Utility-Integrated Biorefineries

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Introduction

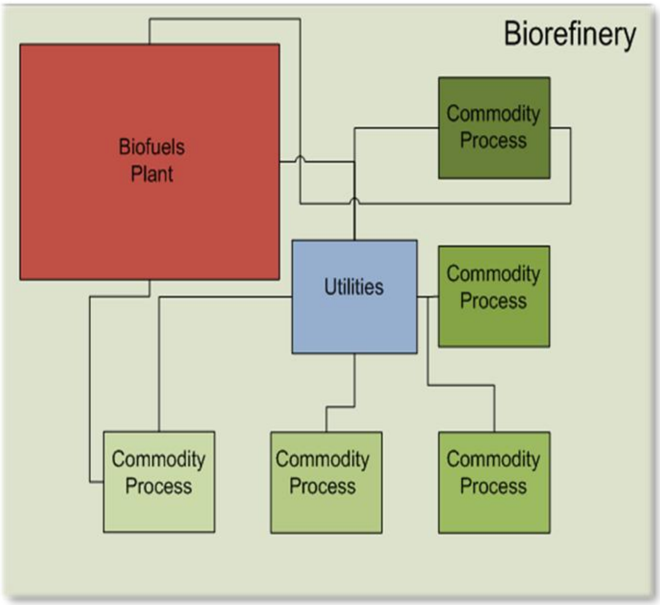
The purpose of this report is to evaluate the feasibility and profitability of a proposed biorefinery. A biorefinery is a chemical plant or cluster of plants that generates value-added products such as biofuels and commodity chemicals from biomass. Biorefineries allow for the integration of multiple processes that require the same biomass feed in one place in order to reduce the cost of each individual process. This integration increases the economic viability of individual processes by reducing operating, transportation, and utility costs. Production of commodity chemicals and fuels from biomass is currently an emerging area of opportunity for several reasons. Small commodity production from biomass is often more cost effective than current production techniques. Since increased demand for biomass directly benefits farming, many government benefits are available to companies investing in this area. The advantages of bio-technology in the area of fuels production include decreased reliance on non-renewable resources such as fossil fuels and decreased CO_2 emissions. There is a high level of public interest in finding viable biomass feedstocks. In recent years, the production of ethanol from corn has been highly publicized. However, corn has several major problems. It generally requires high quality farmland to produce, which could be used for other profitable crops. In addition, using corn to produce fuel puts the fuel and food markets in direct competition, which has major social consequences. In fact, the United Nations has claimed that U.S. subsidies on ethanol production are partially responsible for the current global food crisis. Biorefining from cellulosic feedstocks, specifically switchgrass, eliminates many of these problems. Cellulosic biomass grows naturally in a wider range of climates than other feedstock options and the use of cellulosic biomass for biorefining will not increase demand in other markets. Switchgrass has been shown to be the premier cellulosic feedstock available by several published research studies and is considered the best choice for a biorefinery.

The model used in this study optimizes the planning and development of a biorefinery in the United States. The model takes into account the biorefinery location, raw materials locations, transportation, market locations for products, demand and sales price of products, capital investment, yearly operating costs, and centralized utilities. This model will be used to determine the optimal grouping of commodities processes and biofuels production to maximize net present value.

Background

Biofuels have the potential to reduce the United States' dependence on fossil fuel resources while stemming the tide of global warming. This study will investigate the necessary steps to make biofuels production a reality. The first goal of this study is to determine whether or not the production of biofuels is profitable on its own. Along with this, current government incentives for production of biofuels will be investigated. Another goal of this study is to conclude whether the grouping of biofuels production with commodity production will increase profitability. While the profit generated by commodity production may be large enough to offset the deficit caused by biofuels production, that alone is not enough to support the consolidation of the two processes. The biofuels process must offer enough potential profit from government incentives, decrease in capital, operating, and utility costs, and biofuels sales to support its incorporation in the biorefinery. The final goal is to investigate the carbon emissions generated by the biorefinery and strategies for reducing them. These are all important aspects of the problem that will be addressed completely in this study.

