calculations are given in Table A.18.

A.7 Total annualized cost per gallon of ethanol

The calculations from above for capital costs and operating costs are summarized in Table A.19. The capital costs are annualized using a capital charge factor of 0.176. The resulting price per gallon of ethanol production is $1.08. The cost model for the NREL report gives a production cost of $1.07, so once again, the simplified model is consistent with the original model

A.8 Aspen simulation model interaction with Excel economic model

A primary objective of the simplified model is the capability to modify aspects of the simulation, either process design changes or potential improvements in process parameters, to see the economic impacts of those changes. These changes include simple changes to the cost model to represent improvements in raw material production, but more importantly, changes to parameters such as reaction yield or solids content percentages. Some of these changes require the running of the process simulation multiple times. Due to this requirement, a quick Visual Basic code was introduced to enable the automation of the Aspen simulation with subsequent updating of the economic model. The code for this follows:

```
Sub Macro1()
'
'
'  Call out primary variables
   Dim go_Simulation As HappLS
   Set go_Simulation = GetObject("filename.bkp")
   Dim ihTable As IHNode
   Dim ihBlock As IHNode
   Dim NDim As Integer
   Dim NPoints As Integer
   Dim SimStatus As Integer

'  Open simulation
   go_Simulation.SuppressDialogs = 1 ' disable the confirmation dialog
   Call go_Simulation.Engine.Reinit(IAP_REINIT_SIMULATION)
   go_Simulation.SuppressDialogs = 0 ' restore the ability to display confirmation dialogs

   For k = 0 To 10

      go_Simulation.Visible = True
```

```
    go_Simulation.Engine.Reinit

' Retrieve data from Excel spreadsheet and insert into Aspen simulation
    go_Simulation.Tree.Data.Streams.Elements("001BMASS").Input.TOTFLOW.CISOLID.Value = _
      Range("Feed").Offset(k, 0).Value

    go_Simulation.Tree.Data.Elements("Flowsheeting Options").Elements("Design-Spec"). _
      SACCONC.Input.EXPR2.Value = Range("SacConc").Offset(k, 0).Value

' Run simulation
    On Error GoTo 2
    go_Simulation.Engine.Run

' Check for errors
    SimStatus = go_Simulation.Tree.Data.AttributeValue(HAP_COMPSTATUS)
    Range("Status").Offset(k, 0).Value = SimStatus
    go_Simulation.Visible = False

' Copy entire stream table from Aspen into Excel
    Range("StreamTable").ClearContents
    Set ihTable = go_Simulation.Tree.Data.Elements("Results Summary"). _
      Elements("Stream-Sum").Elements("Stream-Sum").Table
    Set ihBlock = go_Simulation.Tree.Data.Blocks

    NDim = ihTable.Elements.RowCount(0)
    NPoints = ihTable.Elements.RowCount(1)

    For j = 0 To NPoints - 1
      For i = 0 To NDim - 1
        If ihTable.Elements.Item(i, j).Value <> 0 Then Range("Start2"). _
          Offset(i, j).Value = ihTable.Elements.Item(i, j).Value
```

```
            Next i
        Next j

'   Copy specific data from Aspen into Excel, primarily for heat exhanger and column sizing
        Range("BeerReb").Value = ihBlock.BEERCOL.Output.DUTY.Elements("32").Value
        Range("RectCond").Value = ihBlock.RECTIFY.Output.DUTY.Elements("1").Value
        Range("RectReb").Value = ihBlock.RECTIFY.Output.DUTY.Elements("60").Value
        Range("RectDrum").Value = ihBlock.RECTIFY.Output.HYD_LVF.Elements("1").Value
        Range("BeerDiam").Value = ihBlock.BEERCOL.Output.DIAM4.Elements("1").Value
        Range("RectTop").Value = ihBlock.RECTIFY.Output.DIAM4.Elements("1").Value
        Range("RectBot").Value = ihBlock.RECTIFY.Output.DIAM4.Elements("2").Value
        Range("ScrubDiam").Value = ihBlock.SCRUBBER.Output.DIAM2.Elements("1").Value
        Range("Results").copy
        Range("SacConc").Offset(k, 4).PasteSpecial Paste:=xlValues, Operation:=xlNone, _
            SkipBlanks:=False, Transpose:=False
        Set ihTable = Nothing
        Set ihBlock = Nothing

        GoTo 1

2         go_Simulation.SuppressDialogs = 1 ' disable the confirmation dialog
        Call go_Simulation.Engine.Reinit(IAP_REINIT_SIMULATION)
        go_Simulation.SuppressDialogs = 0 ' restore the ability to display confirmation dialogs

1    Next k
    Set go_Simulation = Nothing

End Sub
```

	001A	001B	001BMASS	002AVAP	002BLIQ	002DHYD	002EHYD	002FMIX	002GWW	002HYDRL	003AGLUC	003GLUC	004ABEER	004BBEER	004BEER	004CBEER	004DBEER
TO:	M202HI	M202HI	M202LO	BEERHX	DETOXHX	HYDHEAT	SACCHAR	WWHX		T203	FERMENT	SACCOOL	BEERPUMP	BEERHX	FERMVENT	FDBOTHX	BEERCOL
Substream: MIXED FROM:	M202LO	M202MIX		T203	T203	DETOXMIX	HYDHEAT	BEERHX	WWHX	M202HI	SACCOOL	SACCHAR	FERMVENT	BEERPUMP	FERMENT	BEERHX	FDBOTHX
Mass Flow kg/hr	LIQUID	LIQUID	LIQUID	VAPOR	LIQUID	LIQUID	LIQUID	MIXED	LIQUID	LIQUID	LIQUID	LIQUID	LIQUID	LIQUID	MIXED	LIQUID	LIQUID
GLUCOSE	0	0	0	0	5240.702	5730.106	5730.106	0	0	5240.702	34582.67	34582.67	1414.431	1414.431	1414.431	1414.431	1.41E+03
XYLOSE	0	0	0	4.88E-07	2.13E+04	21721.02	21721.02	4.88E-07	4.88E-07	2.13E+04	21721.02	21721.02	1585.635	1585.635	1585.635	1585.635	1.59E+03
SOLSLDS	7505.56	0	7505.56	0	7505.56	9526.02	9526.02	0	0	7505.56	9526.02	9526.02	9526.02	9526.02	9526.02	9526.02	9.53E+03
ACETATE	0	0	0.00E+00	0	0	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
H2O	56768.24	9.65E+04	14700.24	52291.93	1.35E+05	3.36E+05	3.36E+05	5.23E+04	5.23E+04	1.88E+05	3.33E+05	3.33E+05	3.73E+05	3.73E+05	3.33E+05	3.73E+05	3.73E+05
FURFURAL	0	0	0	384.7624	372.8188	371.0777	371.0777	384.7624	384.7624	757.5812	371.0777	371.0777	371.4612	371.4612	371.0777	371.4612	3.71E+02
HMF	0	0	0	39.17842	58.04403	57.77296	57.77296	39.17842	39.17842	97.22245	57.77296	57.77296	57.80189	57.80189	57.77296	57.80189	5.78E+01
H2SO4	0	2090.094	0	0.0863463	2090.008	137.9405	137.9405	0.0863463	0.0863463	2090.094	137.9405	137.9405	137.9405	137.9405	137.9405	137.9405	137.9405
CO2	0	0	0	0	0	0	0	0	0	0	0	0	403.898	403.898	23696.23	403.898	403.898
LACID	0	0	0	0	0	0	0	0	0	0	0	0	1689.112	1689.112	1689.111	1689.112	1.69E+03
AACID	321.5911	738.6884	0	283.3589	3276.91	4700.464	4700.464	283.3589	283.3589	3560.268	4700.464	4700.464	7814.315	7814.315	7813.759	7814.315	7.81E+03
Total Flow kmol/hr	3609.041	5387.796	1268.557	2911.678	8214.868	19474.52	19474.52	2911.678	2911.678	11126.55	1.95E+04	19474.52	22009.71	22009.71	20303.75	22009.71	22009.71
Total Flow kg/hr	64595.39	9.93E+04	22205.8	52999.32	1.75E+05	3.78E+05	3.78E+05	5.30E+04	5.30E+04	2.28E+05	4.04E+05	4.04E+05	4.21E+05	4.21E+05	4.04E+05	4.21E+05	4.21E+05
Total Flow l/min	1561.96	1743.528	605.1948	1.47E+06	3351.445	6853.709	6926.516	3.37E+05	8.92E+02	4797.013	7008.094	7169.098	7763.53	7764.65	2.59E+05	8.21E+03	8.26E+03
Temperature C	130	73.75516	45	102.5	102.5	54.23538	65	99.96675	30	190	41	65	41	41.14677	41	95	100
Pressure atm	4	3	1	1	1	1	1	1	1	12.05	1	1	0.9	5	1	5	5
Vapor Frac	0	0	0	1	0.00E+00	0	0	0.2299547	0	0	0	0	0	0	0.0288827	0.00E+00	0
Liquid Frac	1	1	1	0	1.00E+00	1	1	0.7700453	1	1	1	1	1	1	0.9711173	1	1
Solid Frac	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Enthalpy cal/mol	-59531.4	-67960.07	-48048.92	-57238.42	-68417.79	-67984.74	-67796.07	-64769.1	-68182.55	-6.61E+04	-7.01E+04	-6.97E+04	-66939.4	-66936.87	-67501.12	-65957.28	-65861.89
Enthalpy kcal/kg	-3326.108	-3687.884	-2744.904	-3144.566	-3208.654	-3502.171	-3492.452	-3558.286	-3745.814	-3221.159	-3379.801	-3359.469	-3498.339	-3498.207	-3392.307	-3447.012	-3442.027
Enthalpy MMkcal/hr	-214.8543	-3.66E+02	-6.10E+01	-166.6622	-562.0512	-1.32E+03	-1.32E+03	-1.89E+02	-1.99E+02	-7.35E+02	-1365.493	-1.36E+03	-1.47E+03	-1.47E+03	-1.37E+03	-1.45E+03	-1.45E+03
Entropy cal/mol-K	-25.54403	-36.38483	-2.961503	-8.926879	-44.26983	-39.99461	-39.61429	-29.10548	-38.60768	-38.64097	-41.51334	-40.75009	-36.54269	-36.53678	-35.31062	-34.33811	-34.13836
Entropy kcal/kg-K	-1.427183	-1.97444	-0.1691826	-0.4904251	-2.076164	-2.060285	-2.040694	-1.598997	-2.12103	-1.884348	-2.00107	-1.964279	-1.909768	-1.909459	-1.774555	-1.794554	-1.784114
Density mol/cc	0.0385097	0.0515028	0.0349352	3.29E-05	0.0408523	0.0473576	0.0468598	1.44E-04	5.44E-02	0.0386579	0.0463143	0.0452742	0.0472502	0.0472434	1.31E-03	4.47E-02	4.44E-02
Density gm/cc	0.6892557	0.9490904	0.611533	5.99E-04	0.8710908	0.9193142	0.9096509	2.62E-03	9.90E-01	0.7927297	0.9608178	0.9392397	0.904115	0.9039847	0.0259993	0.854575	8.50E-01
Average MW	17.89822	18.42793	17.50477	18.20233	21.32289	19.41217	19.41217	18.20233	18.20233	20.50628	20.74557	20.74557	19.13462	19.13462	19.8983	19.13462	19.13462
Liq Vol 60F l/min	1077.184	1641.583	369.5553	883.7302	2825.056	6225.191	6225.191	883.7302	883.7302	3708.787	6688.036	6688.036	7123.74	7123.74	6919.891	7123.74	7123.74
Substream: $TOTAL																	
Total Flow kg/hr	1.40E+05	9.93E+04	98038.8	52999.32	2.24E+05	4.27E+05	4.27E+05	5.30E+04	5.30E+04	2.77E+05	4.27E+05	4.27E+05	4.44E+05	4.44E+05	4.27E+05	4.44E+05	4.44E+05
Enthalpy MMkcal/hr	-350.1647	-366.1602	-198.4075	-166.6622	-659.9929	-1422.27	-1418.437	-188.5895	-198.5285	-831.2952	-1426.734	-1418.362	-1534.579	-1534.522	-1431.787	-1512.595	-1510.459
Substream: CISOLID																	
Mass Flow kg/hr																	
CELLULOS	30833.2	0	30833.2	0	28366.54	28225.42	28225.42	0	0	28366.54	2258.033	2258.033	2258.033	2258.033	2258.033	2258.033	2258.033
XYLAN	17499.92	0	17499.92	0	874.9962	870.643	870.643	0	0	874.9962	870.643	870.643	870.643	870.643	870.643	870.643	870.643
LIGNIN	14999.93	0	14999.93	0	14999.93	14925.31	14925.31	0	0	14999.93	14925.31	14925.31	14925.31	14925.31	14925.31	14925.31	14925.31
GYPSUM	0	0	0	0	0	27.22346	27.22346	0	0	0	27.22346	27.22346	27.22346	27.22346	27.22346	27.22346	27.22346
ACETATE	2499.989	0	2499.989	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C5SOLID	3333.319	0	3333.319	0	166.6659	165.8368	165.8368	0	0	166.6659	165.8368	165.8368	165.8368	165.8368	165.8368	165.8368	165.8368
C6SOLID	2499.989	0	2499.989	0	124.9995	124.3776	124.3776	0	0	124.9995	124.3776	124.3776	124.3776	124.3776	124.3776	124.3776	124.3776
CAH2O2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ASH	4166.648	0	4166.648	0	4166.648	4145.919	4145.919	0	0	4166.648	4145.919	4145.919	4145.919	4145.919	4145.919	4145.919	4145.919
Total Flow kmol/hr	576.0243	0	576.0243	0	354.7294	353.1228	353.1228	0	0	354.7294	192.9711	192.9711	192.9711	192.9711	192.9711	192.9711	192.9711
Total Flow kg/hr	75833	0	75833	0	48699.79	48484.73	48484.73	0	0	48699.79	22517.34	22517.34	22517.34	22517.34	22517.34	22517.34	22517.34
Total Flow l/min	660.019	0	660.019	0	364.3142	362.6985	362.6985	0	0	364.3142	79.76384	79.76384	79.76384	79.76384	79.76384	79.76384	79.76384
Temperature C	130		45		102.5	54.23538	65			190	41	65	41	41.14677	41	95	100
Pressure atm	4	3	1	1	1	1	1	1	1	12.05	1	1	0.9	5	1	5	5
Vapor Frac	0		0		0	0	0			0	0	0	0	0	0	0	0
Liquid Frac	0		0		0	0	0			0	0	0	0	0	0	0	0
Solid Frac	1		1		1	1	1			1	1	1	1	1	1	1	1
Enthalpy cal/mol	-2.35E+05		-2.39E+05		-2.76E+05	-2.78E+05	-2.78E+05			-2.72E+05	-3.17E+05	-3.17E+05	-3.17E+05	-3.17E+05	-3.17E+05	-3.15E+05	-3.15E+05
Enthalpy kcal/kg	-1784.295		-1812.56		-2011.105	-2027.024	-2023.741			-1978.048	-2719.695	-2712.681	-2719.695	-2719.653	-2719.695	-2703.375	-2701.766
Enthalpy MMkcal/hr	-135.3104		-137.4538		-97.94178	-98.2811	-98.12193			-96.33188	-61.24119	-61.08325	-61.24119	-61.24025	-61.24119	-60.8737	-60.83746
Entropy cal/mol-K	-724.3837		-734.7028		-823.779	-829.5276	-828.173			-812.9554	-875.9132	-873.4035	-875.9132	-875.8977	-875.9132	-870.3281	-869.8215
Entropy kcal/kg-K	-5.502389		-5.580772		-6.00041	-6.041595	-6.031729			-5.92157	-7.506475	-7.484968	-7.506475	-7.506343	-7.506475	-7.458612	-7.454271
Density mol/cc	0.0145456		0.0145456		0.0162281	0.0162266	0.0162266			0.0162281	0.0403213	0.0403213	0.0403213	0.0403213	0.0403213	0.0403213	0.0403213
Density gm/cc	1.91492		1.91492		2.227921	2.227963	2.227963			2.227921	4.705002	4.705002	4.705002	4.705002	4.705002	4.705002	4.705002
Average MW	131.649		131.649		137.2871	137.3028	137.3028			137.2871	116.6877	116.6877	116.6877	116.6877	116.6877	116.6877	116.6877

Table A.7 Material and energy balance A

	EVBOT1	EVBOT2	EVBOT3	EVCOND	EVCOND2	EVCOND3	EVFD2	EVHT1IN	EVHT1MID	EVHT2IN	EVHT2MID	EVHT3IN	EVHT3MID	EVMIXOUT	EVSOLID	EVVAP1	EVVAP2	EVVAP3	EVWAT
TO:	EVPNUFIL	EVCV3		EVMIX	EVMIX	EVMIX	EVCV2	EVHEAT1	EVAP1	EVHEAT2	EVAP2	EVHEAT3	EVAP3			EVCOOL1	EVCOOL2	EVCOND	
Substream: MIXED FROM:	EVAP1	EVAP2	EVAP3	EVCOND	EVCOOL1	EVCOOL2	EVPNUFIL	EVCV1	EVHEAT1	EVCV2	EVHEAT2	EVCV3	EVHEAT3	EVMIX	EVPNUFIL	EVAP1	EVAP2	EVAP3	EVPNUFIL
Mass Flow kg/hr	LIQUID	LIQUID	LIQUID	LIQUID	LIQUID	LIQUID	LIQUID	MIXED	MIXED	MIXED	MIXED	MIXED	MIXED	LIQUID	LIQUID	VAPOR	VAPOR	VAPOR	LIQUID
GLUCOSE	1414.431	975.9575	975.9575	0	0	0	975.9575	1414.431	1414.431	975.9575	975.9575	975.9575	975.9575	0	113.1545	0	0	0	325.3192
XYLOSE	1585.635	1094.088	1094.088	4.70E-09	5.58E-09	1.82E-09	1094.088	1585.635	1585.635	1094.088	1094.088	1094.088	1094.088	1.21E-08	126.8508	5.58E-09	1.82E-09	4.70E-09	3.65E+02
SOLSLDS	*9526.02*	*6572.954*	*6572.954*	0	0	0	6572.954	9526.02	9526.02	6572.954	6572.954	6572.954	6572.954	0	762.0816	0	0	0	2190.985
ACETATE	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H2O	2.60E+05	1.02E+05	23992.62	78116.98	73390.24	77481.67	1.80E+05	3.34E+05	3.34E+05	1.80E+05	1.80E+05	1.02E+05	1.02E+05	2.29E+05	20822.18	73390.24	77481.67	78116.98	59863.76
FURFURAL	104.0975	21.98698	6.152395	15.83459	118.6968	49.84028	71.82726	222.7943	222.7943	71.82726	71.82726	21.98698	21.98698	184.3717	8.327798	118.6968	49.84028	15.83459	23.94242
HMF	25.35906	7.184965	2.59597	4.588995	18.3218	10.31279	17.49775	43.68087	43.68087	17.49775	17.49775	7.184965	7.184965	33.22359	2.028725	18.3218	10.31279	4.588995	5.832585
H2SO4	137.9361	95.1739	95.16675	7.15E-03	2.19E-03	2.04E-03	95.17594	137.9383	137.9383	95.17594	95.17594	95.1739	95.1739	1.14E-02	11.03489	2.19E-03	2.04E-03	7.15E-03	3.17E+01
CO2	0	0	0	0	0	0	0	0.00E+00	0.00E+00	0	0	0	0	0	0	0	0	0	0
LACID	1686.693	1162.415	1157.392	5.022735	1.355692	1.402966	1163.818	1688.048	1688.048	1163.818	1163.818	1162.415	1162.415	7.781393	134.9354	1.355692	1.402966	5.022735	387.9393
AACID	*6377.398*	*3046.586*	*1042.16*	*2004.426*	1023.54	1353.819	4400.405	7400.938	7400.938	4400.405	4400.405	3046.586	3046.586	4381.784	510.1919	1023.54	1353.819	2004.426	1466.802
Total Flow kmol/hr	15168.97	6141.95	1772.094	4369.856	4095.119	4324.637	10466.59	19264.08	19264.08	10466.59	10466.59	6141.95	6141.95	12789.61	1213.517	4095.119	4324.637	4369.856	3488.862
Total Flow kg/hr	2.81E+05	1.15E+05	34939.23	80150.07	74685.83	78924.25	1.94E+05	3.56E+05	3.56E+05	1.94E+05	1.94E+05	1.15E+05	1.15E+05	2.34E+05	22494.32	74685.83	78924.25	80150.07	64671.18
Total Flow l/min	5528.247	2341.252	838.7295	1387.724	1336.398	1387.882	3812.84	9.61E+05	3.37E+06	4.53E+05	6.59E+06	2.05E+05	9.70E+06	4.11E+03	442.2597	3.37E+06	6.58E+06	9.70E+06	1.27E+03
Temperature C	*87.41636*	71.91218	67.60587	55	86.08517	70.15871	87	87.21447	87.41636	71.2091	71.91218	63.07641	67.60595	70.25416	87.41636	87.41636	71.91218	67.60587	87.41636
Pressure atm	0.6	0.31	0.21	0.21	0.6	0.31	3.2	0.6	0.6	0.31	0.31	0.21	0.21	2	0.6	0.6	0.31	0.21	0.6
Vapor Frac	0	0	0	0	0	0	0	0.060315	0.2125798	0.0282891	0.4131851	0.0150672	0.7114802	0	0.00E+00	1	1	1	0.00E+00
Liquid Frac	1	1	1	1	1	1	1	0.939685	0.7874202	0.9717109	0.5868149	0.9849328	0.2885198	1	1	0	0	0	1
Solid Frac	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	0	0	0	0	0	0
Enthalpy cal/mol	-65704.4	-64822.93	-57712.35	-68034.61	-67319.63	-67662.5	-65712	-65451.23	-63945.86	-65711.83	-61843.26	-64822.74	-57745.76	-67679.86	-65704.4	-57432.04	-57611.46	-57759.36	-65704.4
Enthalpy kcal/kg	-3544.602	-3459.393	-2927.131	-3709.31	-3691.221	-3707.552	-3545.012	-3543.081	-3461.59	-3545.003	-3336.302	-3459.384	-3081.708	-3702.937	-3544.602	-3149.072	-3156.807	-3149.094	-3544.602
Enthalpy MMkcal/hr	-9.97E+02	-3.98E+02	-102.2732	-297.3057	-275.6858	-292.6199	-687.7903	-1260.876	-1231.876	-687.7885	-647.2971	-398.1437	-354.6767	-865.6115	-79.73456	-235.1944	-249.1522	-252.4037	-229.2369
Entropy cal/mol-K	-33.15186	-31.84978	-20.98198	-37.30186	-35.6654	-36.48435	-33.16625	-32.0122	-27.83855	-32.88248	-21.67012	-31.57892	-10.74854	-36.4885	-33.15186	-8.157437	-7.212733	-6.598737	-33.15186
Entropy kcal/kg-K	-1.788467	-1.699722	-1.064192	-2.033732	-1.955579	-1.999152	-1.789243	-1.732921	-1.506988	-1.773935	-1.169054	-1.685266	-0.5736154	-1.996379	-1.788467	-0.4472826	-0.3952201	-0.3597693	-1.788467
Density mol/cc	0.0457317	0.0437226	0.0352138	0.0524822	0.0510715	0.0519333	0.0457514	3.34E-04	9.52E-05	3.85E-04	2.65E-05	5.00E-04	1.06E-05	5.18E-02	0.0457317	2.03E-05	1.09E-05	7.51E-06	4.57E-02
Density gm/cc	0.8477041	0.819286	0.6942888	0.9626081	0.9314319	0.9477783	0.8480711	6.17E-03	1.76E-03	7.13E-03	4.91E-04	9.36E-03	1.98E-04	9.48E-01	0.8477041	3.70E-04	2.00E-04	1.38E-04	8.48E-01
Average MW	*18.53647*	*18.73823*	*19.71635*	*18.34158*	*18.23777*	*18.24991*	*18.53647*	*18.47297*	*18.47297*	*18.53647*	*18.53647*	*18.73823*	*18.73823*	*18.27735*	*18.53647*	*18.23777*	*18.24991*	*18.34158*	*18.53647*
Liq Vol 60F l/min	4678.021	1910.906	573.9719	1336.934	1246.646	1316.928	3227.835	5924.667	5924.667	3227.835	3227.835	1910.906	1910.906	3900.509	374.2417	1246.646	1316.928	1336.934	1075.945
Substream: $TOTAL																			
Total Flow kg/hr	3.04E+05	1.15E+05	35276.99	80150.07	74685.83	78924.25	1.94E+05	3.78E+05	3.78E+05	1.94E+05	1.94E+05	1.15E+05	1.15E+05	2.34E+05	4.46E+04	74685.83	78924.25	80150.07	64783.77
Enthalpy MMkcal/hr	-1.06E+03	-3.99E+02	-103.1891	-297.3057	-275.6858	-292.6199	-688.7042	-1321.805	-1292.804	-688.7041	-648.2126	-399.0602	-355.5927	-865.6115	-139.444	-235.1944	-249.1522	-252.4037	-229.5415
Substream: CISOLID																			
Mass Flow kg/hr																			
CELLULOS	2258.033	33.8705	33.8705	0	0	0	33.8705	2258.033	2258.033	33.8705	33.8705	33.8705	33.8705	0	2212.873	0	0	0	11.29017
XYLAN	870.643	13.05965	13.05965	0	0	*0*	13.05965	*870.643*	*870.643*	13.05965	13.05965	13.05965	13.05965	*0*	853.2302	0	*0*	0	4.353215
LIGNIN	14925.31	223.8796	223.8796	0	0	0	223.8796	14925.31	14925.31	223.8796	223.8796	223.8796	223.8796	0	14626.8	0	0	0	74.62655
GYPSUM	27.22346	0.4083519	0.4083519	0	0	0	0.4083519	27.22346	27.22346	0.4083519	0.4083519	0.4083519	0.4083519	0	26.67899	0	0	0	0.1361173
ACETATE	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C5SOLID	165.8368	2.487552	2.487552	0	0	0	2.487552	165.8368	165.8368	2.487552	2.487552	2.487552	2.487552	0	162.52	0	0	0	0.8291839
C6SOLID	124.3776	1.865664	1.865664	0	0	0	1.865664	124.3776	124.3776	1.865664	1.865664	1.865664	1.865664	0	121.89	0	0	0	0.6218879
CAH2O2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ASH	4145.919	62.18879	62.18879	0	0	0	62.18879	4145.919	4145.919	62.18879	62.18879	62.18879	62.18879	0	4063.001	0	0	0	20.7296
Total Flow kmol/hr	192.9711	2.894566	2.894566	0	0	*0*	*2.894566*	192.9711	192.9711	2.894566	2.894566	2.894566	2.894566	*0*	*189.1116*	*0*	*0*	*0*	*0.9648553*
Total Flow kg/hr	22517.34	337.7601	337.7601	0	0	0	337.7601	22517.34	22517.34	337.7601	337.7601	337.7601	337.7601	0	22067	0	0	0	112.5867
Total Flow l/min	79.76384	1.196458	1.196458	0	0	0	1.196458	79.76384	79.76384	1.196458	1.196458	1.196458	1.196458	0	78.16856	0	0	0	0.3988192
Temperature C	87.41636	71.91218	67.60587				87	87.21447	87.41636	71.2091	71.91218	63.07641	67.60595		87.41636				87.41636
Pressure atm	0.6	0.31	0.21	0.21	0.6	0.31	3.2	0.6	0.6	0.31	0.31	0.21	0.21	2	0.6	0.6	0.31	0.21	0.6
Vapor Frac	0	0	0				0	0	0	0	0	0	0		0				0
Liquid Frac	0	0	0				0	0	0	0	0	0	0		0				0
Solid Frac	1	1	1				1	1	1	1	1	1	1		1				1
Enthalpy cal/mol	-3.16E+05	-3.16E+05	-3.16E+05				-3.16E+05	-3.16E+05	-3.16E+05	-3.16E+05	-3.16E+05	-3.17E+05	-3.16E+05		-3.16E+05				-3.16E+05
Enthalpy kcal/kg	-2705.784	-2710.59	-2711.897				-2705.915	-2705.848	-2705.784	-2710.804	-2710.59	-2713.258	-2711.897		-2705.784				-2705.784
Enthalpy MMkcal/hr	-60.92795	-0.9155425	-0.9159838				-0.9139635	-60.92938	-60.92794	-0.9156148	-0.9155425	-0.9164434	-0.9159838		-59.70939				-0.3046397
Entropy cal/mol-K	-871.0996	-872.6892	-873.1338				-871.1421	-871.1202	-871.0996	-872.7617	-872.6892	-873.6029	-873.1338		-871.0996				-871.0996
Entropy kcal/kg-K	-7.465224	-7.478846	-7.482656				-7.465588	-7.4654	-7.465224	-7.479468	-7.478846	-7.486677	-7.482656		-7.465224				-7.465224
Density mol/cc	0.0403213	0.0403213	0.0403213				0.0403213	0.0403213	0.0403213	0.0403213	0.0403213	0.0403213	0.0403213		0.0403213				0.0403213
Density gm/cc	4.705002	4.705002	4.705002				4.705002	4.705002	4.705002	4.705002	4.705002	4.705002	4.705002		4.705002				4.705002
Average MW	116.6877	116.6877	116.6877				116.6877	116.6877	116.6877	116.6877	116.6877	116.6877	116.6877		116.6877				116.6877

Table A.8 Material and energy balance B

	005ACO2	005BCO2	005CCO2	005CO2	005DWAT	006ETWAT	007ASTIL	007STILL	008AZTRP	009WATER	010ETREC	011AETOH	011BETOH	011CETOH	011DETOH	011EETOH	011ETOH
TO:	MIXCO2	SCRUBBER		MIXCO2	FERMVENT	RECTIFY	EVCV1	FDBOTHX	MOLSHEAT		RECTIFY	MOLSIEVE	MOLSCOOL	MOLSIVHX	MOLSPUMP	MOLSIVHX	
Substream: MIXED FROM:	BEERCOL	MIXCO2	SCRUBBER	FERMVENT	SCRUBBER	BEERCOL	FDBOTHX	BEERCOL	RECTIFY	RECTIFY	MOLSIVHX	MOLSHEAT	MOLSIEVE	MOLSIEVE	MOLSCOOL	MOLSPUMP	ETOHCOOL
Mass Flow kg/hr	VAPOR	MIXED	VAPOR	VAPOR	LIQUID	VAPOR	LIQUID	LIQUID	VAPOR	LIQUID	LIQUID	VAPOR	VAPOR	VAPOR	LIQUID	LIQUID	LIQUID
GLUCOSE	7.00E-17	7.00E-17	0.00E+00	0.00E+00	0.00E+00	1.27E-13	1.41E+03	1.41E+03	0	0	0	0	0	0	0	0	0
XYLOSE	1.74E-11	1.74E-11	0.00E+00	0.00E+00	0.00E+00	2.79E-08	1.59E+03	1.59E+03	2.22E-26	2.79E-08	0.00E+00	2.22E-26	0.00E+00	0.00E+00	0	0	0
SOLSLDS	4.71E-16	4.71E-16	0.00E+00	0.00E+00	0.00E+00	8.54E-13	9.53E+03	9.53E+03	0	0	0	0	0	0	0	0	0
ACETATE	0	0	0	0	0	0	0.00E+00	0	0	0	0	0	0	0	0	0	0
H2O	1.04E+02	9.69E+02	4.31E+02	8.65E+02	4.10E+04	3.93E+04	3.34E+05	3.34E+05	2.49E+03	3.92E+04	2.37E+03	2493.358	2368.69	124.6679	2368.69	2368.69	124.6679
FURFURAL	3.87E-01	3.99E+00	2.97E-03	3.60E+00	3.98E+00	148.2777	2.23E+02	2.23E+02	6.12E-02	1.48E+02	0.00E+00	6.12E-02	0.00E+00	6.12E-02	0.00E+00	0.00E+00	6.12E-02
HMF	2.90E-02	3.70E-01	3.44E-05	3.41E-01	3.70E-01	14.09182	4.37E+01	43.68087	3.84E-06	1.41E+01	0.00E+00	3.84E-06	0.00E+00	3.84E-06	0.00E+00	0.00E+00	3.84E-06
H2SO4	1.62E-06	3.40E-06	5.98E-35	1.78E-06	3.40E-06	2.20E-03	137.9383	137.9383	1.75E-21	2.20E-03	0	1.75E-21	0	0	0	0	0
CO2	403.8999	23733.61	23696.23	23329.71	3.74E+01	4.04E-04	0.00E+00	0.00E+00	4.04E-04	0.00E+00	0.00E+00	4.04E-04	0.00E+00	4.04E-04	0.00E+00	0.00E+00	4.04E-04
LACID	8.13E-04	2.16E-03	5.45E-25	1.35E-03	2.16E-03	1.06E+00	1.69E+03	1688.048	9.89E-19	1.06E+00	0.00E+00	9.89E-19	0.00E+00	0.00E+00	0	0	0
AACID	5.55E-01	1.10E+01	9.37E-08	1.04E+01	1.10E+01	412.8224	7.40E+03	7400.938	1.16E-09	4.13E+02	0.00E+00	1.16E-09	0.00E+00	1.16E-09	0.00E+00	0.00E+00	1.16E-09
Total Flow kmol/hr	20.81192	614.9848	562.4483	594.1729	2300.129	2724.665	19264.08	19264.08	805.9268	2183.725	264.987	805.9268	264.987	540.9398	264.987	264.987	540.9398
Total Flow kg/hr	7.78E+02	2.57E+04	24131.35	24939.16	42076.59	6.45E+04	3.56E+05	3.56E+05	3.32E+04	3.98E+04	8519.126	33245.6	8519.126	24726.47	8519.126	8519.126	24726.47
Total Flow l/min	5.13E+03	2.94E+05	2.58E+05	2.84E+05	7.21E+02	7.56E+05	7.11E+03	7.16E+03	2.37E+05	7.40E+02	1.79E+02	2.52E+05	8.30E+04	1.69E+05	1.71E+02	1.71E+02	5.32E+02
Temperature C	60.00002	42.02456	28.4431	41	41.0509	113.8377	117.8446	123.3103	92.40671	119.7636	70	116	116	116	35	35.00871	38
Pressure atm	1.85	9.00E-01	0.9	9.00E-01	0.9	1.906452	2.1	2.1	1.7	1.95	1.8	1.7	1.7	1.7	1.7	1.8	1.7
Vapor Frac	1.00E+00	1.00E+00	1.00E+00	1.00E+00	0	1.00E+00	0.00E+00	0.00E+00	1.00E+00	0.00E+00	0.00E+00	1.00E+00	1.00E+00	1	0	0	0.00E+00
Liquid Frac	0.00E+00	2.38E-04	0.00E+00	0.00E+00	1	0.00E+00	1	1.00E+00	0	1	1.00E+00	0.00E+00	0.00E+00	0.00E+00	1	1.00E+00	1.00E+00
Solid Frac	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Enthalpy cal/mol	-72911.89	-89328.76	-92410.25	-89903.79	-67946.34	-56655.71	-65462.88	-65354.16	-55363.02	-66614.31	-65982.62	-54965.66	-55770.74	-54571.28	-66903.13	-66902.91	-65881.35
Enthalpy kcal/kg	-1951.028	-2136.174	-2153.878	-2141.948	-3714.306	-2393.25	-3543.712	-3537.826	-1342.089	-3657.268	-2052.387	-1332.456	-1734.746	-1193.853	-2081.019	-2081.012	-1441.283
Enthalpy MMkcal/hr	-1.517458	-54.93662	-51.97673	-53.41916	-156.2876	-154.3701	-1.26E+03	-1259.006	-44.61918	-145.4694	-17.48479	-44.29894	-14.77874	-29.5202	-17.72872	-17.72866	-35.63835
Entropy cal/mol-K	-15.60925	-0.6318655	0.8640884	-0.2028283	-38.27106	-16.83927	-32.48416	-32.27132	-43.36142	-33.93485	-56.33741	-42.30831	-28.63233	-49.55434	-59.1225	-59.12179	-80.72909
Entropy kcal/kg-K	-4.18E-01	-1.51E-02	2.01E-02	-4.83E-03	-2.09E+00	-7.11E-01	-1.758469	-1.746948	-1.051151	-1.863096	-1.752373	-1.025622	-0.8906075	-1.084098	-1.839003	-1.838981	-1.766106
Density mol/cc	6.77E-05	3.48E-05	3.64E-05	3.49E-05	5.32E-02	6.00E-05	4.51E-02	4.49E-02	5.67E-05	4.92E-02	2.47E-02	5.32E-05	5.32E-05	5.32E-05	2.58E-02	2.58E-02	1.70E-02
Density gm/cc	2.53E-03	1.46E-03	1.56E-03	1.47E-03	9.72E-01	1.42E-03	8.34E-01	8.29E-01	2.34E-03	8.96E-01	7.94E-01	2.20E-03	1.71E-03	2.43E-03	8.31E-01	8.31E-01	7.75E-01
Average MW	37.37101	41.81718	42.90411	41.97291	18.29314	23.67313	18.47297	18.47297	41.25139	18.21423	32.14922	41.25139	32.14922	45.71021	32.14922	32.14922	45.71021
Liq Vol 60F l/min	15.60105	518.8194	487.9027	503.2184	707.0675	1183.407	5924.667	5924.667	688.8313	663.5688	168.9931	688.8313	168.9931	519.8381	168.9931	168.9931	519.8381
Substream: $TOTAL																	
Total Flow kg/hr	7.78E+02	2.57E+04	24131.35	24939.16	42076.59	6.45E+04	3.78E+05	3.78E+05	3.32E+04	3.98E+04	8519.126	33245.6	8519.126	24726.47	8519.126	8519.126	24726.47
Enthalpy MMkcal/hr	-1.517458	-54.93662	-51.97673	-53.41916	-156.2876	-154.3701	-1321.806	-1319.67	-44.61918	-145.4694	-17.48479	-44.29894	-14.77874	-29.5202	-17.72872	-17.72866	-35.63835
Substream: CISOLID																	
Mass Flow kg/hr																	
CELLULOS	0	0	0	0	0	0	2258.033	2258.033	0	0	0	0	0	0	0	0	0
XYLAN	0	0	0	0	0	0	870.643	870.643	0	0	0	0	0	0	0	0	0
LIGNIN	0	0	0	0	0	0	14925.31	14925.31	0	0	0	0	0	0	0	0	0
GYPSUM	0	0	0	0	0	0	27.22346	27.22346	0	0	0	0	0	0	0	0	0
ACETATE	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C5SOLID	0	0	0	0	0	0	165.8368	165.8368	0	0	0	0	0	0	0	0	0
C6SOLID	0	0	0	0	0	0	124.3776	124.3776	0	0	0	0	0	0	0	0	0
CAH2O2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ASH	0	0	0	0	0	0	4145.919	4145.919	0	0	0	0	0	0	0	0	0
Total Flow kmol/hr	0	0	0	0	0	0	192.9711	192.9711	0	0	0	0	0	0	0	0	0
Total Flow kg/hr	0	0	0	0	0	0	22517.34	22517.34	0	0	0	0	0	0	0	0	0
Total Flow l/min	0	0	0	0	0	0	79.76384	79.76384	0	0	0	0	0	0	0	0	0
Temperature C							117.8446	123.3103									
Pressure atm		0.9			0.9		2.1	2.1			1.8	1.7	1.7	1.7	1.7	1.8	1.7
Vapor Frac							0	0									
Liquid Frac							0	0									
Solid Frac							1	1									
Enthalpy cal/mol							-3.15E+05	-3.14E+05									
Enthalpy kcal/kg							-2695.887	-2694.044									
Enthalpy MMkcal/hr							-60.70509	-60.66359									
Entropy cal/mol-K							-868.026	-867.4798									
Entropy kcal/kg-K							-7.438884	-7.434203									
Density mol/cc							0.0403213	0.0403213									
Density gm/cc							4.705002	4.705002									
Average MW							116.6877	116.6877									