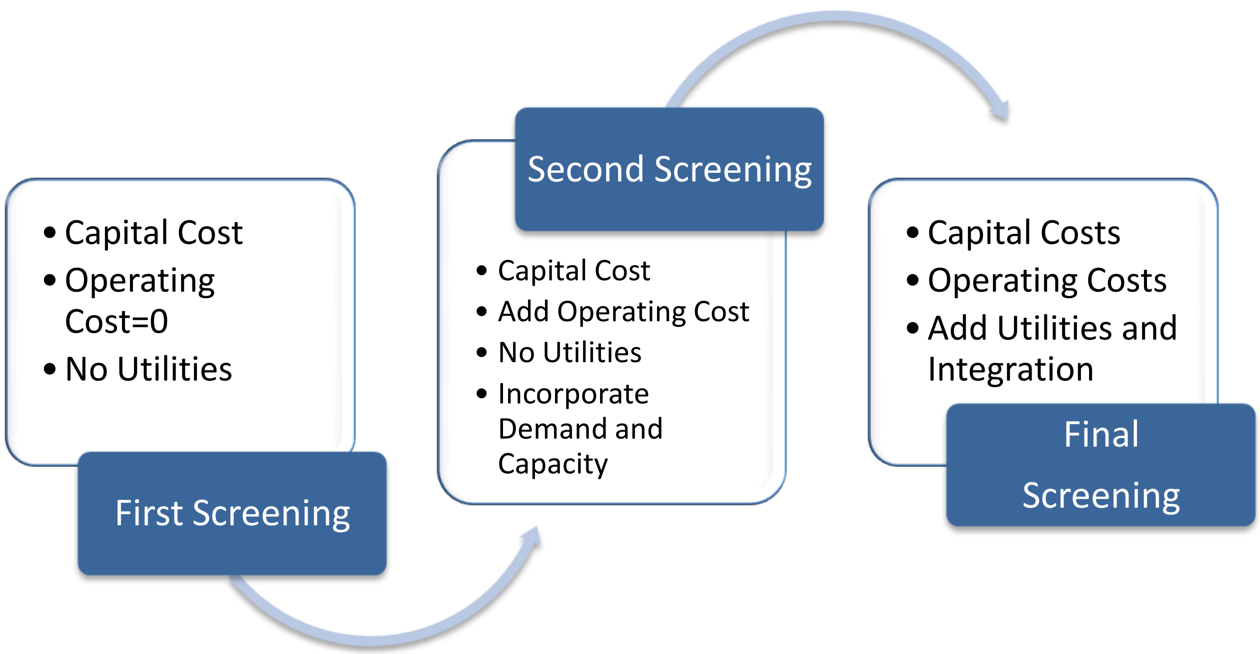
Centralized Utilities

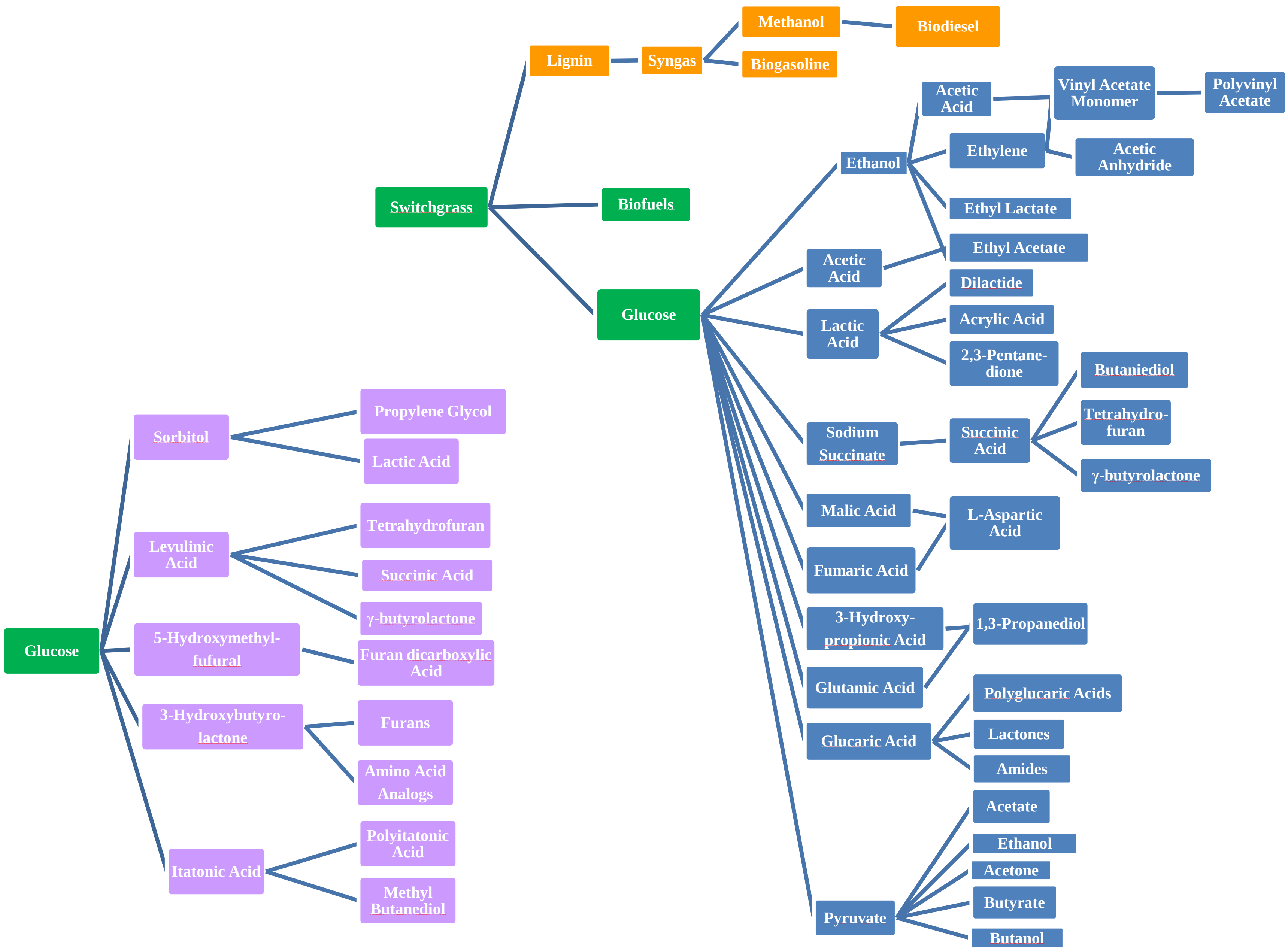


The basic concept of centralized utilities is recycling the utilities from one process within the biorefinery to use them in another process. Centralizing the utilities used by multiple processes in a refinery greatly decreases both the capital and operating costs associated with utilities. There are five major utilities that are taken into account in the model: steam, cooling water, electricity, air, and process water. Process water is water that directly contacts and mixes with process components while cooling water and steam are used for heat exchange and never directly contact process streams. Heat transfer between processes is modeled through the use of steam and cooling water. When modeling the use of utilities in a biorefinery, both the cost of each utility used based on the input stream and the operating and capital costs of operating equipment associated with utilities such as water treatment plants, boilers, and cooling towers were taken into account. In order to maximize the profitability of the biorefinery it is important to minimize utility costs and utility integration is an effective way to do that.

Value-Added Commodities

There are a wide range of value-added chemicals that can be produced from biomass. The first list of processes used in this study was based on previous study in the area of biorefining and included fifty-eight processes. After developing a basic model, the number of processes was reduced by removing any processes that were not profitable if operating cost and utility cost were set equal to zero. This produced a list of seventeen processes that returned a positive net present value under the zero costs condition. The second optimization model incorporated capital investment, operating cost, and product demand. A few processes were eliminated on the basis that the current demand is too low to support even the minimum capacity of a refinery setting. The final screening included capital cost, operating cost, product demand, and utilility costs. The results of this screening made up our base-case scenario. A flow diagram of the systematic screening process and a diagram of the initial process list are included below.