Table A.9 Material and energy balance C

	011FETOH	012AFEED	012BLIQ	012CSOL	012DCOND	012EHYD	012FGYP	101LPST	201HPST	301COND	302COND	303COND	304COND	306COND	401SACID	402SACID	501LIME
TO:	ETOHCOOL	PNUFILT	CONDTNR	DETOXMIX	DRUMFILT	DETOXMIX		M202LO	M202HI	M202LO	M202MIX	DETOXHX	SCRUBBER	DETOXMIX	M202MIX	CONDTNR	CONDTNR
Substream: MIXED FROM:	MOLSIVHX	DETOXHX	PNUFILT	PNUFILT	CONDTNR	DRUMFILT	DRUMFILT										
Mass Flow kg/hr	MIXED	LIQUID	LIQUID	LIQUID	LIQUID	LIQUID	LIQUID	VAPOR	VAPOR	LIQUID	LIQUID	LIQUID	LIQUID	LIQUID	LIQUID	LIQUID	LIQUID
GLUCOSE	0	5582.845	5214.377	368.4677	5214.377	5188.305	26.07188	0	0	0	0	342.1426	0	173.3331	0	0	0
XYLOSE	0	21648.79	20219.97	1428.82	20219.97	20118.87	101.0998	0	0	0	0	342.1426	0	173.3331	0	0	0
SOLSLDS	0	8874.13	8288.438	585.6926	8288.438	8246.995	41.44219	0	0	0	0	1368.57	0	693.3324	0	0	0
ACETATE	0	0	0	0.00E+00	0.00E+00	0	0	0	0	0	0	0	0	0	0	0	0
H2O	1.25E+02	2.69E+05	2.34E+05	3.50E+04	2.34E+05	2.33E+05	1.17E+03	1.18E+04	37149.53	30279.04	9.65E+04	1.34E+05	40491.01	67807.9	0	0	1.00E+00
FURFURAL	6.12E-02	372.8188	348.2127	24.60604	348.2127	346.4717	1.741064	0	0	0	0	0	0	0	0	0	0
HMF	3.84E-06	58.04403	54.21312	3.830906	54.21312	53.94206	0.2710656	0	0	0	0	0	0	0	0	0	0
H2SO4	0	2090.008	1952.068	137.9405	0	0	0	0	0	0	0	0	0	0	2090.094	1149.552	0
CO2	4.04E-04	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.00E+00
LACID	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
AACID	1.16E-09	4234.909	3955.405	279.504	3955.405	3935.628	19.77702	0	0	321.5911	738.6884	957.9992	0	485.3326	0	0	0
Total Flow kmol/hr	540.9398	15747.11	13751.6	1995.512	13731.75	13663.09	6.87E+01	654.3867	2062.113	1686.097	5366.486	7532.244	2247.593	3815.916	21.31021	11.72062	0.0555084
Total Flow kg/hr	2.47E+04	3.12E+05	2.74E+05	3.78E+04	2.72E+05	2.71E+05	1.36E+03	1.18E+04	37149.53	30600.63	9.72E+04	1.37E+05	40491.01	69333.24	2090.094	1149.552	1.00E+00
Total Flow l/min	1.59E+05	5.64E+03	4.97E+03	6.70E+02	4.98E+03	4953.868	24.89381	88511.99	1.17E+05	523.9549	1715.294	2417.826	679.9157	1224.897	19.1761	10.54686	1.69E-02
Temperature C	92.40347	50	50	50	57.66824	57.66824	57.66824	164	268.1895	45	74	45	26	45	20	20	30
Pressure atm	1.7	1	1	1	1	1	1	4.42	13	1	3	1	1	1	3.4	3.4	1
Vapor Frac	9.98E-01	0.00E+00	0	0	0	0	0	1	1	0	0	0	0	0	0	0	0
Liquid Frac	1.56E-03	1.00E+00	1.00E+00	1	1	1	1	0	0	1	1	1	1	1	1	1	1
Solid Frac	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Enthalpy cal/mol	-55022.1	-68370.82	-68409.83	-68102.1	-68102.29	-6.81E+04	-68102.29	-56626.86	-5.58E+04	-6.80E+04	-67477.07	-67486.42	-68217.71	-6.75E+04	-1.90E+05	-1.90E+05	-68150.99
Enthalpy kcal/kg	-1203.716	-3450.538	-3430.844	-3593.328	-3434.932	-3434.932	-3434.932	-3143.269	-3094.757	-3748.241	-3725.62	-3714.272	-3786.658	-3714.272	-1933.03	-1933.03	-3782.955
Enthalpy MMkcal/hr	-29.76407	-1076.659	-940.7581	-1.36E+02	-9.35E+02	-930.5013	-4.675886	-37.0564	-114.9704	-114.7002	-362.12	-508.3315	-153.3278	-257.5262	-4.040274	-2.22E+00	-3.78E-03
Entropy cal/mol-K	-50.75031	-41.03649	-41.28985	-39.30712	-41.0209	-41.0209	-41.0209	-10.43844	-10.78865	-37.78956	-36.25175	-36.87864	-38.80218	-36.87864	-79.48341	-79.48341	-38.58265
Entropy kcal/kg-K	-1.110262	-2.071029	-2.070741	-2.073994	-2.069006	-2.069006	-2.069006	-0.5794213	-0.5988613	-2.082208	-2.001573	-2.029702	-2.153848	-2.029702	-0.8103979	-0.8103979	-2.141663
Density mol/cc	5.68E-05	4.65E-02	4.61E-02	4.96E-02	4.60E-02	0.0459677	4.60E-02	1.23E-04	2.93E-04	0.0536336	0.0521435	0.0519216	0.0550948	0.0519216	0.0185215	0.0185215	5.49E-02
Density gm/cc	2.59E-03	9.22E-01	9.20E-01	9.40E-01	9.11E-01	0.9113745	9.11E-01	2.22E-03	5.27E-03	0.9733864	0.944404	0.9433889	0.9925498	0.9433889	1.816579	1.816579	9.89E-01
Average MW	45.71021	19.81454	19.93965	18.95238	19.82638	19.82638	19.82638	18.01528	18.01528	18.14879	18.11164	18.16949	18.01528	18.16949	98.07948	98.07948	18.01528
Liq Vol 60F l/min	519.8381	5108.486	4483.668	624.8176	4465.893	4443.563	22.32946	196.8613	620.3522	510.767	1622.533	2283.43	676.1508	1156.81	19.05033	10.47768	0.0166987
Substream: $TOTAL																	
Total Flow kg/hr	2.47E+04	3.61E+05	2.74E+05	8.63E+04	2.78E+05	2.71E+05	7.02E+03	1.18E+04	37149.53	30600.63	9.72E+04	1.37E+05	40491.01	69333.24	2090.094	1149.552	2.34E+03
Enthalpy MMkcal/hr	-29.76407	-1175.416	-941.2519	-234.1642	-950.9229	-930.5801	-20.3428	-37.0564	-114.9704	-114.7002	-362.12	-508.3315	-153.3278	-257.5262	-4.040274	-2.222151	-7.44859
Substream: CISOLID																	
Mass Flow kg/hr																	
CELLULOS	0	28366.54	141.8327	28224.71	141.8327	0.7091635	141.1235	0	0	0	0	0	0	0	0	0	0
XYLAN	0	874.9962	4.374981	870.6212	4.374981	0.0218749	4.353106	0	0	0	0	0	0	0	0	0	0
LIGNIN	0	14999.93	74.99967	14924.93	74.99967	0.3749984	74.62467	0	0	0	0	0	0	0	0	0	0
GYPSUM	0	0	0	0	5444.692	27.22346	5417.468	0	0	0	0	0	0	0	0	0	0
ACETATE	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C5SOLID	0	166.6659	0.8333297	165.8326	8.33E-01	4.17E-03	0.829163	0	0	0	0	0	0	0	0	0	0
C6SOLID	0	124.9995	0.6249973	124.3745	6.25E-01	3.12E-03	0.6218723	0	0	0	0	0	0	0	0	0	0
CAH2O2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2343.072
ASH	0	4166.648	20.83324	4145.815	20.83324	0.1041662	20.72908	0	0	0	0	0	0	0	0	0	0
Total Flow kmol/hr	0	354.7294	1.773647	352.9558	33.39718	0.1669859	33.23019	0	0	0	0	0	0	0	0	0	31.62353
Total Flow kg/hr	0	48699.79	243.4989	48456.29	5688.19	28.44095	5659.75	0	0	0	0	0	0	0	0	0	2343.072
Total Flow l/min	0	364.3142	1.821571	362.4926	41.1876	0.205938	40.98166	0	0	0	0	0	0	0	0	0	16.85979
Temperature C		50	50	50	57.66824	57.66824	57.66824										30
Pressure atm	1.7	1	1	1	1	1	1	4.42	13	1	3	1	1	1	3.4	3.4	1
Vapor Frac		0	0	0	0	0	0										0
Liquid Frac		0	0	0	0	0	0										0
Solid Frac		1	1	1	1	1	1										1
Enthalpy cal/mol		-2.78E+05	-2.78E+05	-2.78E+05	-4.71E+05	-4.71E+05	-4.71E+05										-2.35E+05
Enthalpy kcal/kg		-2027.854	-2027.854	-2027.854	-2768.088	-2768.088	-2768.088										-3177.324
Enthalpy MMkcal/hr		-98.75746	-0.4937873	-98.26368	-15.74564	-0.0787281	-15.66691										-7.444807
Entropy cal/mol-K		-830.3611	-830.3611	-830.3611	-212.2517	-212.2517	-212.2517										-69.88529
Entropy kcal/kg-K		-6.048354	-6.048354	-6.048354	-1.246198	-1.246198	-1.246198										-0.9432145
Density mol/cc		0.0162281	0.0162281	0.0162281	0.0135142	0.0135142	0.0135142										0.0312612
Density gm/cc		2.227921	2.227921	2.227921	2.301741	2.301741	2.301741										2.316232
Average MW		137.2871	137.2871	137.2871	170.3195	170.3195	170.3195										74.09268

Table A.10 Material and energy balance D

					Original													
Equipment	Scaling		Shell	Tube	Duty		LMTD	LMTD	overall U	Overdesign	Area		Scale	Factor	2002 Cost	Equip.	Spare	2002 Cost
	Block	Type	Material	Material	cal/sec	BTU/h	Farenheit	K	BTU/h/ft^2/F	Factor	square feet				ea $1,000	Number		$1,000
					MMkcal/hr	MMbtu/hr						m^2			from capcost			
H-201	BEERHX	S/T Float	SS304	SS304	21.927	87.051	44.9	24.9	150	1.0	6469.5	601.0	592.0	0.75	$290.4	2	1	$881.2
H-244	WWHX	S/T Float	SS304	SS304	-9.939	39.458	42.1	23.4	150	1.0	3124.8	290.3	170.0	0.65	$123.7	2	1	$525.5
H-301	HYDHEAT	S/T Fixed	SS304	SS304	3.833	15.217	99.4	55.2	300	1.0	510.4	47.4	45.0	0.6	$47.3	1	1	$97.6
H-302	SACCOOL	S/T Fixed	SS304	CS	-8.372	33.237	40.1	22.3	300	1.0	921.2	85.6	83.0	0.6	$46.0	3	0	$140.6
FermentCool		S/T Fixed	SS304	CS	-5.053	20.060	18.4	10.2	300	0.25	182.2	16.9	16.9	0.6	$20.0	5	1	$120.1
H-501	BEERCOL	S/T Fixed	SS304	SS304	35.534	141.071	45.3	25.2	175	1.0	17781.2	1651.9	900.0	0.75	$318.0	1	1	$1,002.9
H-505 Startup	RECTIFY	S/T Fixed	SS304	SS304	-22.337	88.680	112.1	62.3	175	1.0	4520.8	420.0	403.0	0.70	$179.0	1	0	$184.3
Evaporator1					-29.001	115.134	9.2	5.1	175	1.0	35899.8	3335.2	3700.0	0.70	$1,800.0	2	0	$3,347.7
Evaporator2					-40.492	160.751	26.7	14.8	175	1.0	34414.6	3197.2	3700.0	0.70	$1,450.0	1	0	$1,309.1
Evaporator3					-43.468	172.566	10.0	5.6	175	1.0	49091.8	4560.8	3700.0	0.70	$1,450.0	2	0	$3,357.3
Evap Condensor		S/T Float	SS304	SS304	-44.902	178.261	56.3	31.3	300	1.00	10551.8	980.3	825.0	0.75	$374.0	1	1	$851.3

Table A.11 Heat exchanger calculations

		Materials	Stream	Type	l/min	atm	kW	scale	factor	Number	Spares	Capcost	Cost
P-244	Saccharificatio	SS304	002DHYD	Total Volume Flow	7216.4	13.5	82.3	78	0.56	2	1	$199,000	$615,146
P-300	Ferment Recirc	SS304	004BEER	Hrx from ferment	-5.053	Mmkcal/hr		-5	0.8			$250,000	$252,118
P-501	Beer Pump	SS304	007STILL		7237.6	4.38	53.5	50	0.56	1		$282,000	$293,023
P-511	Effect Pump	SS304	EVBOT1	Total Volume Flow	5608.0	3.21	15.2	14	0.56	2	1	$74,000	$232,567

Table A.12 Pump calculations

Equipment		Scaling	Material	Flow	Res Time	Tank #	Design	Vol/tank	H/L	Diameter	Original	Original	Scale	Installation	Installed Cos
		Stream					Factor				Size	Cost	Factor	Factor	
				l/min	hours			gallons	meters	meters	gallons				
Sacchar and Ferment	F-300,T-310, w/ agitators	002EHYD	SS304	7,289	72	10	1.2	998343			950000	$533,000	0.6	1.2	$6,589,344
Seed Fermenters	F-301, jacketed			729		2		21			20.0	$14,700	0.6	2.8	$84,277
	F-302, jacketed			729		2		208			200	$32,600	0.6	2.8	$186,901
	F-303, jacketed			729		2		2080			2000	$81,100	0.6	2.8	$464,958
	F-304, add coil, agitator			729		2		20799			19200	$55,000	0.6	1.2	$138,489
	F-304, add coil, agitator			729	36	2	1	207988			192000	$176,000	0.6	1.2	$443,166
Seed Hold Tank	T-301			729		1	1.2	249586			240000	$213,300	0.6	1.2	$262,046
Beer Hold Tank	T-306			7,289	4	1	1.1	508415			484000	$272,700	0.6	1.2	$337,047
Rectifier Reflux Drum	T-505	Volume Flow Stage 1		2294	0.25	1	2	18181	10.6	2.80	17441	$168,600	0.6	1	$172,855
Evaporator Cond Drum	T-514	EVCOND	SS304	4112	0.166667	1	1.333333	14484	9.9	2.59	12228	$132,100	0.6	1	$146,228

Table A.13 Tank calculations

Equipment	Scaling	Diameter	Theoretical	Actual	Efficiency	Tray Space	Height	2002 Cost	Scale (Dia)	Factor	Installed Cost
	Block	meter	Stages	Stages		meter	meter	$1,000			
D-501	BEERCOL	3.38		30		0.610	22.3	$1,117.0	3.300	0.800	$1,139
D-502	RECTIFY-Top	3.91		43		0.457	23.7	$1,354.0	3.840	0.800	$1,374
D-502	RECTIFY-Bot	1.28		15		0.457	6.9	$199.0	1.260	0.800	$201
T-512	SCRUBBER	1.85	4			1.200	7.8	$299.0	1.860	0.800	$298

Table A.14 Tower calculations

Total Installed Equipment Cost	**$114.6**		
Warehouse	$1.7	1.50%	of Equipment
Site Development	$6.1	9.00%	of ISBL
Total Installed Cost (TIC)	**$122.4**		
Indirect Costs			
Field Expenses	$24.5	20.00%	of TIC
Home Office & Construction Fee	$30.6	25.00%	of TIC
Project Contingency	$3.7	3.00%	of TIC
Total Capital Investment (TCI)	**$181.2**		
Other Costs (Startup, Permits, etc.)	$18.1	10.00%	of TCI
Total Project Investment	**$199.3**		

Table A.15 Total project investment calculation

				Aspen link		flow	scale flow	scale factor	base price	scaled price	installation factor	installed price
									$MM	$MM		$MM
Feedstock Handling												
	Total area					98038.8				7.60	1	7.60
Hydrolysis												
	Reactor			002HYDRL	Total Mass Flow	276864	281000	0.6	7.5	7.43	2.3	17.10
	Beer Column Economizer			BEERHX	Actual Exchanger Area							0.88
	Waste Vapor Condensor			WWHX	Heat Duty, Tin, Tout							0.53
	Saccharification Pump			002DHYD	Total Volume Flow							0.62
												0.96
	Total Area											20.07
Detox												
	Pnuematic Filter			012AFEED	Solids Mass Flow	48700	48700	0.7	5.02	5.02	1	5.02
	Reacid Tank/Agitator			012BLIQ	Total Mass Flow	274446	256000	0.7	1.03	1.08	1	1.08
	Lime Materials			501LIME	Solids Mass Flow	2343.072	2400	0.7	0.97	0.95	1	0.95
												0.35
	Total Area											7.41
Sacchar and Ferment												
	Sacchar and Ferr	F-300,T-310, w/ agitat		002EHYD								6.59
	Seed Fermenters	F-301, jacketed		002EHYD								0.08
		F-302, jacketed		002EHYD								0.19
		F-303, jacketed		002EHYD								0.46
		F-304, add coil, agitat		002EHYD								0.14
		F-305, add coil, agitat		002EHYD								0.44
	Seed Hold Tank			002EHYD								0.26
	Beer Hold Tank			002EHYD								0.34
	Hyrolyzate Heater			HYDHEAT	Heat Duty, Tin, Tout							0.10
	Sacchar Cooler			SACCOOL	Heat Duty, Tin, Tout							0.14
	Ferment Cooler			FERMENT	Heat Duty							0.12
	Ferment Recirc Pump			FERMENT	Heat Duty							0.25
												0.46
	Total Area											9.57
Distillation												
	Beer Column			BEERCOL	Diameter							1.14
	Rectify Column			RECTIFY	Diameter							1.57
	Scrubber			SCRUBBER	Diameter							0.30
	Beer Col Reboiler			BEERCOL	Heat Duty, Tin, Tout							1.00
	Rectify Startup Cond			RECTIFY	Heat Duty, Tin, Tout							0.18
	Rectify Reflux Drum			RECTIFY	Heat Duty, Tin, Tout							0.17
	Evaporator1			EVHEAT1	Heat Duty, Tin, Tout							3.35
	Evaporator2			EVHEAT2	Heat Duty, Tin, Tout							1.31
	Evaporator3			EVHEAT3	Heat Duty, Tin, Tout							3.36
	Effect Pump			EVBOT1	Total Volume Flow							0.23
	Evap Condensor			EVCOND	Heat Duty, Tin, Tout							0.85
	Evap Cond Drum			EVMIXOUT	Total Volume Flow							0.15
	Molecular Sieve			011ETOH	Total Mass Flow	24726.47	24927	0.7	3.17	3.15	1	3.15
	Pnuematic Filter			012AFEED	Solids Mass Flow	22067	22573	0.7	5.4	5.31	1	5.31
												0.84
	Total Area											22.92
Storage, Utilities, Wast												
	Wastewater Treatment			011ETOH		24726.47	24930	0.6	3.1	3.08	1	3.08
	Storage			011ETOH		24726.47	24930	0.6	2	1.99	1	1.99
	Utilities			011ETOH		24726.47	24930	0.6	4.6	4.58	1	4.58
	Combuster, Boiler, Turbogenerator			011ETOH		30792.12	32022.75	0.6	38.3	37.41	1	37.41
	Total area											47.06
Overall Total Capital Cost												114.63

Table A.16 Capital costs of individual sections plus overall installed capital cost

Biomass available	30,792	kg/hr			
Biomass heating value	3,820	kcal/kg			
	1st stage	2nd stage	3rd stage	4th stage	
Steam temperature	510	268	164	115	C
Steam pressure	86	13	4	2	atm
Steam heating value	650	515	515	529	kcal/kg
Steam from previous stage	180963	180963	129336	20100	kg/hr
Steam required					
Hydrolyzate heater				7245	kg/hr
Beer column reboiler			68957		kg/hr
Rectifier reboiler			7964		kg/hr
Evaporator first effect				12595	kg/hr
Molecular sieve heater			621		kg/hr
LP steam to pretreat			11789		kg/hr
HP steam to pretreat		37150			kg/hr
Total steam required	0	37150	89331	19839	kg/hr
Recycle fraction	0	0.08	0.11	0	
Recycled steam		14477	19906	0	kg/hr
Steam for power	180963	129336	20100	260	kg/hr
Stage power generation	0.1205	0.0529	0.0400	0.0940	kW/kg/hr
Power generated	21806	6842	804	24	kW
Total power generated				29476	kW
Electricity used				11869	kW
Net				17608	kW

Table A.17 Spreadsheet calculation for turbogenerator

Variable Operating Costs									
Raw Material	**Stream No.**		**kg/hr**	**lb/hr**	**2000 Cost (cents / ton)**	**2000 Cost ($/lb)**	**$/hour**	**MM$/yr (2001)**	**Cents/Gallon Ethanol (2001)**
Feedstock	001BMASS	Total Mass Flo	83,339	183,762	3000.00	0.0150	2,756.42	23.15	33.50
Sulfuric Acid	401SACID, 40	Total Mass Flo	3,240	7,143	2500.00	0.0125	89.29	0.75	1.09
Hydrated Lime	501LIME	Total Mass Flo	2,343	5,166	7000.00	0.0350	180.83	1.52	2.20
Corn Steep Liquor	003GLUC	Total Mass Flo	1,280	2,821	16000.00	0.0800	225.72	1.90	2.74
Purchased Cellulase Enzyme	002EHYD	Cellulose Mas	6,774	14,937	11000.00	0.0550	821.53	6.90	9.99
							203.69	1.71	2.48
Subtotal							**4,277.48**	**35.93**	**51.99**
Waste Streams									
Disposal of Steam 809	EVBOT3, EVS	Ash Mass Flov	4,125	9,096	1900.00	0.0095	86.41	0.73	1.05
Disposal of Stream 229	012FGYP	Total Mass Flo	7,021	15,481	1900.00	0.0095	147.07	1.24	1.79
Subtotal							**233.48**	**1.96**	**2.84**
By-Product Credits			KW			**$/kWh**			
Electricity Net			17637			0.0400	705.50	5.93	8.57
Co-product									
Subtotal							**705.50**	**5.93**	**8.57**
Total Variable Operating Costs							**3,805.46**	**31.97**	**46.25**
Fixed Operating Costs									
Plant Manager	80000		1	80,000					
Plant Engineer	65000		1	65,001					
Maintenance Supr	60000		1	60,000					
Lab Manager	50000		1	50,000					
Shift Supervisor	37000		5	185,003					
Lab Technician	25000		2	50,001					
Maintenance Tech	28000		8	224,004					
Shift Operators	25000		20	500,008					
Yard Employees	20000		32	640,010					
General Manager	100000		1	100,000					
Clerks & Secretaries	20000		5	100,002					
Salary Inflation				0.1					
Total Salaries				2,259,430				2.26	3.27
Overhead/Maint	60%		of Labor & Supervison	1,355,658				1.36	1.96
Maintenance	2%		of Installed Equipment Cost	2,292,691				2.29	3.32
Insurance & Taxes	1.5%		of Total Installed Cost	1,836,533				1.84	2.66
Total Fixed Operating Costs								**7.74**	**11.21**
Total Cash Cost								**39.71**	**57.46**

Table A.18 Operating cost calculations

Minimum Ethanol Selling Price $1.08

Ethanol Production (MM Gal. / Year)	69.1	Ethanol at 68°F
Ethanol Yield (Gal / Dry US Ton Feedstock)	89.7	
Feedstock Cost $/Dry US Ton	$30	
Fermentation Concentration	5.82%	
Pentose Conversion	80%	

Capital Costs ($MM)	
Feed Handling	$7.60
Pretreatment	$20.07
Neutralization/Conditioning	$7.41
Saccharification & Fermentation	$9.57
Distillation and Solids Recovery	$22.92
Wastewater Treatment	$3.08
Storage	$1.99
Utilities	$4.58
Boiler/Turbogenerator	$37.41
Total Installed Equipment Cost	$114.63
Added Costs	$85
(% of TPI)	42%
Total Project Investment	$199

Operating Costs (cents/gal ethanol)	
Feedstock	33.5
Sulfuric Acid	1.1
Hydrated Lime	2.2
Corn Steep Liquor	2.7
Purchased Cellulase Enzyme	10.0
Other Feeds	2.5
Waste Disposal	2.8
Electricity	-8.6
Fixed Costs	11.2
Capital Cost	50.8
Total Production Cost	108.2
Excess Electricity (KWH/gal)	2.14
Plant Electricity Use (KWH/gal)	1.44
Plant Steam Use (kg steam/gal)	0.0
Boiler Feed -- LHV (kJ/kg)	16,000
Boiler Feed -- Water Fraction	0.561

Table A.19 Summary of total annualized ethanol production costs (NREL format)

Appendix B Details for the corn grain ethanol balance

Chapter 5 provides the overview of an analysis of the energy balance of corn grain ethanol while considering the uncertainty throughout the process. The details of nitrogen application and upstream nitrogen production are given, but the remaining details are left for the appendix. The following section describes how the probability distributions for the other inputs to corn production were determined.