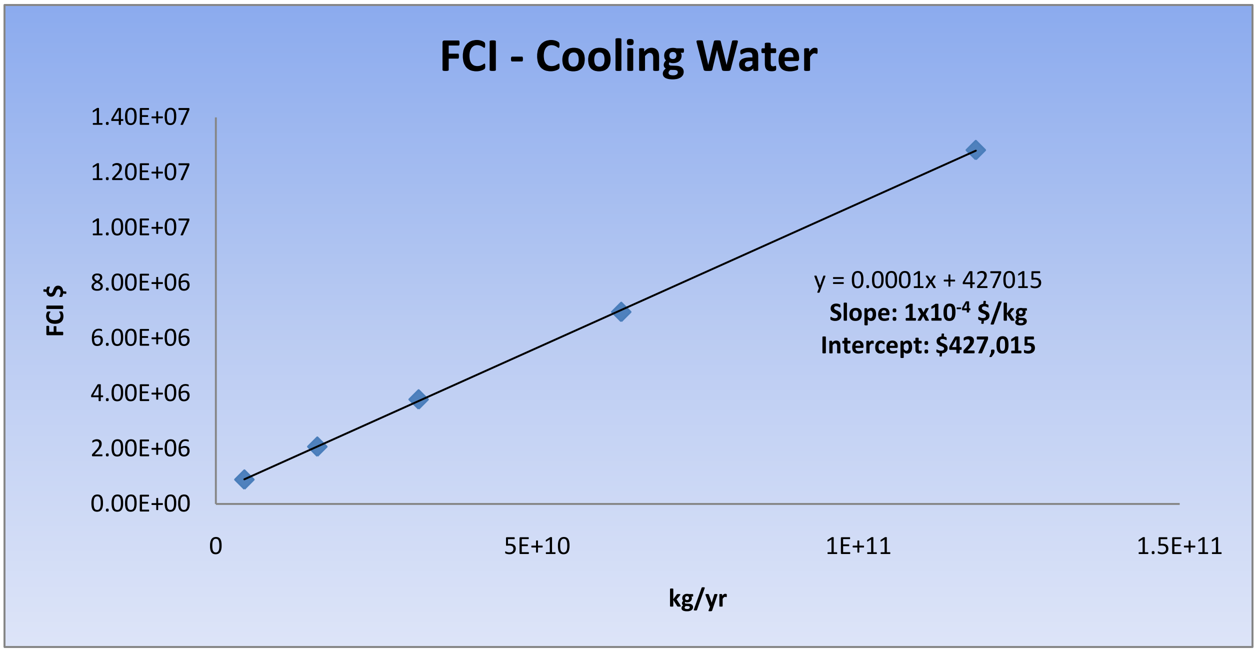




Methanol
Biodiesel
Lignin
Syngas
Biogasoline
Acetic Acid
Vinyl Acetate Monomer
Polyvinyl Acetate
Ethylene
Acetic Anhydride
Ethanol
Switchgrass
Biofuels
Ethyl Lactate
Ethyl Acetate
Acetic Acid
Dilactide
Glucose
Acrylic Acid
Lactic Acid
2,3-Pentane-dione
Butaniediol
Propylene Glycol
Sorbitol
Tetrahydro-furan
Sodium Succinate
Succinic Acid
Lactic Acid
γ-butyrolactone
Malic Acid
L-Aspartic Acid
Tetrahydrofuran
Levulinic Acid
Fumaric Acid
Succinic Acid
γ-butyrolactone
3-Hydroxy-propionic Acid
1,3-Propanediol
Glucose
5-Hydroxymethyl-fufural
Furan dicarboxylic Acid
Glutamic Acid
Polyglucaric Acids
3-Hydroxybutyro-lactone
Furans
Glucaric Acid
Lactones
Amino Acid Analogs
Amides
Acetate
Ethanol
Polyitatonic Acid
Itatonic Acid
Acetone
Butyrate
Methyl Butanediol
Pyruvate
Butanol

Capital Investment and Operating Costs

To obtain Capital and Operating Costs for use in our mathematical model, an incremental model was used. That is, it was assumed that $cost = \alpha \cdot capacity + \beta$ where alpha and beta are



constants. To determine the value of alpha and beta, the processes were simulated in SuperPro at varying capacities. The cost is then plotted against the capacity and a linear fit is obtained. The figure above shows a sample of the plot generated.

This process was used to find analytical models for all of the processes included in our model. Capital and Operating Costs constants for the utilities were calculated separately from overall costs; the same basic method was used to determine alpha and beta coefficients for the capital investment and operating costs associated with utilities. These estimations were based off the major pieces of equipment associated with each utility. For example, the estimation of costs associated with steam was based on the cost of a boiler plant.