B.1 Potassium, Phosphate, Lime

Potassium and phosphate are additional fertilizers which are applied to the field during corn production. While the requirements of the maize plant are less for these chemicals than for nitrogen, the need still exists for replenishing the nutrients to the soil before the next crop. Potassium and phosphate are required for photosynthesis, osmotic regulation, and the activation of enzyme systems. Their deficiency causes delayed maturity and low yield. Lime acts more as a soil conditioner rather than a nutrient. With all of the nitrogen, potassium, and phosphate added, the soil begins to become more acidic. A farmer may choose to apply lime to raise the pH of the soil. The combined contribution of these fertilizers to the overall energy inputs for agriculture is less than that of nitrogen, but they still contribute considerably to the discrepancy in the studies. In this section, the production of potassium and phosphate will be investigated similarly to nitrogen to determine what are adequate values for the embodied energy in the two fertilizers. The difference in the lime contribution in the two studies is based on a significantly different application rate rather than differences in the embodied energy.

In contrast to ammonia, which has a high energy intensity because of its reliance on natural gas as a feedstock, the production of phosphate and potassium fertilizers is based on mineral ores and requires much less energy. Additionally, because the industry has a much lower intensity, there have been less remarkable improvements in efficiency and reports from 20 years ago are still fairly accurate. These ores can also be found in abundance in the U.S. and Canada so the production systems are fairly modern. The production of phosphate is primarily based on the reaction of phosphate rock and sulfuric acid. Phosphate rock is a mineral salt which is upgraded after mining by beneficiation and concentration steps. Sulfuric acid production is based on an exothermic reaction of elemental sulfur, typically produced as a waste product in gas processing. Therefore, the embodied energy of phosphate consists of the mining, upgrading, and transportation of the phosphate rock, along with the electricity and steam required in the production process. As in nitrogen production, a variety of phosphate forms may be produced; however, they all have lower energy requirements. The production of potassium is even simpler with the potash or potassium chloride mineral ore being applied directly as field. The basic inputs into the system are shown in Figure B.1.

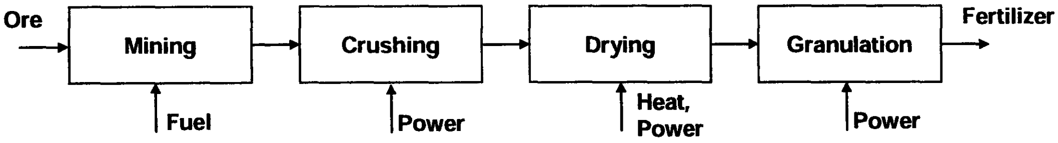


Figure B.1 Schematic for potassium and phosphate production

The analyses for phosphate and potassium production are less prevalent than for nitrogen fertilizer. However, there is still considerable discrepancy in the results which are found. Unfortunately, the embodied energy data given in the Pimentel report is not cited. Shapouri cites the Fertilizer Institute (2000) again for this data. The sources chosen for this assessment are Kongshaug (1998) and Bhat (1994). As stated earlier, the Kongshaug data represents the European industry. The Bhat publication is based on surveys of the U.S. phosphate industry. It is an older report, but the phosphate and potassium industries have remained pretty constant as opposed to the considerable increase in efficiency in the nitrogen industry. Combining the data from these reports results in the data ranges given in Table B.1 for all of the inputs into phosphate and potassium production. Following a similar Monte Carlo simulation of an LCA for the two fertilizer productions, a representative prior distribution for both is a uniform function with a range from 5-10 MJ/kg. Referencing back to Table 5.2, the values from the Shapouri report fall in line with that range, while those for Pimentel almost two times greater. Once again, for fertilizer production, the Pimentel report appears to overestimate the embodied energy in the chemical production life cycle. Furthermore, because the data in the Pimentel report is not cited, it is difficult to ascertain its basis.

Input	Distribution	Mean	MinRatio	MaxRatio
Phosphorus				
Thermal natural gas	Uniform	0.75	0.75	1.25
Electricity	Uniform	2	0.75	1.25
Mechanical diesel	Uniform	3	0.75	1.25
Potassium				
Thermal natural gas	Uniform	3	0.75	1.25
Electricity	Uniform	1	0.75	1.25
Mechanical diesel	Uniform	2	0.75	1.25

Table B.1 Inputs for K, P production

The production of lime is even less energy intensive than phosphate and potassium, but the confusion for its contribution to overall energy requirements comes from vast differences in the assumptions for its application rate in corn production. Unfortunately, the data available for lime application are somewhat thin. Whereas the USDA keeps an abundance of statistics for other agricultural impacts, it does not track the amount of lime applied to which acreage. Therefore, one must sift through the available references to find an accurate depiction of this application rate. While most of the studies suggest that lime is applied at a rate of approximately 4000 kg/ha, the frequency of this application is what is contentious. In a standard survey of corn farmers, prior to 1996 only about 5% annually answered that they applied to lime to the corn acreage. However, the following year the question was changed to "have you ever applied lime," and the answers have been consistently about 50% annually since. It is difficult to ascertain if the application rate has risen that high due to technology advancement and educational awareness or if those surveyed are answering the wrong question. Therefore, using this USDA survey data, a uniform distribution is established as the initial prior with a range of 200 – 2000 kg/ha. In the downstream sensitivity analysis it will be determined if this range needs to be tightened. Comparing the values from Pimentel and Shapouri, it appears that Shapouri is considerably underestimating the application rate while Pimentel is in the reasonable range. However, it must be noted that the confidence of this range is considerably low.

B.2 Herbicide and Insecticide

Pesticides are added to the field during corn growth to stop or prevent infestations of insects which can destroy the crops or weeds which compete for nutrients and water. The application rates of these diverse chemicals are relatively low compared to the other inputs, but they are typically very refined chemicals which require significant upstream processing. The contribution of pesticides to the overall energy utilization in corn production is relatively small, but the variance in both the application rate and the embodied energy is significant such that this is one of the critical parameters in the comparison between the two studies of interest

The embodied energy in herbicides and pesticides is more challenging to determine than nitrogen as the number of varieties of chemicals used as pesticides is quite large, and the different forms are quite varied. For their studies, Shapouri cites Wang (1999) while Pimentel does not have a citation. Another review which gives quite a few values and references for this item is Graboski (2002). The embodied energy reported there is repeated in Table B.2 Because of the wide variety of data sources, the initially defined distribution for the embodied energy will be uniform with the parameters, U~(150,500) MJ/kg, with the input being a product named "fuel mix energy" which is defined as 1/3 each of coal, natural gas, and oil. While this does not help in the differentiation between the previous studies, it enables the methodology which is presented in this work to identify whether or not this large range is consequential in the final analysis. The sensitivity analysis step will show if the assumed distributions for the application rates and embodied energies need to be refined.

Chemical	MJ/kg
2,4,D	85
Alachlor	278
Atrazine	190
Dicamba	295
Glyphosate	453
Metalochlor	276
Paraquat	459
Trifluralin	150
Carbofuran	453
Methyl parathion	160
Transport/packaging	41

Table B.2 Embodied energy in pesticides (Graboski, 2002)

The application rates for pesticides vary greatly between Shapouri and Pimentel, despite both citing the same data source. A possible reason is that the USDA data is divided into more detailed information. For each farming region, ERS provides data for the number of pesticide applications per year and the treatment rate per application. Therefore, an accurate accounting of the inputs for corn production should include a statistical analysis of the product of those two parameters. Performing an analysis of ERS data for the application rates of herbicides and insecticides, the statistics were too varied, and uniform distributions were chosen instead using the upper and lower bounds of the distribution. The prior distributions assumed for the herbicide and insecticide application rates are uniform with ranges of $U(5.5,9.2)$ kg/ha and $U(0.25,1.25)$ kg/ha, respectively. Comparing these distributions to the previous studies demonstrates that the Shapouri value is underestimated for the herbicide application rate, while the Pimentel number overestimates the insecticide application rate. It is unclear how either of the previous studies used the available data to arrive at their assumed conclusions.

B.3 Seed Corn Production

Corn is a highly hybridized crop, and nearly 100% of the corn grown in the U.S uses hybrid seed which is unable to produce kernels which can be further used in sexual reproduction. Therefore, new seed must be purchased before each growing season. This seed corn is produced in a process which is more labor and energy intensive than standard corn production. Therefore, seed corn production must be investigated in further detail to determine its energy requirements.

The agronomic practices in hybrid seed corn production are in general similar to those used in commercial corn production (Corn, 2004). However, several additional steps and inputs are required. In the field, roguing, the manual removal of unwanted plants, and detasseling, the removal of the pollen producing part of the female plant are required. These two additional steps will require excess field work. Then, because the crop is harvested at a higher moisture content than typical, additional energy is required in the drying step which occurs directly after harvest. On average, the moisture will have to be reduced from about 35% to 12% quickly.

The actual seed corn production is at a lower yield than standard production as the seeding rate is not as dense. Additionally, only the female plants (about 75% of the total) produced seed. These two factors contribute to the overall yield being 33-50% of normal. While the fertilizer, pesticide, and water inputs are slightly lower than commercial production, the difference is not that great. Using these factors, the specification given for inputs to hybrid seed corn production will be the same on a per acre basis as standard corn production, with the following adjustments. The yield will be reduced by 66-75% to account for the lower plant density and ratio of male-female plants. The amount of fossil fuel required will increase by 2-3 times to account for the additional field operations, roguing and detasseling. For the drying step, an energy value of 1500-3500 btu/lb water is assumed. With a drop in moisture content from 35% to 12%, the total energy input amounts to 0.75-2.25 MJ/acre. Note that the overall calculation assumes that the above ranges are treated as uniform distributions.

After performing a Monte Carlo analysis of the LCA for hybrid seed corn production, the energy utilized for the seed corn can be approximated with a lognormal distribution with geometric mean and variance parameters, LN~(15,1.4) MJ/kg. Comparing to the values from the studies, Shapouri assumes a multiplier (4.7) applied to standard corn production to reach an embodied energy of 8.8 MJ/kg, slightly underestimating the distribution. By contrast, Pimentel has chosen a value of 100 MJ/kg, which is base on his own previous report. This amounts to a multiplier parameter which suggests the production of seed corn is 33 times as energy intensive as regular corn production. Based on the analysis in this report, this value is considerably overestimating the potential data range.

B.4 Machinery Production

The question of how to account for the energy implicit in the steel and other materials required for the agricultural infrastructure including machinery is controversial. On one side, Pimentel claims that this infrastructure is so ubiquitous that it must be considered a critical parameter. By contrast Shapouri makes the point that the fuels which ethanol would be replacing consist of their own infrastructure, such as oil exploration and production rigs and facilities. Moreover, Shapouri is critical of the data which Pimentel uses as it is based on a very old report. The primary problem addressed here is how to draw the system boundaries for the analysis. In the overview of the methodology, a primary theme is using equivalent boundaries when making comparisons. But how can that be done when the assessors are adamant about the correctness of their own boundaries. The suggestion here is to start by picking the larger boundary in the initial analysis, and the results of the sensitivity analysis will suggest whether more work needs to be done in determining the proper boundary. In cases where adequate data is not available for the expanded boundaries, a preliminary distribution must be assumed based on whatever information can be found. Because the data available for the infrastructure and machinery in corn production is limited, the assumptions will be based on two different methodologies: 1) a theoretical inventory of equipment used per acres of farmland, 2) a percentage of the energy used as fuel during the operation of the machinery.

The first method, the hypothetical inventory is based on a couple of reports and personal communication (Winter, 2005). Once the inventory has been assembled, reports giving average weights for different pieces of equipment will be used to calculate an overall amount of steel which is used by the farm. An uncertainty range of +100% was added to the inventory. That value will be divided by the number of acres assumed to be farmed by the inventory and subsequently divided by the life time of the equipment which is assumed to be 10 years.

The second method requires only an accounting of the fuel which is used during corn production and a parameter for the multiplying factor for arriving at the embodied energy in the machinery. The determination of the fuel usage is described in the following section. For the other factor, values from Heywood (2005) give a range of 0.2-0.4. That means for every 1 MJ of fuel used on an annual basis, the amortized embodied energy is approximately 0.3 MJ. Assuming an embodied energy in refined steel of 78 MJ/kg (Pimentel 2005), this results in a steel usage rate of 0.0025-0.005 kg steel per 1 MJ fuel.

Using the two methods described above, the overall use of machined steel in corn production can be estimated to come up with data ranges. For the first method, the resulting range is a lognormal distribution with geometric parameters LN~(12.8, 1.7) kg/ha. Whereas, the second method results in a slightly higher lognormal distribution with geometric parameters LN~(18.2, 1.4) kg/ha. Either way, the estimator of 55 kg/ha used by Pimentel is exceptionally high.

B.5 Human Labor

Another input which is included in the Pimentel boundary but left out by Shapouri is the impact of human labor. While standard protocol for LCA requires the inclusion of building materials and machinery in at least the first tier of inputs for most processes, recognition of energy required for human input is rarely considered. The case could be made that agricultural processes are more labor intensive with more distribution than other industrial processes, but the question becomes how to determine what those energy requirements are. Should it be based on caloric intake, on fuel for commuting, or on something else? Pimentel chooses 8000 l of oil equivalents per year for a 2000 hr work-year. Additionally, a NASS report is cited which states that it requires 11.4 hours of manpower to farm 1 ha of corn.

First investigating the energy requirements for an hour of labor, solely based on caloric intake with a daily rate of 3200 kcal for 365 days, the total energy consume is just over 120 l oil equivalent, so the assumption must include much more inputs. In fact, it appears Pimentel has simply divided the U.S. overall energy consumption by the U.S. population to arrive at this value. However, this method would actually be double counting energy utilization as the other energy inputs into the corn production process are included in the overall national energy use value. At the very least, this overall energy utilization is not for the sole purpose of work, and the consumption should be divided by the 8760 hours in a year, not simply the 2000 hours worked.

As for the labor hours required for corn production, the latest survey of corn farmers by the USDA reports that the range of values is between 5-8 hrs per acre farmed, a little over half of what is given in Pimentel's work. So multiplying the labor hours required in corn production to the energy required for a human hour from above gives an overall contribution of 0.2 – 0.3 GJ/ha, which is an order of magnitude lower than the 2 GJ/ha suggested by Pimentel. While this hasn't shown a comparison between energy required for resource extraction between different energy sources, it has shown that the contribution of labor might be lower than Pimentel states.

B.6 Other Inputs

In the previous sections, the inputs to corn production have been investigated in further detail for the values which cause the most discrepancy between Shapouri (2004) and Pimentel (2005) in their respective assessments of the overall energy utilization for ethanol production. While these parameter alone are sufficient to describe the inaccuracies in the previous studies, to have a complete assessment of the overall energy efficiency issue, the other inputs should be presented. In this section, the other inputs to corn production along with the primary inputs to transportation, distribution, and ethanol production will be described. The results form this report will be compared to the previous studies for accuracy sake, but the differences in the alternative studies are not as great as the discrepancies of the above inputs.

B.6.1 Fossil Fuel Inputs to Corn Production

Next to nitrogen application, the second most energy consuming input into corn production is the fuel used to drive the tractors, pump the irrigation water, and power any other agricultural machinery. The ERS division within USDA surveys this data in the Agriculture Resource Management Study (ARMS) which is performed every four years. The fuel consumption data is estimated for machinery operations, including tractor and truck use, irrigation, and drying by combining engineering coefficients describing fuel use per hour with data on engine horsepower, fuel type, and hours of machine use collected in the ARMS (ERS, 2006). Using the state by state data from the last three surveys, inputs of diesel, gasoline, LPG, natural gas, and electricity can be determined. As with the other inputs, this data covers spatial and temporal variations. Therefore, the requirements of the different fuels for corn production are presented as probability distributions. Note that while diesel is probably used in most small scale irrigation systems, the larger scale ones can be driven by natural gas. Therefore, for the purpose of dividing allocating the fuels to different inputs, it is assumed that the natural gas requirements are equivalent to irrigation inputs. Note that this does not have any effect on the overall energy balance.

The variance shown for the overall energy from fuel is significantly large. Much of this comes from the high variability in irrigation practices across the U.S. While the higher corn producing states such as Iowa and Illinois utilize very little irrigation, dryer states such as Nebraska, Kansas, and Texas consume large amounts of water. The utilization of water itself is out of the scope of this work, but the fuel used for the pumping is critical. Therefore, the energy assessment must take into consideration this variability. The overall acreage which uses irrigation is not very large, but the large amounts of energy used in those few acres is not insignificant. For this initial assessment, the variance will be included as is, and the sensitivity analysis and subsequent data refinement will be used to help a decision maker determine whether the irrigation numbers are important or not

Appendix C EnvEvalTool

The EnvEvalTool is a combined database/spreadsheet developed by Alejandro Cano-Ruiz (2000) for performing life cycle assessment calculations. This is a description of how to use the tool based on both Cano-Ruiz (2000) and Chen (2005). See these two theses for a more detailed description. Following the brief discussion is the documentation for the matrices utilized in the case studies for this thesis.

C.1 User's Manual of Environmental Evaluation Tools

These steps are to be followed to set up a new case study in EnvEvalTool, populate the inventory databases and transfer the data to the spreadsheet calculation too. The initial step is to open the EnvEvalTool Access database file

C.1.1 Creating a New Case Study

Each individual LCA within the database must be identified by its own case study. On the opening list of tables, click on "Case Studies," and choose to open a new one, giving the case study an identifying name, and choosing the primary product to be produces. All of the previously input products and processes can be used in this case study, if they are an input or output to a product or process in the supply chain tree for the product of interest.

C.1.1.1 Specify the Processes and Products

Open the "products" table and enter the name of the new product along with the units of measurement that will be used for entering input-output coefficients. Open the "processes" table and enter data for the new processes. Add the process into the "Sources of Input-Output Data" sheet.

C.1.1.2 Specify the Input-Output Data

Each of the new products defined requires at least one entry in the "Make coefficients" table. Multi-product processes will have more than one entry in this table. Usage coefficient distributions also need to be entered in the "Use coefficients" table for each of the processes that make the products of interest. If a process uses a product not previously existing in the database, the product and the process that makes the product need to be defined first before you are able to use it as an entry in the "use coefficients" table. The "Make coefficients" and "Use coefficients" tables are corresponding to the Fabrication Matrix and the Usage Matrix mentioned in the text.

C.1.1.3 Define the Environmental Exchange Factors

Finally, the environmental exchange inventory must be defined. If the emission substance is not currently in the database, it needs to be added in the "chemical information" table. The characterization factors for this chemical also needs to be added in the "characterization factors" table, otherwise the emissions of that chemical will not be evaluated for impact. Similarly, new impact categories need to be defined in the "Impact Categories" table. The valuation factor for the new category should be defined in the "Valuation Factors" table. After the emissions, the characterization factors, and the impact categories are completed, emission inventories can be entered in the "Emission factors" table.

If there is correlation within the newly entered characterization factors or valuation factors, or among these two, their correlation coefficients need to be entered in "CF to CF correlation", "VF to VF correlation", and "CF to VF correlation" tables.

C.1.2 Define the Valuation Method

Open the "Case Studies (valuation)" table and enter the name of the new case study and the code of the valuation method you to be used. Valuation methods are defined in two tables. The "valuation method" table gives the valuation method code, valuation method name, and reference. There are currently three defined valuation methods in the tool: The EPS method, the XLCA method, and the "Cano Thesis" method, which was used in this valuation. The distributions for the valuation factors used in each method are given in "valuation factors" table.

C.1.2.1 Specify the Final Product and Economic Information

Open the "Case Studies (products)" table and enter the name of the case study and the product code for the products to be included as final demand products in the study. If the study is to compare several different processes to make the same product, a market share scenario needs to be specified in the "market share" table. The distributions entered in this table are the market shares that different processes have in the production of the product of interest. For products produced in multi-product processes, prices of these products also need to be specified. The default price for all the products are 999 $/unit.

C.1.3 Export the Data into the PIO-LCA spreadsheet

After the data has been input into the Access database, a macro for querying the appropriate data and setting up the calculation matrices in Excel is performed

C.1.3.1 Specify the Path for Output Files

Select "Modules" from the list of objects on the left side of the Access window. Double click on the "Export to spreadsheet" module. On the 11th line of the code, the pathname can be specified for where the exported file to be. The directory should exist before the exportation. It is recommended not to change the last part of the path (i.e. "\Environmental Evaluation Tool\Temp").

C.1.3.2 Export Data

Select "Macros" from the list of objects on the left side of the Access window. Double click on "Export to Spreadsheet". A dialogue window will pop up asking for the name of the case study. Input the case study name and hit "OK".

C.1.3.3 Read Data into PIO-LCA Model

After running successfully the "export to spreadsheet" macro, a series of Excel files will exist in the "Environmental Evaluation Tool\Temp" directory. Firstly, set the pathname used in the read-data macros to be consistent with the file structure of the computer. Go to the menu in Excel Tools→Macros→Visual Basic Editor and double click on the Sheet1 object under Project Explorer. Scroll down to the CommandButton2_Click() section and edit the Path Name. Then go to "PIO-LCA macros version 3.1" excel workbook and press the "Load Data" button in Sheet1. The files generated by the databse will be read into the sheets.

C.1.4 Specify the Demand Vector

After loading the data, the demand vector remains zero for all the entries. The demand for the final product of interest needs to be specified.

C.2 Biomass Ethanol Case Study Matrices

The following tables are the input output matrices used for the life cycle assessment calculation using the EnvEvalTool. The distributions used in the uncertainty analysis for the biomass ethanol processes can be found in Chapter 4 and 5 and Appendix B and in Cano-Ruiz (2000) for the upstream processes. The deterministic entries in these tables represent the expected values of those distributions.

Build PIO-LCA tables

PROCESS

PRODUCT INPUTS	UNITS	Bioethanol	Coal furnace	Coal production	Coal-fired power plant	Coke production	Cooling water	Corn dry mill	Corn production	Corn stover collection	Custom farming	Diesel engine	Diesel fuel production	Ethanol engine	Fuel mix furnace	Gas-fired power plant	Gasoline engine	Gasoline production	Herbicide production	Hydroelectric plant	Industrial gas furnace	Insecticide production	Iron ore mining	Iron production	K production	Limestone production	LPG engine	LPG fuel production	N production	Natural gas productio	Nuclear power plant	Oil furnace	Oil production	Oil-fired power plant	Oxygen production	P production	Petroleum refining NR	Railroad transport	Seed production	Sinter pellet productio	Steel production	Steel sheet production	Utility gas furnace
Coal	kg	0	1	0	0	1.33	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Coke	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
Cooling water	m3	0	0	0	0	0	0	0.134	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Corn	kg	0	0	0	0	0	0	3.442	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	6	0	0	0	0
Corn stover	kg	3.38	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Custom labor	MJ	0	0	0	0	0	0	0	200	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
DDGS	kg	0	0	0	0	0	0	-1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Diesel fuel	kg	0	0	0	0	0	0	0	0	0	0	0.023	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	4E-04	0	0	0	0	0	0
Electricity	MJ	-2.74	0	0.052	0	0.14	0.36	1.3	101	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0.75	0.124	0	0	0.142	0	2.668	2	0.94	0	0.75	0	0	1.407	0
Ethanol	kg	0	0	0	0	0	0	0	0	0	0	0	0	0.038	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Fuel mix energy	MJ	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	300	0	0	300	0	0	0	0	0	0	1.67	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Gasoline	kg	0	0	0	0	0	0	0.046	0	0	0	0	0	0	0	0	0.023	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Herbicide	kg	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Insecticide	kg	0	0	0	0	0	0	0	0.3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Iron	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.85	0	0
Iron ore	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1.45	0	0	0
K fertilizer	kg	0	0	0	0	0	0	0	27	0.007	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Limestone	kg	0	0	0	0	0	0	0.004	440	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.13	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.15	0	0
LPG	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.022	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Mechanical energy from diesel engines	MJ	4E-05	0	2.53	0	0	0	0	863	0.3	0.6	0	0	0	0	0	0	0	0	0	0	0	0.1	0	2	122	0	0	2	0	0	0	0	0	0	3	0	0.269	0	0	0	0	0
Mechanical energy from ethanol	MJ	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Mechanical energy from gasoline	MJ	0	0	0	0	0	0	0	296	0	0.1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Mechanical energy from LPG	MJ	0	0	0	0	0	0	0	395	0	0.3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
N fertilizer	kg	0	0	0	0	0	0	0.006	60.3	0.006	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Natural gas	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	19.5	0	0	0	0	0	0	0	0.54	0	0	0	0	0	0	0	0.02	0	0	0	0	0	19.5
Oil	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1.01	0	0	0	0	0	23.24	0	0	0	0	1.03	0	0	0	0	0	0
Oxygen	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.03	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.08	0	0
P fertilizer	kg	0	0	0	0	0	0	0	24.6	8E-04	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Railroad transport	kg-km	0	467.2	0	0	0	0	3125	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Refined oil	kg	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	1	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Seeds	kg	0	0	0	0	0	0	0	9.7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Sinter pellets	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Steel	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0
Steel sheet	kg	0	0	0	0	0	0	0	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Thermal energy from coal furnace	MJ	0	0	0.01	10.25	0	0	0	0	0	0	0	0	0	0.34	0	0	0	0	0	0	0	0	18	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.85	0	0
Thermal energy from industrial gas furnace	MJ	0	0	0	0	6.18	0	0	0	0	0	0	0	0	0.33	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1.271	0	0	0.53	0	0	0	0	0	0	0	0	0	0
Thermal energy from oil furnace	MJ	0	0	0	0	0	0	0	0	0	0	0	0	0	0.33	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.027	0	0	0.064	9.73	0	0	0	0	0	0	0	0	0
Thermal energy from utility gas furnace	MJ	0	0	0	0	0	0	13.5	220	0	0	0	0	0	0	10.25	0	0	0	0	0	0	0	0	3	0	0	0	12.6	0	0	0	0	0	0	0.75	0	0	1.5	0	0	0	0

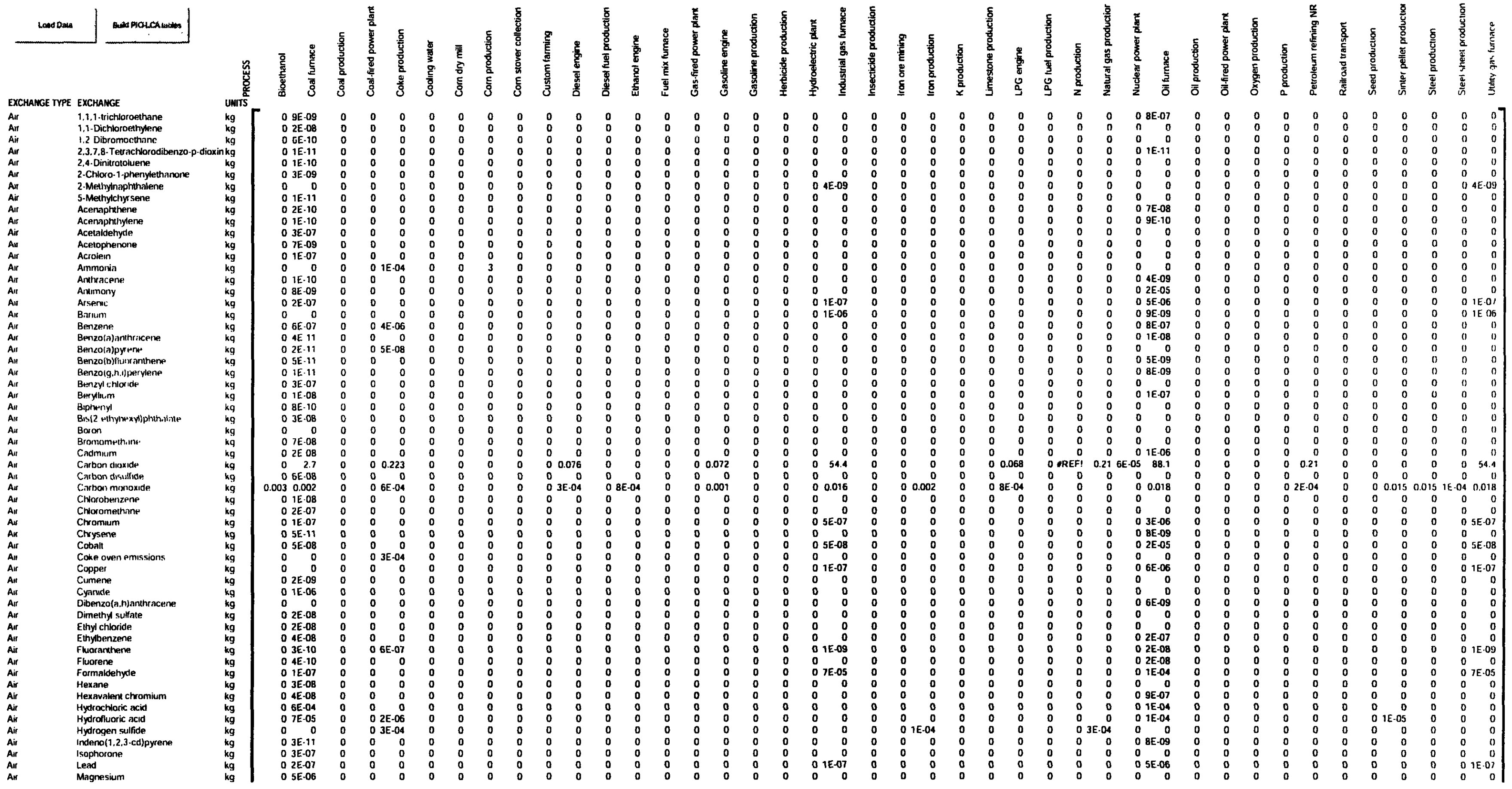
Figure C.1 Use matrix - C

Build PIO-LCA tables

PROCESS

PRODUCT OUTPUTS	UNITS	Bioethanol	Coal furnace	Coal production	Coal-fired power plant	Coke production	Cooling water	Corn dry mill	Corn production	Corn stover collection	Custom farming	Diesel engine	Diesel fuel production	Ethanol engine	Fuel mix furnace	Gas-fired power plant	Gasoline engine	Gasoline production	Herbicide production	Hydroelectric plant	Industrial gas furnace	Insecticide production	Iron ore mining	Iron production	K production	Limestone production	LPG engine	LPG fuel production	N production	Natural gas productior	Nuclear power plant	Oil furnace	Oil production	Oil-fired power plant	Oxygen production	P production	Petroleum refining NR	Railroad transport	Seed production	Sinter pellet productio	Steel production	Steel sheet production	Utility gas furnace
Coal	kg	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Coke	kg	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Cooling water	m3	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Corn	kg	0	0	0	0	0	0	0	3600	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Corn stover	kg	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Custom labor	MJ	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
DDGS	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Diesel fuel	kg	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Electricity	MJ	0	0	0	3.6	0	0	0	0	0	0	0	0	0	0	3.6	0	0	0	3.6	0	0	0	0	0	0	0	0	0	0	3.6	0	0	3.6	0	0	0	0	0	0	0	0	0
Ethanol	kg	1	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Fuel mix energy	MJ	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Gasoline	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.95	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Herbicide	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Insecticide	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Iron	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Iron ore	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
K fertilizer	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Limestone	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1000	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
LPG	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Mechanical energy from diesel engines	MJ	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Mechanical energy from ethanol	MJ	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Mechanical energy from gasoline	MJ	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Mechanical energy from LPG	MJ	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1.05	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
N fertilizer	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Natural gas	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
Oil	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
Oxygen	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
P fertilizer	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
Railroad transport	kg-km	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1000	0	0	0	0	0
Refined oil	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
Seeds	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
Sinter pellets	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
Steel	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0
Steel sheet	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0
Thermal energy from coal furnace	MJ	0	29.57	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Thermal energy from industrial gas furnace	MJ	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1055	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Thermal energy from oil furnace	MJ	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1055	0	0	0	0	0	0	0	0	0	0	0
Thermal energy from utility gas furnace	MJ	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1055

Figure C.2 Make matrix - B



		PROCESS	Bioethanol	Coal furnace	Coal production	Coal-fired power plant	Coke production	Cooling water	Corn dry mill	Corn production	Corn stover collection	Custom farming	Diesel engine	Diesel fuel production	Ethanol engine	Fuel mix furnace	Gas-fired power plant	Gasoline engine	Gasoline production	Herbicide production	Hydroelectric plant	Industrial gas furnace	Insecticide production	Iron ore mining	Iron production	K production	Limestone production	LPG engine	LPG fuel production	N production	Natural gas productior	Nuclear power plant	Oil furnace	Oil production	Oil-fired power plant	Oxygen production	P production	Petroleum refining NR	Railroad transport	Seed production	Sinter pellet productior	Steel production	Steel sheet production	Utility gas furnace
EXCHANGE TYPE	EXCHANGE	UNITS																																										
Air	1,1,1-trichloroethane	kg	0	9E-09	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	8E-07	0	0	0	0	0	0	0	0	0	0	0
Air	1,1-Dichloroethylene	kg	0	2E-08	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Air	1,2 Dibromoethane	kg	0	6E-10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Air	2,3,7,8-Tetrachlorodibenzo-p-dioxin	kg	0	1E-11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1E-11	0	0	0	0	0	0	0	0	0	0	0
Air	2,4-Dinitrotoluene	kg	0	1E-10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Air	2-Chloro-1-phenylethanone	kg	0	3E-09	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Air	2-Methylnaphthalene	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	4E-09	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	4E-09
Air	5-Methylchrysene	kg	0	1E-11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Air	Acenaphthene	kg	0	2E-10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	7E-08	0	0	0	0	0	0	0	0	0	0	0
Air	Acenaphthylene	kg	0	1E-10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	9E-10	0	0	0	0	0	0	0	0	0	0	0
Air	Acetaldehyde	kg	0	3E-07	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Air	Acetophenone	kg	0	7E-09	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Air	Acrolein	kg	0	1E-07	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Air	Ammonia	kg	0	0	0	0	1E-04	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Air	Anthracene	kg	0	1E-10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	4E-09	0	0	0	0	0	0	0	0	0	0	0
Air	Antimony	kg	0	8E-09	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2E-05	0	0	0	0	0	0	0	0	0	0	0
Air	Arsenic	kg	0	2E-07	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1E-07	0	0	0	0	0	0	0	0	0	0	5E-06	0	0	0	0	0	0	0	0	0	0	1E-07
Air	Barium	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1E-06	0	0	0	0	0	0	0	0	0	0	9E-09	0	0	0	0	0	0	0	0	0	0	1E-06
Air	Benzene	kg	0	6E-07	0	0	4E-06	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	8E-07	0	0	0	0	0	0	0	0	0	0	0
Air	Benzo(a)anthracene	kg	0	4E-11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1E-08	0	0	0	0	0	0	0	0	0	0	0
Air	Benzo(a)pyrene	kg	0	2E-11	0	0	5E-08	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Air	Benzo(b)fluoranthene	kg	0	5E-11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	5E-09	0	0	0	0	0	0	0	0	0	0	0
Air	Benzo(g,h,i)perylene	kg	0	1E-11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	8E-09	0	0	0	0	0	0	0	0	0	0	0
Air	Benzyl chloride	kg	0	3E-07	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Air	Beryllium	kg	0	1E-08	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1E-07	0	0	0	0	0	0	0	0	0	0	0
Air	Biphenyl	kg	0	8E-10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Air	Bis(2-ethylhexyl)phthalate	kg	0	3E-08	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Air	Boron	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Air	Bromomethane	kg	0	7E-08	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Air	Cadmium	kg	0	2E-08	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1E-06	0	0	0	0	0	0	0	0	0	0	0
Air	Carbon dioxide	kg	0	2.7	0	0	0.223	0	0	0	0	0	0.076	0	0	0	0	0.072	0	0	0	54.4	0	0	0	0	0	0.068	0	#REF!	0.21	6E-05	88.1	0	0	0	0	0.21	0	0	0	0	0	54.4
Air	Carbon disulfide	kg	0	6E-08	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Air	Carbon monoxide	kg	0.003	0.002	0	0	6E-04	0	0	0	0	0	3E-04	0	8E-04	0	0	0.001	0	0	0	0.016	0	0	0.002	0	0	8E-04	0	0	0	0	0.018	0	0	0	0	2E-04	0	0	0.015	0.015	1E-04	0.018
Air	Chlorobenzene	kg	0	1E-08	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Air	Chloromethane	kg	0	2E-07	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Air	Chromium	kg	0	1E-07	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	5E-07	0	0	0	0	0	0	0	0	0	0	3E-06	0	0	0	0	0	0	0	0	0	0	5E-07
Air	Chrysene	kg	0	5E-11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	8E-09	0	0	0	0	0	0	0	0	0	0	0
Air	Cobalt	kg	0	5E-08	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	5E-08	0	0	0	0	0	0	0	0	0	0	2E-05	0	0	0	0	0	0	0	0	0	0	5E-08
Air	Coke oven emissions	kg	0	0	0	0	3E-04	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Air	Copper	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1E-07	0	0	0	0	0	0	0	0	0	0	6E-06	0	0	0	0	0	0	0	0	0	0	1E-07
Air	Cumene	kg	0	2E-09	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Air	Cyanide	kg	0	1E-06	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Air	Dibenzo(a,h)anthracene	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	6E-09	0	0	0	0	0	0	0	0	0	0	0
Air	Dimethyl sulfate	kg	0	2E-08	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Air	Ethyl chloride	kg	0	2E-08	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Air	Ethylbenzene	kg	0	4E-08	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2E-07	0	0	0	0	0	0	0	0	0	0	0
Air	Fluoranthene	kg	0	3E-10	0	0	6E-07	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1E-09	0	0	0	0	0	0	0	0	0	0	2E-08	0	0	0	0	0	0	0	0	0	0	1E-09
Air	Fluorene	kg	0	4E-10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2E-08	0	0	0	0	0	0	0	0	0	0	0
Air	Formaldehyde	kg	0	1E-07	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	7E-05	0	0	0	0	0	0	0	0	0	0	1E-04	0	0	0	0	0	0	0	0	0	0	7E-05
Air	Hexane	kg	0	3E-08	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Air	Hexavalent chromium	kg	0	4E-08	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	9E-07	0	0	0	0	0	0	0	0	0	0	0
Air	Hydrochloric acid	kg	0	6E-04	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1E-04	0	0	0	0	0	0	0	0	0	0	0
Air	Hydrofluoric acid	kg	0	7E-05	0	0	2E-06	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1E-04	0	0	0	0	0	0	0	1E-05	0	0	0
Air	Hydrogen sulfide	kg	0	0	0	0	3E-04	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1E-04	0	0	0	0	0	3E-04	0	0	0	0	0	0	0	0	0	0	0	0	0
Air	Indeno(1,2,3-cd)pyrene	kg	0	3E-11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	8E-09	0	0	0	0	0	0	0	0	0	0	0
Air	Isophorone	kg	0	3E-07	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Air	Lead	kg	0	2E-07	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1E-07	0	0	0	0	0	0	0	0	0	0	5E-06	0	0	0	0	0	0	0	0	0	0	1E-07
Air	Magnesium	kg	0	5E-06	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Figure C.3 Environmental exchange matrix part 1 - E

Load Data

Build PIO-LCA tables

		PROCESS	Bioethanol	Coal furnace	Coal production	Coal-fired power plant	Coke production	Cooling water	Corn dry mill	Corn production	Corn stover collection	Custom farming	Diesel engine	Diesel fuel production	Ethanol engine	Fuel mix furnace	Gas-fired power plant	Gasoline engine	Gasoline production	Herbicide production	Hydroelectric plant	Industrial gas furnace	Insecticide production	Iron ore mining	Iron production	K production	Limestone production	LPG engine	LPG fuel production	N production	Natural gas productior	Nuclear power plant	Oil furnace	Oil production	Oil-fired power plant	Oxygen production	P production	Petroleum refining NR	Railroad transport	Seed production	Sinter pellet productior	Steel production	Steel sheet production	Utility gas furnace
EXCHANGE TYPE	EXCHANGE	UNITS																																										
Air	Manganese	kg	0	2E-07	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2E-07	0	0	0	0	0	0	0	0	0	0	1E-05	0	0	0	0	0	0	0	0	0	0	2E-07
Air	Mercury	kg	0	4E-08	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	4E-07	0	0	0	0	0	0	0	0	0	0	0
Air	Methane	kg	0	3E-05	0	0	0	0	0	0	0	0	3E-06	0	2E-05	0	0	2E-05	0	0	0	0.001	0	0	0	0	0	2E-05	0	0	0.025	0	1E-03	0	0	0	0	1E-05	0	0	0	0	0	1E-04
Air	Methyl ethyl ketone	kg	0	2E-07	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Air	Methyl methacrylate	kg	0	9E-09	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Air	methyl t-butyl ether	kg	0	2E-08	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Air	Methylene chloride	kg	0	1E-07	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Air	Methylhydrazine	kg	0	8E-08	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Air	Molybdenum	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	3E-07	0	0	0	0	0	0	0	0	0	0	3E-06	0	0	0	0	0	0	0	0	0	0	3E-07
Air	Naphthalene	kg	0	6E-09	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1E-07	0	0	0	0	0	0	0	0	0	0	4E-06	0	0	0	0	0	0	0	0	0	0	1E-07
Air	Nickel	kg	0	1E-07	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2E-06	0	0	0	0	0	0	0	0	0	0	3E-04	0	0	0	0	0	0	0	0	0	0	2E-06
Air	Nitrous oxide	kg	0.003	2E-05	0	0	0	0	0	#REF!	0	0	2E-06	0	5E-06	0	0	5E-06	0	0	0	0.001	0	0	0	0	0	5E-06	0	0.001	0	0	4E-04	0	0	0	0	5E-06	0	0	0	0	0	3E-04
Air	Non-methane volatile organic comp	kg	0	2E-05	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.001	0	0	0	0	0	0	0	0	0	0	0.003	0	0	0	0	0	0	0	0	0	0	6E-05
Air	NOx (as NO2)	kg	0	0.005	0	0	2E-04	0	0	3	0	0	5E-04	0	5E-05	0	0	5E-05	0	0	0	0.063	0	0	2E-04	0	0	5E-05	0	0	0	0.002	0.14	0	0	0	0	5E-04	0	0	7E-04	0	1E-04	0.024
Air	Phenanthrene	kg	0	1E-09	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	5E-09	0	0	0	0	0	0	0	0	0	0	4E-08	0	0	0	0	0	0	0	0	0	0	5E-09
Air	Phenol	kg	0	7E-09	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Air	Phosphorus	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	3E-05	0	0	0	0	0	0	0	0	0	0	0
Air	PM10	kg	0	0.008	0	0	0	0	0	0	0	0	4E-05	0	5E-06	0	0	6E-06	0	0	0	0.003	0	0	0	0	0	4E-06	0	0	0	0	0.044	0	0	0	0	0	0	0	0	0	0	0.001
Air	Polycyclic aromatic hydrocarbons	kg	0	0	0	0	7E-07	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Air	propionaldehyde	kg	0	2E-07	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Air	Pyrene	kg	0	2E-10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2E-09	0	0	0	0	0	0	0	0	0	0	2E-08	0	0	0	0	0	0	0	0	0	0	2E-09
Air	Selenium	kg	0	6E-07	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2E-06	0	0	0	0	0	0	0	0	0	0	0
Air	Styrene	kg	0	1E-08	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Air	Sulfur dioxide	kg	6E-04	0.017	0	0	0.002	0	0	0	0	0	1E-05	0	1E-06	0	0	1E-05	0	0	0	3E-04	0	0	3E-04	0	0	0	0	0	0	6E-04	0.6	0	0	0	0	0.001	0	0	7E-04	0	0	3E-04
Air	Tetrachloroethylene	kg	0	2E-08	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Air	Thallium	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Air	Toluene	kg	0	1E-07	0	0	3E-06	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1E-06	0	0	0	0	0	0	0	0	0	0	2E-05	0	0	0	0	0	0	0	0	0	0	1E-06
Air	Total Suspended Particles	kg	4E-04	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1E-04	0	0	0	0	0	0	2E-04	0	0	0	0	0	3E-04	0	0	5E-04	2E-04	0.007	0
Air	Tribromomethane	kg	0	2E-08	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Air	trichloromethane	kg	0	3E-08	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Air	Vanadium	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1E-06	0	0	0	0	0	0	0	0	0	0	1E-05	0	0	0	0	0	0	0	0	0	0	1E-06
Air	Vinyl acetate	kg	0	3E-09	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Air	Volatile Organic Compounds	kg	3E-04	0	0	0	0.002	0	1E-04	0	0	0	5E-05	0	3E-05	0	0	4E-05	0	0	0	0	0	0	0	0	0	2E-05	0	0	0	0	0	0	0	0	0	0	0	0	7E-05	0	1E-05	0
Air	Waste gases, vent gas, C1-6	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.001	0	0	0	0	0	0
Air	Xylenes	kg	0	2E-08	0	0	3E-06	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	4E-07	0	0	0	0	0	0	0	0	0	0	0
Air	Zinc	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1E-04	0	0	0	0	0	0	0	0	0	0	0
Water	Ammonia	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1E-04	0	0	0	0	0	0
Water	Arsenic	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Water	Biological oxygen demand	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	7E-04	0	0	0	0	0	0
Water	Cadmium	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Water	Chemical Oxygen Demand	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.006	0	0	0	0	2E-04	0
Water	Chromium	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2E-06	0	0	0	0	0	0
Water	Copper	kg	0	0	0	0	3E-08	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2E-06	0	0	0	0	0	0
Water	Dissolved Solids	kg	0	0	0	2E-05	0	0	0	0	0	0	0	0	0	0	5E-05	0	0	0	0	0.005	0	0	0	0	0	0	0	0	0	0	0.336	0	0.004	0	0	0	0	0	0	0	0	0
Water	Hydrochloric acid	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2E-04	0	0	0
Water	Iron	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2E-06	0	0	0	0	0	0
Water	Lead	kg	0	0	0	0	1E-07	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Water	Mercury	kg	0	0	0	0	6E-09	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Water	Nickel	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2E-06	0	0	0	0	0	0
Water	Nitrate	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Water	Oil	kg	0	0	0	0	5E-06	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	3E-04	0	0	0	0	0.001	0
Water	Orthophosphate	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Water	Phenol	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1E-05	0	0	0	0	0	0
Water	Polycyclic aromatic hydrocarbons	kg	0	0	0	0	1E-08	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Water	Sulfate	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Water	Sulfuric acid	kg	0	0	0	9E-04	0	0	0	0	0	0	0	0	0	0	5E-06	0	0	0	0	5E-04	0	0	0	0	0	0	0	0	0	0	0.001	0	1E-05	0	0	0	0	0	0	0	0	0
Water	Suspended Solids	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1E-05	0	0	0	0	0	0	0	0	0	0	0	0	0.003	0	0	0.001	2E-04	0.005	0
Water	Total Nitrogen	kg	0	0	0	0	0.001	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Water	Zinc	kg	0	0	0	0	7E-08	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Figure C.4 Environmental exchange matrix part 2 - E

Product by product total requirements matrix	Coal (per kg)	Coke (per kg)	Cooling water (per m3)	Corn (per kg)	Corn stover (per kg)	Custom labor (per MJ)	DDGS (per kg)	Diesel fuel (per kg)	Electricity (per MJ)	Ethanol (per kg)	Fuel mix energy (per MJ)	Gasoline (per kg)	Herbicide (per kg)	Insecticide (per kg)	Iron (per kg)	Iron ore (per kg)	K fertilizer (per kg)	Limestone (per kg)	LPG (per kg)	Mechanical energy from diesel engines (per MJ)	Mechanical energy from ethanol (per MJ)	Mechanical energy from gasoline (per MJ)	Mechanical energy from LPG (per MJ)	N fertilizer (per kg)	Natural gas (per kg)	Oil (per kg)	Oxygen (per kg)	P fertilizer (per kg)	Railroad transport (per kg-km)	Refined oil (per kg)	Seeds (per kg)	Sinter pellets (per kg)	Steel (per kg)	Steel sheet (per kg)	Thermal energy from coal furnace (per MJ)	Thermal energy from industrial gas furnace (per MJ)	Thermal energy from oil furnace (per MJ)	Thermal energy from utility gas furnace (per MJ)
Coal (kg)	1.007	1.348	0.02	0.011	0.001	0.001	0	0.061	0.056	0.12	0.012	0.064	3.504	3.504	1.965	1E-04	0.059	2E-04	0.061	0.001	0.004	0.001	0.001	0.069	0.007	0.008	0.148	0.115	4E-07	0.061	0.109	1.348	1.711	1.789	0.034	1E-04	2E-04	1E-04
Coke (kg)	-0	1	3E-18	0.001	-0	3E-19	0	4E-17	8E-18	0.005	2E-17	2E-17	2E-15	7E-15	1	-0	2E-17	-0	4E-17	-0	2E-04	0	0	0	0	0	2E-17	7E-18	1E-20	4E-17	0.009	1	0.85	0.85	-0	-0	-0	0
Cooling water (m3)	0	2E-19	1	-0	2E-19	-0	0	2E-19	2E-19	0.134	1E-19	5E-19	0	0	2E-18	-0	1E-17	-0	2E-19	5E-21	0.005	5E-21	-0	-0	2E-20	6E-20	0	1E-18	3E-21	2E-19	6E-18	0	2E-18	2E-18	0	8E-21	-0	3E-19
Corn (kg)	0	4E-18	-0	1.016	6E-18	-0	0	4E-18	4E-18	3.498	3E-18	1E-17	3E-18	3E-18	6E-17	-0	3E-16	-0	4E-18	1E-19	0.131	1E-19	-0	-0	5E-19	2E-18	0	3E-17	7E-20	4E-18	6.099	8E-20	6E-17	6E-17	2E-20	2E-19	-0	8E-18
Corn stover (kg)	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Custom labor (MJ)	0	2E-19	-0	0.056	3E-19	1	0	2E-19	2E-19	0.194	2E-19	7E-19	2E-19	2E-19	3E-18	-0	1E-17	-0	2E-19	7E-21	0.007	7E-21	-0	-0	3E-20	8E-20	0	2E-18	4E-21	2E-19	0.339	5E-21	4E-18	3E-18	1E-21	1E-20	-0	4E-19
DDGS (kg)	0	-0	0	6E-18	-0	2E-19	1	-0	-0	-1	-0	-0	0	0	-0	9E-21	-0	9E-21	-0	-0	-0.04	-0	4E-20	1E-16	-0	-0	0	-0	-0	-0	-0	0	-0	-0	0	-0	2E-19	-0
Diesel fuel (kg)	0.059	0.078	0.001	0.009	0.008	0.014	0	1.004	0.003	0.056	7E-04	0.004	0.214	0.214	0.12	0.002	0.05	0.003	0.004	0.023	0.002	1E-04	9E-05	0.05	4E-04	5E-04	0.009	0.076	6E-06	0.004	0.057	0.082	0.105	0.11	0.002	8E-06	1E-05	8E-06
Electricity (MJ)	0.116	0.31	0.363	0.086	0.023	0.025	0	1.099	1.007	1.767	0.003	1.157	0.962	0.962	0.468	0.003	1.065	0.003	1.099	0.025	0.066	0.026	0.023	0.91	0.128	0.145	2.688	2.092	7E-06	1.099	1.276	0.314	0.617	2.034	0.004	0.002	0.003	0.002
Ethanol (kg)	0	1E-18	0	-0	2E-18	-0	0	1E-18	1E-18	1	9E-19	3E-18	0	0	2E-17	-0	8E-17	-0	1E-18	4E-20	0.038	4E-20	-0	-0	1E-19	4E-19	0	9E-18	2E-20	1E-18	5E-17	0	2E-17	2E-17	0	6E-20	-0	3E-18
Fuel mix energy (MJ)	6E-18	-0	3E-20	0.308	0.01	-0	0	-0	-0	1.07	1	9E-17	300	300	-0	-0	-0	-0	-0	-0	0.04	-0	-0	1.67	8E-19	-0	-0	-0	9E-20	-0	1.848	1E-18	-0	-0	4E-17	-0	7E-16	-0
Gasoline (kg)	-0	1E-17	4E-19	0.002	-0	0.002	0	-0	-0	0.053	3E-19	1	-0	-0	0	-0	0	0	-0	-0	0.002	0.023	-0	-0	4E-18	-0	2E-18	1E-17	2E-20	-0	0.012	1E-17	0	0	0	-0	-0	4E-19
Herbicide (kg)	2E-20	0	0	8E-04	0	0	0	-0	-0	0.003	0	3E-19	1	0	-0	0	-0	0	-0	-0	1E-04	-0	0	-0	0	-0	-0	-0	4E-22	-0	0.005	0	-0	-0	1E-19	-0	2E-18	-0
Insecticide (kg)	0	4E-22	1E-22	8E-05	5E-22	-0	0	0	0	3E-04	2E-22	8E-22	0	1	3E-21	-0	2E-20	-0	0	0	1E-05	1E-23	-0	-0	5E-23	1E-22	0	3E-21	6E-24	0	5E-04	0	7E-21	3E-21	0	2E-23	-0	6E-22
Iron (kg)	-0	-0	2E-18	0.001	6E-19	-0	0	2E-17	4E-18	0.005	-0	5E-18	-0	-0	1	-0	2E-18	-0	2E-17	-0	2E-04	4E-19	-0	5E-18	9E-19	1E-18	-0	8E-18	-0	2E-17	0.009	3E-18	0.85	0.85	1E-17	-0	0	-0
Iron ore (kg)	-0	-0	3E-18	0.002	3E-19	-0	0	4E-17	2E-17	0.007	-0	1E-17	2E-15	2E-15	1.45	1	1E-17	-0	4E-17	2E-19	3E-04	9E-19	2E-20	0	-0	4E-18	-0	0	2E-22	4E-17	0.013	1.45	1.233	1.233	-0	-0	-0	-0
K fertilizer (kg)	-0	4E-18	4E-18	0.008	0.007	0	0	-0	2E-17	0.026	5E-19	-0	5E-16	5E-16	4E-17	-0	1	0	-0	-0	1E-03	-0	-0	5E-16	-0	2E-18	0	7E-17	-0	-0	0.046	-0	-0	3E-17	4E-19	-0	0	0
Limestone (kg)	-0	5E-19	1E-18	0.125	7E-19	-0	0	7E-18	2E-18	0.433	-0	6E-18	1E-16	1E-16	0.13	-0	3E-17	1	7E-18	-0	0.016	1E-19	-0	-0	8E-20	7E-19	-0	1E-17	5E-20	7E-18	0.748	1E-18	0.261	0.261	9E-19	-0	-0	2E-18
LPG (kg)	-0	9E-21	0	0.003	1E-20	0.006	0	0	0	0.009	5E-21	2E-20	-0	-0	0	-0	7E-19	-0	1	3E-22	3E-04	0	0.021	-0	0	2E-21	0	9E-20	6E-25	0	0.016	-0	1E-19	0	0	6E-22	-0	2E-20
Mechanical energy from diesel engines (MJ)	2.548	3.412	0.053	0.392	0.333	0.604	0	0.161	0.148	2.419	0.031	0.17	9.305	9.305	5.213	0.1	2.156	0.122	0.161	1.004	0.091	0.004	0.003	2.184	0.019	0.021	0.394	3.307	3E-04	0.161	2.466	3.557	4.558	4.765	0.09	3E-04	5E-04	3E-04
Mechanical energy from ethanol (MJ)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Mechanical energy from gasoline (MJ)	0	3E-19	1E-19	0.089	5E-19	0.1	0	4E-19	4E-19	0.307	2E-19	1E-18	3E-17	3E-17	7E-18	-0	2E-17	-0	4E-19	1E-20	0.012	1	-0	-0	5E-20	1E-19	9E-19	3E-18	6E-21	4E-19	0.535	0	7E-18	3E-18	2E-19	2E-20	-0	7E-19
Mechanical energy from LPG (MJ)	-0	4E-19	0	0.128	7E-19	0.3	0	0	0	0.442	2E-19	9E-19	-0	-0	0	-0	3E-17	-0	0	1E-20	0.017	0	1	-0	0	1E-19	0	4E-18	3E-23	0	0.771	-0	7E-18	0	0	3E-20	-0	1E-18
N fertilizer (kg)	4E-19	-0	0	0.017	0.006	-0	0	0	-0	0.065	-0	4E-18	1E-17	1E-17	-0	0	-0	-0	0	1E-19	0.002	0	-0	1	4E-19	0	-0	-0	-0	0	0.102	9E-19	-0	-0	-0	2E-19	-0	0
Natural gas (kg)	0.002	0.121	0.002	0.018	0.006	8E-04	0	0.036	0.005	0.333	0.006	0.038	1.907	1.907	0.123	8E-05	0.064	1E-04	0.036	8E-04	0.012	9E-04	8E-04	0.808	1.025	0.011	0.013	0.027	2E-07	0.036	0.142	0.121	0.106	0.113	8E-05	0.019	2E-04	0.019
Oil (kg)	0.061	0.082	0.002	0.017	0.008	0.023	0	1.037	0.005	0.136	0.008	1.092	2.407	2.407	0.125	0.002	0.053	0.004	1.037	0.024	0.005	0.025	0.022	0.066	0.001	1.002	0.013	0.082	6E-06	1.037	0.104	0.085	0.109	0.116	0.002	2E-05	0.022	2E-05
Oxygen (kg)	-0	-0	2E-19	2E-04	3E-20	-0	0	2E-18	2E-19	6E-04	-0	2E-18	1E-17	1E-17	0.03	4E-22	2E-19	4E-21	2E-18	-0	2E-05	4E-20	-0	9E-19	-0	6E-20	1	4E-19	-0	2E-18	0.001	2E-19	0.106	0.106	-0	-0	-0	3E-20
P fertilizer (kg)	0	4E-20	1E-20	0.007	8E-04	-0	0	3E-20	0	0.024	2E-20	5E-20	0	0	4E-19	-0	2E-18	-0	3E-20	8E-22	9E-04	0	-0	-0	0	1E-20	0	1	5E-22	3E-20	0.042	0	4E-19	4E-19	1E-20	1E-21	-0	5E-20
Railroad transport (kg-km)	3.158	8.214	9.351	4.309	0.642	0.636	0	28.33	25.97	3178	5.456	29.82	1637	1637	296.8	0.065	27.46	0.083	28.33	0.652	119.2	0.671	0.594	32.45	3.301	3.726	69.3	53.95	1	28.33	45.42	8.308	271.3	307.9	15.91	0.061	0.082	0.061
Refined oil (kg)	0.059	0.078	0.001	0.014	0.008	0.023	0	1.004	0.003	0.121	7E-04	1.057	0.214	0.214	0.12	0.002	0.05	0.003	1.004	0.023	0.005	0.024	0.021	0.05	4E-04	5E-04	0.009	0.076	6E-06	1.004	0.086	0.082	0.105	0.11	0.002	8E-06	1E-05	8E-06
Seeds (kg)	0	2E-20	-0	0.003	0	-0	0	-0	0	0.009	4E-21	0	6E-19	6E-19	5E-20	5E-23	4E-19	0	-0	0	4E-04	-0	-0	-0	3E-21	7E-21	0	1E-19	-0	-0	1.016	1E-20	1E-19	5E-20	4E-21	2E-21	-0	-0
Sinter pellets (kg)	-0	-0	2E-18	0.001	2E-19	-0	0	3E-17	1E-17	0.005	-0	7E-18	2E-15	2E-15	1	3E-21	7E-18	-0	3E-17	1E-19	2E-04	6E-19	1E-20	0	-0	3E-18	-0	0	1E-22	3E-17	0.009	1	0.85	0.85	-0	-0	-0	-0
Steel (kg)	-0	9E-19	7E-18	0.002	4E-19	-0	0	2E-17	1E-17	0.006	-0	2E-17	7E-16	7E-16	1E-16	2E-20	7E-18	3E-20	2E-17	2E-19	2E-04	4E-19	0	0	-0	2E-18	-0	2E-17	1E-22	2E-17	0.01	7E-18	1	1	-0	-0	3E-18	0
Steel sheet (kg)	-0	9E-19	7E-18	0.002	4E-19	-0	0	2E-17	1E-17	0.006	-0	2E-17	7E-16	7E-16	1E-16	2E-20	7E-18	3E-20	2E-17	2E-19	2E-04	4E-19	0	0	-0	2E-18	-0	2E-17	1E-22	2E-17	0.01	7E-18	9E-18	1	-0	-0	3E-18	0
Thermal energy from coal furnace (MJ)	0.2	0.52	0.592	0.273	0.041	0.04	0	1.793	1.644	3.341	0.345	1.887	103.6	103.6	18.78	0.004	1.738	0.005	1.793	0.041	0.125	0.042	0.038	2.054	0.209	0.236	4.386	3.415	1E-05	1.793	2.875	0.526	17.17	19.49	1.007	0.004	0.005	0.004
Thermal energy from industrial gas furnace (MJ)	0.035	6.377	0.003	0.143	0.015	0.013	0	0.596	0.009	0.878	0.342	0.627	102.7	102.7	6.402	0.001	0.109	0.002	0.596	0.014	0.033	0.014	0.012	1.613	1.303	0.545	0.024	0.077	4E-06	0.596	0.898	6.379	5.445	5.458	0.001	1.024	0.012	0.024
Thermal energy from oil furnace (MJ)	0.012	0.029	0.025	0.109	0.006	0.003	0	0.142	0.069	0.49	0.331	0.149	99.27	99.27	0.043	3E-04	0.077	5E-04	0.142	0.003	0.018	0.003	0.003	0.639	0.036	0.074	0.183	0.147	9E-07	0.142	0.706	0.03	0.052	0.148	4E-04	7E-04	1.002	7E-04
Thermal energy from utility gas furnace (MJ)	0.03	0.08	0.094	0.331	0.105	0.006	0	0.285	0.261	15.1	8E-04	0.3	0.249	0.249	0.121	7E-04	3.276	8E-04	0.285	0.007	0.566	0.007	0.006	12.84	0.033	0.037	0.696	1.292	2E-06	0.285	3.683	0.081	0.16	0.527	0.001	6E-04	8E-04	1.001

Figure C.5 Total requirements matrix - A

EXCHANGE TYPE	ENVIRONMENTAL EXCHANGE	UNITS	AETP (air) kg 1,4-dichlorobenzene to water equivalent/kg	AETP (water) kg 1,4-dichlorobenzene to water equivalent/kg	AP kg SO2 equivalent/kg	Cancer DALYs (air) person-yr/kg released in Europe	Cancer DALYs (water) person-yr/kg released in Europe	EP (air) kg NO2 to air equivalent/kg	EP (water) kg N-tot to water equivalent/kg	GWP100 kg CO2 equivalent/kg	NonCancer DALYs (air) DALYs/kg	NonCancer DALYs (water) DALYs/kg	ODP kg CFC-11 equivalent/kg	PM10 Effects kg PM10 equivalent/kg	POCP kg Ethylene equivalent/kg	TETP (air) kg 1,4-dichlorobenzene to ind soil equivalent/kg	TETP (water) kg 1,4-dichlorobenzene to ind soil equivalent/kg
			H = [Characterization factor matrix]														
Air	1,1,1-trichloroethane	kg	0.003	0	0	0	0	0	0	-224.775	0.000000273	0	0.0999	0	0.004023	2	0
Air	1,1-Dichloroethylene	kg	0	0	0	0.0000051	0	0	0	0	1.105E-08	0	0	0	0.173	0	0
Air	1,2-Dibromoethane	kg	0	0	0	0.00021	0	0	0	0	0.0000052	0	0	0	0	0	0
Air	2,3,7,8-Tetrachlorodibenzo-p-dioxi	kg	7200000	0	0	1500	0	0	0	0	1092	0	0	0	0	260000000	0
Air	2,4-Dinitrotoluene	kg	0	0	0	0.000018	0	0	0	0	1.118E-07	0	0	0	0	0	0
Air	2-Chloro-1-phenylethanone	kg	0	0	0	5.91821E-06	0	0	0	0	0.000115863	0	0	0	0	0	0
Air	2-Methylnaphthalene	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Air	5-Methylchrysene	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Air	Acenaphthene	kg	0	0	0	0	0	0	0	0	2.6E-10	0	0	0	0	0	0
Air	Acenaphthylene	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Air	Acetaldehyde	kg	0	0	0	0.00000022	0	0	0	0	4.94E-09	0	0	0	0.623052	0	0
Air	Acetophenone	kg	0	0	0	0	0	0	0	0	1.092E-08	0	0	0	0	0	0
Air	Acrolein	kg	160	0	0	5.91821E-06	0	0	0	0	0.00000273	0	0	0	0	680	0
Air	Ammonia	kg	0	0	1.88	0	0	2.71	0	-16.6	4.16E-09	0	0	0.103	0	0	0
Air	Anthracene	kg	0	0	0	0	0	0	0	0	5.59E-11	0	0	0	0	0	0
Air	Antimony	kg	0	0	0	0	0	0	0	0	0.0026	0	0	0	0	0	0
Air	Arsenic	kg	5.6	0	0	0.16	0	0	0	0	0.0000702	0	0	0	0	72000	0
Air	Barium	kg	0	0	0	0	0	0	0	0	0.0000052	0	0	0	0	0	0
Air	Benzene	kg	0.0013	0	0	0.000002	0	0	0	11	2.21E-08	0	0	0	0.218	0.063	0
Air	Benzo(a)anthracene	kg	0	0	0	0.11	0	0	0	0	0	0	0	0	0	0	0
Air	Benzo(a)pyrene	kg	320	0	0	0.27	0	0	0	0	0	0	0	0	0	64000000	0
Air	Benzo(b)fluoranthene	kg	0	0	0	0.0042	0	0	0	0	0	0	0	0	0	0	0
Air	Benzo(g,h,i)perylene	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Air	Benzyl chloride	kg	0.000000052	0	0	0.00001	0	0	0	0	2.99E-08	0	0	0	0	3.6E-13	0
Air	Beryllium	kg	0	0	0	0.00005025	0	0	0	0	0.000221	0	0	0	0	0	0
Air	Biphenyl	kg	0	0	0	0	0	0	0	0	7.67E-10	0	0	0	0	0	0
Air	Bis(2-ethyhexyl)phthalate	kg	0.29	0	0	0.0000081	0	0	0	0	0.000000169	0	0	0	0	110	0
Air	Boron	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Air	Bromomethane	kg	2.2	0	0	0	0	0	0	0	0.0000156	0	0.677366667	0	0	1700	0
Air	Cadmium	kg	130	0	0	0.13	0	0	0	0	3.41745E-05	0	0	0	0	130000000	0
Air	Carbon dioxide	kg	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
Air	Carbon disulfide	kg	0.051	0	0	0	0	0	0	0	6.37E-09	0	0	0	0	39	0
Air	Carbon monoxide	kg	0	0	0	0	0	0	0	3	0.000000731	0	0	0	0.018	0	0
Air	Chlorobenzene	kg	0.00099	0	0	0	0	0	0	0	3.64E-09	0	0	0	0	0.045	0
Air	Chloromethane	kg	0	0	0	0.000018	0	0	0	0	0.000000702	0	0	0	0.005	0	0
Air	Chromium	kg	2.5	0	0	0.0003075	0	0	0	0	0.000299	0	0	0	0	220000	0
Air	Chrysene	kg	0	0	0	0.000255	0	0	0	0	0	0	0	0	0	0	0
Air	Cobalt	kg	2.6	0	0	0	0	0	0	0	0.0000351	0	0	0	0	17000	0
Air	Coke oven emissions	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Air	Copper	kg	2.9	0	0	0	0	0	0	0	0.000871	0	0	0	0	910000	0
Air	Cumene	kg	0	0	0	0	0	0	0	0	4.03E-10	0	0	0	0.4885	0	0
Air	Cyanide	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Air	Dibenzo(a,h)anthracene	kg	0	0	0	12	0	0	0	0	0	0	0	0	0	0	0
Air	Dimethyl sulfate	kg	0	0	0	0.00105	0	0	0	0	0	0	0	0	0	0	0
Air	Ethyl chloride	kg	0	0	0	8.46084E-05	0	0	0	0	2.6E-10	0	0	0	0	0	0
Air	Ethylbenzene	kg	0	0	0	0	0	0	0	0	4.29E-10	0	0	0	0.71686	0	0
Air	Fluoranthene	kg	0	0	0	0	0	0	0	0	0.000000065	0	0	0	0	0	0
Air	Fluorene	kg	0	0	0	0	0	0	0	0	3.38E-09	0	0	0	0	0	0
Air	Formaldehyde	kg	6.1	0	0	0.0000032	0	0	0	11	9.1E-09	0	0	0	0.519	2600	0
Air	Hexane	kg	0	0	0	0	0	0	0	0	1.209E-09	0	0	0	0.435246	0	0
Air	Hexavalent chromium	kg	2.5	0	0	530	0	0	0	0	0	0	0	0	0	220000	0
Air	Hydrochloric acid	kg	0	0	0.88	0	0	0	0	-15.3	7.48072E-09	0	0	0.095	0	0	0
Air	Hydrofluoric acid	kg	0	0	1.6	0	0	0	0	-14.9	0	0	0	0.092	0	0	0
Air	Hydrogen sulfide	kg	0	0	1.88	0	0	0	0	-34.73	2.89663E-07	0	0	0.230609238	0	0	0
Air	Indeno(1,2,3-cd)pyrene	kg	0	0	0	0.24	0	0	0	0	0	0	0	0	0	0	0
Air	Isophorone	kg	0	0	0	9.75E-10	0	0	0	0	8.06E-12	0	0	0	0	0	0
Air	Lead	kg	1.2	0	0	0.0001125	0	0	0	0	0.034809918	0	0	0	0	11000	0

Figure C.6 Environmental impact characterization matrix part 1 - T

H = [Characterization factor matrix]

EXCHANGE TYPE	ENVIRONMENTAL EXCHANGE	ENVIRONMENTAL IMPACT CATEGORY / UNITS	AETP (air) kg 1,4-dichlorobenzene to water equivalent/kg	AETP (water) kg 1,4-dichlorobenzene to water equivalent/kg	AP kg SO2 equivalent/kg	Cancer DALYs (air) person-yr/kg released in Europe	Cancer DALYs (water) person-yr/kg released in Europe	EP (air) kg NO2 to air equivalent/kg	EP (water) kg N-tot to water equivalent/kg	GWP100 kg CO2 equivalent/kg	NonCancer DALYs (air) DALYs/kg	NonCancer DALYs (water) DALYs/kg	ODP kg CFC-11 equivalent/kg	PM10 Effects kg PM10 equivalent/kg	POCP kg Ethylene equivalent/kg	TETP (air) kg 1,4-dichlorobenzene to ind soil equivalent/kg	TETP (water) kg 1,4-dichlorobenzene to ind soil equivalent/kg
Air	Magnesium	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Air	Manganese	kg	0	0	0	0	0	0	0	0	0.00001274	0	0	0	0	0	0
Air	Mercury	kg	16000	0	0	0	0	0	0	0	0.000570733	0	0	0	0	13000000	0
Air	Methane	kg	0	0	0	0	0	0	0	21	0	0	0	0	0.006	0	0
Air	Methyl ethyl ketone	kg	0	0	0	0	0	0	0	0	1.43E-09	0	0	0	0.358826	0	0
Air	Methyl methacrylate	kg	0	0	0	0	0	0	0	0	1.82E-10	0	0	0	0	0	0
Air	methyl t-butyl ether	kg	0	0	0	0	0	0	0	0	1.157E-10	0	0	0	0.175	0	0
Air	Methylene chloride	kg	0.00044	0	0	0.00000044	0	0	0	9	7.54E-08	0	0	0	0.050796	0.078	0
Air	Methylhydrazine	kg	0	0	0	1.51356E-08	0	0	0	0	0	0	0	0	0	0	0
Air	Molybdenum	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Air	Naphthalene	kg	0	0	0	8.46084E-05	0	0	0	0	1.69E-08	0	0	0	0	0	0
Air	Nickel	kg	80	0	0	0.095	0	0	0	0	0.00001222	0	0	0	0	190000	0
Air	Nitrous oxide	kg	0	0	0.944974589	0	0	1.35	0	310	9.27517E-07	0	0	0.097468437	0.1575	0	0
Air	Non-methane volatile organic comp	kg	0	0	0	0	0	0	0	0	0	0	0	0	0.493136	0	0
Air	NOx (as NO2)	kg	0	0	0.7	0	0	1	0	40	0.00000043	0	0	0.076290946	0.116666667	0	0
Air	Phenanthrene	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Air	Phenol	kg	39	0	0	0	0	0	0	0	5.85E-11	0	0	0	0	11000	0
Air	Phosphorus	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Air	PM10	kg	0	0	0	0	0	0	0	-8.3	8.58901E-08	0	0	1	0	0	0
Air	Polycyclic aromatic hydrocarbons	kg	0	0	0	1.146577223	0	0	0	0	0	0	0	0	0	0	0
Air	propionaldehyde	kg	0	0	0	0	0	0	0	0	0	0	0	0	0.765282	0	0
Air	Pyrene	kg	0	0	0	0	0	0	0	0	8.06E-09	0	0	0	0	0	0
Air	Selenium	kg	0	0	0	0.00676083	0	0	0	0	0.00001092	0	0	0	0	0	0
Air	Styrene	kg	0	0	0	0.000000063	0	0	0	0	3.9E-11	0	0	0	0.142	0	0
Air	Sulfur dioxide	kg	0	0	1	0	0	0	0	-23.3	0.00000109	0	0	0.153901092	0.048	0	0
Air	Tetrachloroethylene	kg	0.0033	0	0	0.0000048	0	0	0	0	0.000000299	0	0	0	0.020503	110	0
Air	Thallium	kg	0	0	0	0	0	0	0	0	0.000533	0	0	0	0	0	0
Air	Toluene	kg	0.000097	0	0	0	0	0	0	0	1.3E-09	0	0	0	0.632541	0.035	0
Air	Total Suspended Particles	kg	0	0	0	0	0	0	0	-8.3	0	0	0	1	0	0	0
Air	Tribromomethane	kg	0	0	0	0.000015	0	0	0	0	0.000000923	0	0	0	0	0	0
Air	trichloromethane	kg	0.02	0	0	0.000026	0	0	0	4	0.000000104	0	0	0	0.023	5.2	0
Air	Vanadium	kg	11	0	0	0	0	0	0	0	0.0000273	0	0	0	0	450000	0
Air	Vinyl acetate	kg	0	0	0	0	0	0	0	0	2.47E-09	0	0	0	0	0	0
Air	Volatile Organic Compounds	kg	0	0	0	0	0	0	0	11	0	0	0	0	0.459311667	0	0
Air	Waste gases, vent gas, C1-6	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Air	Xylenes	kg	0	0	0	0	0	0	0	0	1.066E-09	0	0	0	0	0	0
Air	Zinc	kg	2.6	0	0	0	0	0	0	0	0.00000338	0	0	0	0	660000	0
Water	Ammonia	kg	0	0	0	0	0	0	0	0	0	1.353E-10	0	0	0	0	0
Water	Arsenic	kg	0	190	0	0	0.00067	0	0	0	0	0.0001947	0	0	0	0	0.0000097
Water	Biological oxygen demand	kg	0	0	0	0	0	0	0.1017	0	0	0	0	0	0	0	0
Water	Cadmium	kg	0	4500	0	0	0.0018	0	0	0	0	0.01188	0	0	0	0	0.025
Water	Chemical Oxygen Demand	kg	0	0	0	0	0	0	0.0508	0	0	0	0	0	0	0	0
Water	Chromium	kg	0	84	0	0	0	0	0	0	0	0.00002145	0	0	0	0	0.000011
Water	Copper	kg	0	96	0	0	0	0	0	0	0	0.002277	0	0	0	0	0.00001
Water	Dissolved Solids	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Water	Hydrochloric acid	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Water	Iron	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Water	Lead	kg	0	40	0	0	0.000507	0	0	0	0	0.001848	0	0	0	0	0.0000002
Water	Mercury	kg	0	130000	0	0	0	0	0	0	0	0.000570733	0	0	0	0	8200000
Water	Nickel	kg	0	2700	0	0	0.001	0	0	0	0	0.0000429	0	0	0	0	0.000031
Water	Nitrate	kg	0	0	0	0	0	0	0.24	0	0	0	0	0	0	0	0
Water	Oil	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Water	Orthophosphate	kg	0	0	0	0	0	0	2.38	0	0	0	0	0	0	0	0
Water	Phenol	kg	0	720	0	0	0	0	0	0	0	1.254E-11	0	0	0	0	34
Water	Polycyclic aromatic hydrocarbons	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Water	Sulfate	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Water	Sulfuric acid	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Water	Suspended Solids	kg	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Water	Total Nitrogen	kg	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
Water	Zinc	kg	0	86	0	0	0	0	0	0	0	0.00001155	0	0	0	0	0.000025
			w' = Transpose of valuation factor vector														
	Valuation factor		0.0001	0.0001	0.8	85000	85000	0.8	0.8	0.03	85000	85000	100	40	2	0.0000003	0.0000003

Figure C.7 Environmental impact characterization matrix part 2 - T

Appendix D Large-Scale Uses of Coal

D.1 Introduction

Coal utilization is not limited to power generation. Coal will continue to be used in significant amounts for coke production for steel manufacture and as a source of heat in a number of industrial processes and in combined heat and power systems. In addition, there is renewed interest in further development of technologies using coal as a feedstock for both transportation fuels and chemicals. Both fuels and chemicals are produced from coal today but only in a few specific instances and locations. The following section provides an overview of other potential large-scale uses of coal along with some limited technical, economic, and environmental assessments. This assessment is aimed at providing a basis for considering the potential for coal use growth beyond that in power generation.

Polygeneration is a term often used in conjunction with future coal-based power generation. This refers to the inclusion of co-product production integrated with base-load power generation. Possible byproducts could be transportation fuels, chemicals, and hydrogen and would give the power plant flexibility to optimize the product output based on market conditions. However, the additional processing capability adds a considerable capital requirement above the typical cost for the power generation facility. For base-load power facilities, this capital expense is prohibitive since the primary utilization for the coal feed will be power, and the other processing capacity will suffer from under-utilization. If transportation fuels are produced from coal, it will be in dedicated facilities designed, optimized, and built for that explicit purpose, and in these cases power production primarily for internal use will be an integral part of the facility design. Therefore, this analysis will forego any further discussion of polygeneration and instead focus on facilities that are primarily geared to either fuels and/or chemicals production.

The goal of this section is to provide estimates for the viability of advanced coal technologies for the production of fuels and chemicals. While many of these concepts have been demonstrated and even commercialized in specific cases, those instances are few, and the available technical and economic data for the system performance is very limited. To develop the best assessment, data from various studies are compared on an equivalent basis. The variation that remains in the analysis is simply due to the uncertainty in the technical and economic data.

D.2 Liquid Fuels Production

The production of fuels from coal has been researched since the beginning of the 20th century. Two primary pathways have been studied, direct and indirect liquefaction. Direct liquefaction involves the use of high temperatures and pressures in the presence of high pressure hydrogen to thermally break down the coal structure and then stabilize the fragments by hydrogenation, producing a mix of hydrocarbons and other organic compounds. Indirect liquefaction is a multi-step process in which the coal is initially gasified to form syngas. This syngas is then converted catalytically to the desired products. For example, by Fischer-Tropsch reaction it is converted into very clean hydrocarbons that can then be refined into high-quality transportation fuels, primarily diesel. The Fischer-Tropsch process has received the most development and has been commercialized by Sasol from coal gasification on a large scale in South Africa and by Shell for natural gas. Direct liquefaction, on the other hand, after much R&D effort, is considered too costly and produces a complex, undesirable product mix requiring much costly additional refining to make acceptable products. The indirect process has the advantage of being more flexible since the syngas can be utilized for a number of different applications. Therefore, this section will focus on the indirect liquefaction process.

The first step in coal to liquids involves coal preparation, air separation, coal gasification, syngas cooling, and syngas treating to remove impurities, particularly all sulfur compounds, and is essentially the same as in IGCC. The optimum conditions of the syngas stream – temperature, pressure, and composition – are dependent on the process to which it is aimed. Each gasifier type produces a syngas stream with specific properties and thus the optimum gasifier will depend on the syngas conversion process considered. In all cases, an oxygen-blown gasifier will be required to eliminate the dilution effect of nitrogen, and a pure syngas stream without methane, light hydrocarbons, oils and tars is highly preferred, suggesting an entrained-flow gasifier.

Gasification for fuels and chemicals production typically requires water gas shift conversions to establish the required CO to hydrogen ratio.

Below we briefly describe several processes to illustrate the potential technologies for the production of hydrocarbons, methanol, and dimethyl ether. Because coal derived diesel and gasoline will easily integrate into the existing infrastructure, we assume they will continue to attract the most interest, and we present the critical decisions which are involved in their production.

D.3 Fischer-Tropsch

In the Fischer-Tropsch process, syngas with the proper carbon monoxide to hydrogen ratio is reacted over a catalyst to produce a broad range of hydrocarbon products.

$$\text{Carbon Monoxide (CO)} + \text{Hydrogen } (H_2) \rightarrow \text{Hydrocarbons } (n\text{-}C_nH_m)$$

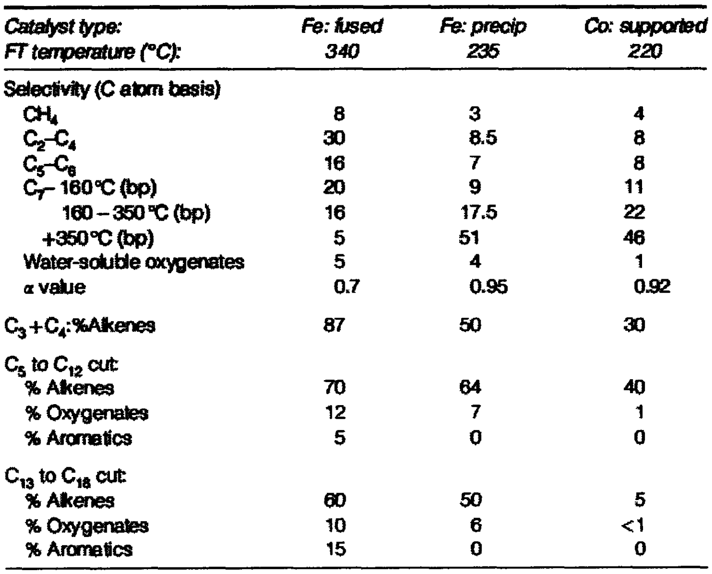
The hydrocarbons produced within the Fischer-Tropsch reactor have a characteristic carbon number distribution that is dependent on catalyst and operating temperature. The reactor outlet is upgraded downstream by hydrogenation, hydro-cracking and hydro-isomerization to produce a product distribution that can be blended into high quality diesel fuel or upgraded furthre to gasoline or chemicals. The most common differentiation between processes are Fischer-Tropsch reactor temperature and type of catalyst used (iron-based or cobalt-based).

D.3.1 Temperature

Low temperature Fischer-Tropsch (LTFT) typically occurs in the range of 220 to 260 °C and results in straight-chain, paraffin-rich hydrocarbons and waxes which can easily be hydrocracked to produce high quality diesel. The high temperature Fischer-Tropsch (HTFT) range is 320 to 350 °C and gives a more highly-branched, olefin-rich naphtha with a lighter product distribution. The HTFT product can be used for gasoline and chemicals production, but requires substantially more refining than the LTFT process. The LTFT operation is typically preferred because a large fraction of the product can be converted to extremely high quality diesel with little additional processing. The diesel can be used directly or blended into other diesel range streams in a refinery. On the other hand, the naptha product from the HTFT version requires much more refining to produce gasoline. While the downstream processing in the LTFT process is easier suggesting its attractiveness, continued demand for gasoline in the U.S. could lead towards possible selection of the HTFT process.

D.3.2 Catalysts

The primary catalysts in Fischer-Tropsch processing are iron and cobalt. Whereas iron is the principal catalyst used in the HTFT process, either iron or cobalt can be used in the LTFT process. The utilization of iron catalyst produces a small fraction of oxygen-containing organics and more olefins. Whereas cobalt catalyst, which is the preferred catalyst today, produces primarily straight chain paraffin hydrocarbons leading to easier downstream refining. Table D.1 shows a typical product breakdown by temperature and catalyst used.



Catalyst type: *FT temperature (°C):*	*Fe: fused* *340*	*Fe: precip* *235*	*Co: supported* *220*
Selectivity (C atom basis)			
CH_4	8	3	4
C_2–C_4	30	8.5	8
C_5–C_6	16	7	8
C_7– 160°C (bp)	20	9	11
160 – 350°C (bp)	16	17.5	22
+350°C (bp)	5	51	46
Water-soluble oxygenates	5	4	1
α value	0.7	0.95	0.92
C_3+C_4:%Alkenes	87	50	30
C_5 to C_{12} cut:			
% Alkenes	70	64	40
% Oxygenates	12	7	1
% Aromatics	5	0	0
C_{13} to C_{18} cut:			
% Alkenes	60	50	5
% Oxygenates	10	6	<1
% Aromatics	15	0	0

Table D.1 Typical Fischer-Tropsch Production distribution (Dry, 2002)

While cobalt is the preferred catalyst for its higher activity and selectivity, a couple of characteristics of coal processing lead iron catalyst to be possibly advantageous. First, iron has water-gas shift activity which means the H_2/CO ratio is not as critical. For cobalt, which doesn't have shift activity, this ratio must be ~2 meaning a coal based syngas with a ratio ~1 would need a separate shift reactor. Second, preventing coal derived catalyst poisons from reaching the Fischer-Tropsch reactor is more difficult than for natural gas, and continually replacing a cobalt catalyst will become prohibitive as the price of cobalt can be ~1000 times more expensive than iron.

D.3.3 Economics

	Coal to Diesel		Coal to SNG	
	w/o capture	w/ capture	w/o capture	w/ capture
PERFORMANCE				
Liquid Production (bbl/day)	50,000	50,000		
SNG Production (MMbtu/hr)			14,000	14,000
h efficiency (HHV)	50.0%	50.0%	60.0%	60.0%
Coal feed, kg/h	973,033	973,033	973,033	973,033
Carbon in coal, kg/h	595,496	595,496	595,496	595,496
CO_2 emitted, kg/h	1,343,208	134,321	1,392,953	139,295
CO_2 captured at 90%, kg/h (3)	0	1,208,888	0	1,253,658
CO_2 emitted, kg/bbl	645	64		
CO_2 emitted, kg/MMBtu			99	10
COSTS				
Total Plant Cost, $/bbl/day	$53,005	$55,753		
Total Capital Required, $/bbl/day	$59,366	$62,443		
Total Plant Cost, $/MMbtu/hr			$109,101	$114,857
Total Capital Required, $/MMbtu/hr			$122,193	$128,640
Inv. Charge, $/bbl @ 15.1% (2)	25.8	27.1		
Fuel, $/bbl @ $1.50/MMBTU	16.80	16.80		
O&M, $/bbl	10.00	14.35		
COE, $/bbl	**52.60**	**58.29**		
Inv. Charge, $/MMBtu @ 15.1% (2)			2.21	2.33
Fuel, $/MMBtu @ $1.50/MMBTU			2.50	2.50
O&M, $/MMBtu			1.49	1.94
COE, $/MMBtu			**6.20**	**6.77**

Table D.2 Economic cost estimations for coal to fuels technology

Using the limited available data from commercial operation and recent design studies, an estimated capital cost for coal to liquids production is of order $55,000 per stream day barrel production for a 100,000 bbl per day facility. That gives a capital cost of $5.5 billion for such a plant. The same type of estimation for a greenfields oil refinery is about $15,000 per stream day barrel. With coal at $1.50/MMBTU and operating and maintenance expenses at $10/bbl, the total operating cost would be about $30 per barrel. The service cost on the capital is about $25 per barrel. Thus, the product would have to recover $55 per barrel to be profitable. An assessment of the economics for both diesel and synthetic natural gas is given in Table D.2

D.3.4 Carbon Emissions

While the coal derived diesel or gasoline would have roughly the same emissions during utilization as that from petroleum, a disadvantage of coal is that over 40% of its carbon is emitted during the Fischer-Tropsch process. Therefore, carbon capture and sequestration would need to be added to the facility, causing the economics of the production to be higher, but not significantly as the CO_2 is typically removed from the process anyway.

D.4 Synthetic Natural Gas

The syngas can also be processed through a methanation reaction, creating synthetic natural gas (SNG). These reactions are exothermic, and low-grade steam can be produced as a byproduct of the process which can be used for power generation or industrial uses. A block flow for both the SNG and Fischer-Tropsch processes is given in Figure D.1

D.5 Methanol and Dimethyl ether (DME)

Catalyst technology was developed decades ago to produce methanol from syngas, predominately produced from natural gas. The same technology can be used to synthesize methanol from syngas produced from coal. Methanol is a primary building block for many chemical products. Methanol can also be dehydrated to produce dimethyl ether. The reactions for the production of methanol and dimethyl ether are:

$$\text{Carbon Monoxide (CO)} + \text{Hydrogen } (H_2) \rightarrow \text{Methanol } (CH_3OH)$$

$$\text{Methanol } (CH_3OH) \rightarrow \text{DME } (CH_3OCH_3)$$

Both of these products can be utilized either as fuels or chemical feedstocks. Methanol can be considered either as an additive or as a fuel itself. The methanol-to-gasoline (MTG) process was commercialized by Mobil Oil to produce gasoline from methanol in New Zealand in 1985. DME is a light weight fuel ether which has similar properties as propane, and it can be used as a substitute for LPG. DME also has potential as a diesel fuel that is clean burning and does not produce particulates.

D.6 Chemicals Production

The gasification of coal for chemicals production has been commercialized for several products. The largest commodity chemical produced worldwide from gasification is ammonia. The typical ammonia process uses natural gas reforming; however, the hydrogen required for the process can also be supplied by coal gasification just as well. World wide there are a number of coal-based plants that produce ammonia from coal. In the United States, Eastman Chemical Company has operated a coal gasification process to produce acetyl and oxochemicals since the early 1980s.

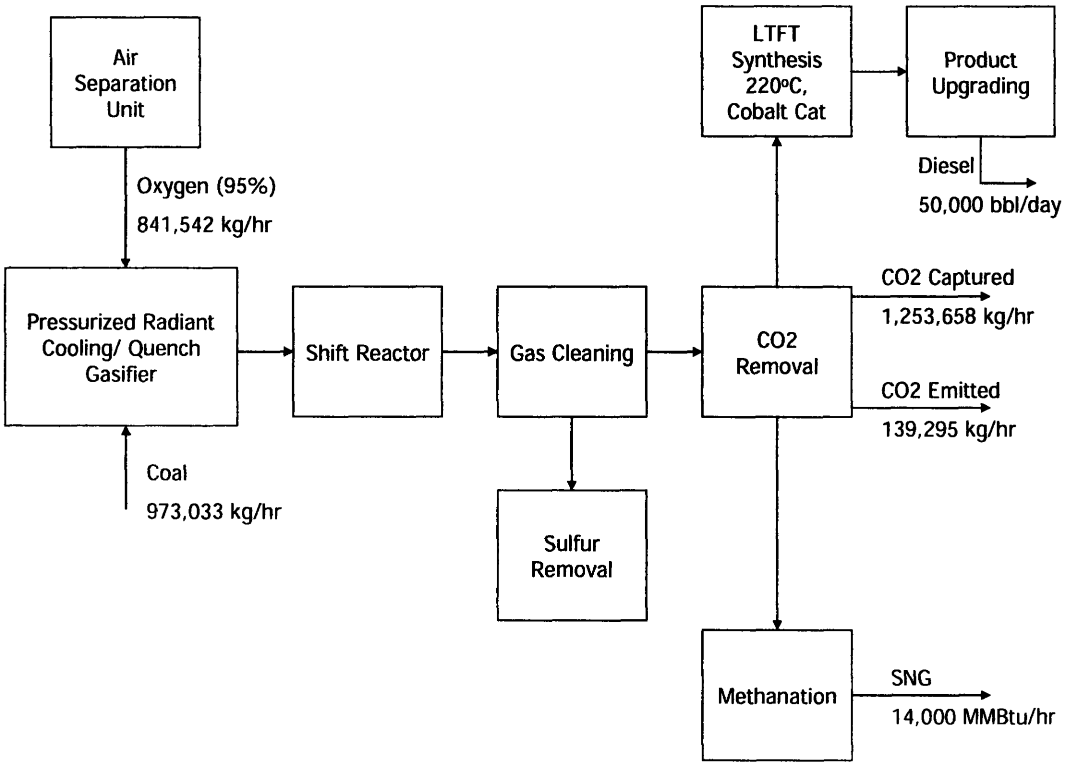


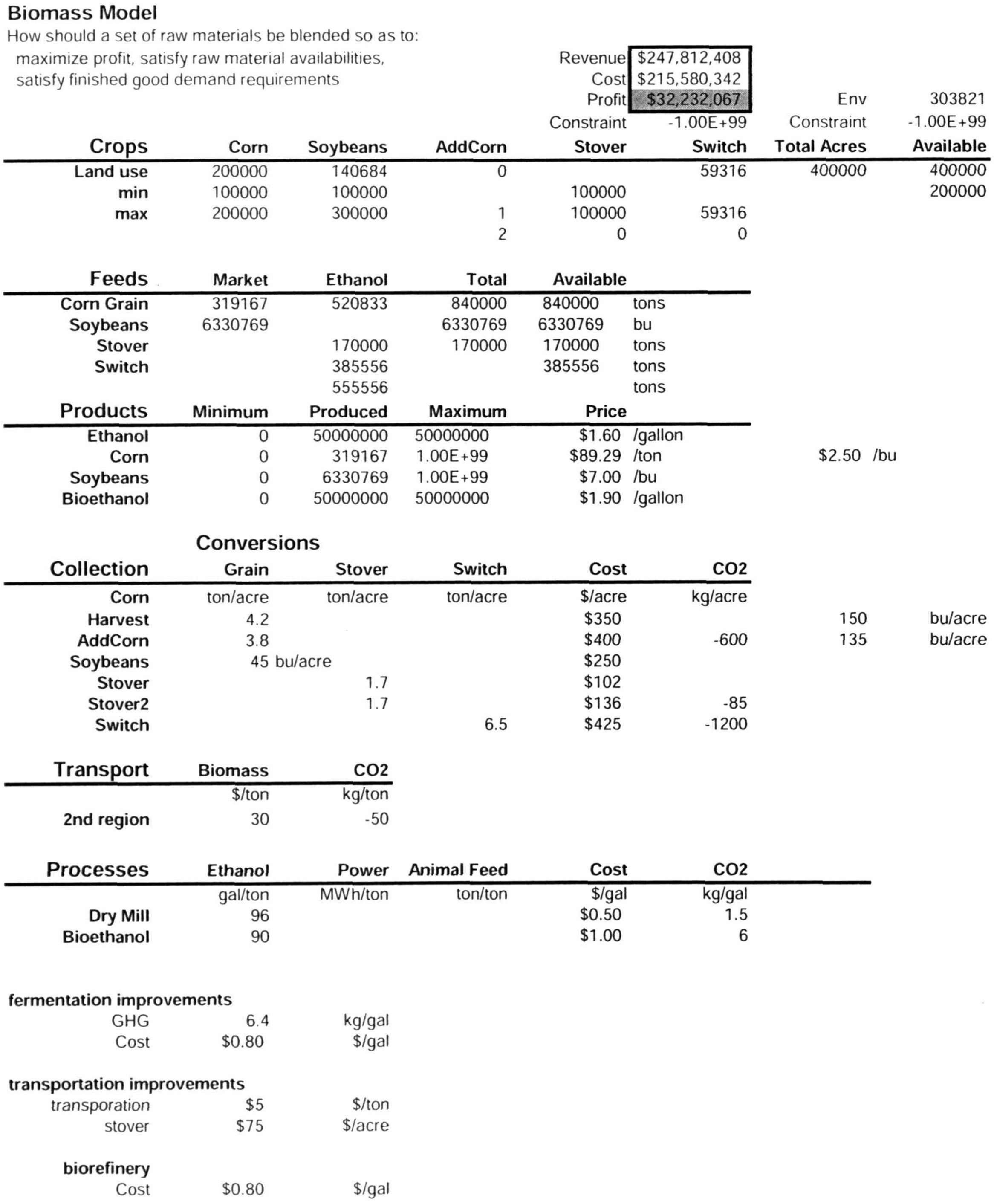
Figure D.1 Process flow diagram for coal to liquids and SNG

Appendix E Network Optimization

Following is the Matlab code used for the formulation of the Pareto frontiers in Chapter 7. Below that is a table with the parameters used in the different case study optimizations.

```
% variable list
Yetoh = 96;
Ycell = 90;
Ycorn = 150*56/2000;
Yaddcorn = 135*56/2000;
Ystover = 1.7;
Ysoy = 45;
Yswitch = 6.5;
Petoh = 1.75;
Cetoh = .5;
Ccell = 1;
Pcornbu = 2.5;
Pcorn = Pcornbu/56*2000;
Psoy = 7;
Ccorn = 350;
Caddcorn = 400;
Cstover = 100;
Csoy = 250;
Cswitch = 425;
Ctrans = 30;
GHGetoh = 1.5;
GHGcell = 6;
GHGaddcorn = -600;
GHGtrans = -50;
GHGswitch = -1000
MaxAcres = 400000;
MaxCorn = 200000;
MaxSoy = 300000;
MinCorn = 100000;
MinSoy = 100000;
MinCornbu = 420000;
MaxStov = 100000;
MaxSwitch = 100000;
MaxEtoh = 500000000;
MaxCell = 500000000;
MaxEtohTot = 100000000;
j=0;
% variables - corn soy addcorn stov stov2 switch switch2 etoh cell corn
soy
% contraints -  land soyacres cornacres stovtot stovacres switchacres
cornbal soybal cellbal etoh cell
     j=j+1
% initial optimizations
      Profit = 1000*[Ccorn; Csoy; Caddcorn; Cstover;
         Cstover+Ctrans*Ystover; Cswitch; Cswitch+Ctrans*Yswitch;
         -(Petoh-Cetoh)*Yetoh; -(Petoh-Ccell)*Ycell; -Pcornbu/56*2000;
```

```
         -Psoy];
      Env = [0; 0; -GHGaddcorn; 0; -GHGtrans*Ystover; -GHGswitch; -
         GHGswitch-GHGtrans*Yswitch;
         -GHGetoh*Yetoh; -GHGcell*Ycell; 0; 0];
      A = [1 1 1 0 0 1 1 0 0 0 0; 0 1 0 0 0 0 0 0 0 0 0; 1 0 0 0 0 0 0
         0 0 0 0; -1 0 -1 1 1 0 0 0 0 0 0;
         0 0 0 1 0 0 0 0 0 0 0; 0 0 0 0 0 1 0 0 0 0 0;
         -Ycorn 0 -Yaddcorn 0 0 0 0 1 0 1 0; 0 -Ysoy 0 0 0 0 0 0 0 0
         1;0 0 0 -Ystover -Ystover -Yswitch -Yswitch 0 1 0 0;
         0 0 0 0 0 0 0 Yetoh 0 0 0; 0 0 0 0 0 0 0 Yetoh Ycell 0 0];
      b = [MaxAcres MaxSoy MaxCorn 0 MaxStov MaxSwitch 0 0 0 MaxEtoh
         MaxEtohTot];
%          Aeq = [1 1 1 0 0 1 1 0 0 0 0; 0 0 0 0 0 1 1 0 0 0 0];
%          beq = [MaxAcres 0];
         Aeq = [1 1 1 0 0 1 1 0 0 0 0];
         beq = [MaxAcres];
      [x1, fprofit] = linprog(Profit,A,b,Aeq,beq,[MinCorn MinSoy 0 0 0
         0 0 0 0 MinCornbu 0],[]);
      [x2, fenv] = linprog(Env,A,b,Aeq,beq,[MinCorn MinSoy 0 0 0 0 0 0
         0 MinCornbu 0],[]);
% specification of minimum and maximum environmental constraints
      minenv(j) = -Env'*x1;
      maxenv(j) = -Env'*x2;
% e-constraint optimizations
      for i = 1:1:11
            A = [1 1 1 0 0 1 1 0 0 0 0; 0 1 0 0 0 0 0 0 0 0 0; 1 0 0 0
               0 0 0 0 0 0 0; -1 0 -1 1 1 0 0 0 0 0 0;
               0 0 0 1 0 0 0 0 0 0 0; 0 0 0 0 0 1 0 0 0 0 0;
               -Ycorn 0 -Yaddcorn 0 0 0 0 1 0 1 0;
               0 -Ysoy 0 0 0 0 0 0 0 1;
               0 0 0 -Ystover -Ystover -Yswitch -Yswitch 0 1 0 0;
               0 0 0 0 0 0 0 Yetoh 0 0 0;
               0 0 0 0 0 0 0 Yetoh Ycell 0 0; 0 0 -GHGaddcorn 0 -
               GHGtrans -GHGswitch -GHGswitch-GHGtrans -GHGetoh*Yetoh -
               GHGcell*Ycell 0 0];
            b = [MaxAcres MaxSoy MaxCorn 0 MaxStov MaxSwitch 0 0 0
               MaxEtoh MaxEtohTot -(minenv(j) + (i-1)/10 * (maxenv(j)-
               minenv(j)))];
            [x, fprofit2] = linprog(Profit,A,b,Aeq,beq,[MinCorn MinSoy
               0 0 0 0 0 0 0 MinCornbu 0],[]);
            P(i)=-Profit'*x;
            E(i)=-Env'*x;
            y(i,:)=x;
        end
        T = [E' P' y];
```



Biomass Model

How should a set of raw materials be blended so as to:
maximize profit, satisfy raw material availabilities,
satisfy finished good demand requirements

Revenue	$247,812,408
Cost	$215,580,342
Profit	$32,232,067
Constraint	-1.00E+99

Env	303821
Constraint	-1.00E+99

Crops	Corn	Soybeans	AddCorn	Stover	Switch	Total Acres	Available
Land use	200000	140684	0		59316	400000	400000
min	100000	100000		100000			200000
max	200000	300000	1	100000	59316		
			2	0	0		

Feeds	Market	Ethanol	Total	Available	
Corn Grain	319167	520833	840000	840000	tons
Soybeans	6330769		6330769	6330769	bu
Stover		170000	170000	170000	tons
Switch		385556		385556	tons
		555556			tons

Products	Minimum	Produced	Maximum	Price			
Ethanol	0	50000000	50000000	$1.60	/gallon		
Corn	0	319167	1.00E+99	$89.29	/ton	$2.50	/bu
Soybeans	0	6330769	1.00E+99	$7.00	/bu		
Bioethanol	0	50000000	50000000	$1.90	/gallon		

Conversions

Collection	Grain	Stover	Switch	Cost	CO2		
Corn	ton/acre	ton/acre	ton/acre	$/acre	kg/acre		
Harvest	4.2			$350		150	bu/acre
AddCorn	3.8			$400	-600	135	bu/acre
Soybeans	45 bu/acre			$250			
Stover		1.7		$102			
Stover2		1.7		$136	-85		
Switch			6.5	$425	-1200		

Transport	Biomass	CO2
	$/ton	kg/ton
2nd region	30	-50

Processes	Ethanol	Power	Animal Feed	Cost	CO2
	gal/ton	MWh/ton	ton/ton	$/gal	kg/gal
Dry Mill	96			$0.50	1.5
Bioethanol	90			$1.00	6

fermentation improvements

GHG	6.4	kg/gal
Cost	$0.80	$/gal

transportation improvements

transporation	$5	$/ton
stover	$75	$/acre

biorefinery

Cost	$0.80	$/gal

Figure E.1 Parameters for network optimization

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