Demand

In the mathematical model, the value for demand determines how much of a product the model is allowed to sell in kg/year. For example, if the demand value for biodiesel is 10^9, the model will produce no more than 10^9 kg/year of biodiesel. Obviously, there is no easy or foolproof way to know how much of each product can be sold. Instead, the values for demand were estimated from known U.S. chemical consumptions (since the chemicals will be sold in the U.S.). These values were found online; the specific websites can be found in the sources appendix in the supporting data. In some cases, only world consumption was available. When data for chemicals with known U.S. and world consumption was examined, it was found that U.S. consumption was consistently around 25% of world consumption for chemical commodities. Given this, the U.S. consumption was calculated for most of the chemicals in the model. However, the U.S. consumption should not be used as the value for demand. To see this, imagine what would happen if a new plant introduced supply of a commodity equal to that commodity's annual consumption. It is obvious that the market for the commodity would be destroyed. To account for this, the demand values were chosen as 20% of U.S. consumption. This was thought to be a production level which would not have a substantial negative impact on the market.

Sample Demand

Commodity	**Gasoline**	**Biodiesel**	**3-Hydropropionic Acid**	**Levulinic Acid**
Demand (kg/yr)	77,400,000,000	27,600,000,000	655,000,000	205,000,000

Incentives

A major goal when manufacturing biofuels is maximizing the benefit obtained from government subsidies. The first step in this direction is awareness of what incentives are available. The Department of Energy maintains a comprehensive database of government subsidies in all areas of renewable energy. For this project, the relevant incentives were identified and incorporated in the mathematical model.

There are two main types of incentives available: tax credits and grants/loans. Tax credits are a flat reduction in taxes. For example, if a $1/gallon tax credit is available of biodiesel and 100,000 gallons of biodiesel is manufactured at facility A, facility A can claim a $100,000 reduction in their taxes for that year. Tax credits are especially prominent in modeling economic ventures because, unlike grants/loans, they are guaranteed. This is extremely important in business where low risk is valued highly. Grants and loans, on the other hand, are distributed by the applicable government agency to projects which they feel are deserving. While this can be extremely rewarding, it also carries the risk of not receiving the subsidy.

National Biofuels Incentives

Program	Agency	Type	Amount	Likelihood
VAPG	USDA	Grant	300,000	Possible
Rural Business-Cooperative Service	USDA	Loan	250,000,000	Possible
B&I Guaranteed Loan Program	USDA	Loan	40,000,000	Possible
Cellulosic Biofuel Producer Tax Credit	Congress	Tax Credit	$1.01/gallon produced	Guaranteed

Selected State Biofuels Incentives

Program	State	Type	Amount	Likelihood
Biodiesel Production Tax Credit	IN	Tax Credit	$1/gal biodiesel up to $5 million	Guaranteed
Biodiesel Production Tax Credit	KY	Tax Credit	$1/gal biodiesel up to $5 million	Guaranteed

Algae

In recent years, algae has rapidly gained attention as a potential feedstock for biofuels. The technology necessary to produce biodiesel from triglycerides (such as algal oil) has been available since the late 1930s. However, available sources of triglycerides (such as soybean oil) have always required heavy consumption of farmland. Since that put them in direct competition with food crops, the production of biodiesel from triglycerides has never been commercially feasible. Algae could change all of that. Recent research suggests that algae could produce higher yields of oil than conventional oil crops. In addition, algae can be cultivated in coastal waters, thus eliminating the competition with food crops. Furthermore, in recent studies, algae has demonstrated the ability to sequester up to 50% of CO_2 from gas streams passed through the algae. Clearly, algae has potential as a feedstock. It remains to be seen whether it can be a profitable addition to a biorefinery.

Since the biorefinery will likely be built inland, only land-based algae cultivation methods were considered. Aquatic cultivation is also viable, but coastal locations are likely not suitable for a biorefinery given the large amounts of land-based feedstock required. In addition, both states identified as optimal locations in terms of government biofuel incentives are landlocked. There are three common approaches to land-based algae cultivation: open pools, closed pools, and photobioreactors. Open pools are exactly what they sound like: open air pools filled with water and seeded with algae. Closed pools are essentially open pools with greenhouses constructed over the top. Photobioreactors are structures designed specifically for growing algae productively. For a biorefinery application, open pools are the only viable choice. The other options produce better yields and eliminate some of the problems associated with open pools, but are impractical on a large scale.

The production of biodiesel from algal oil is performed by transesterification with methanol. The algal oil is a triglyceride with molecular weight of approximately 930 g/mol. When methanol is added to the oil, the methanol groups substitute into the triglyceride to produce glycerol and three methyl esters with molecular weights of approximately 310 g/mol. This falls into the molecular weight range of diesel (or biodiesel in this case). To catalyze the reaction, alkali hydroxides or methoxides are used. The catalyst activates methanol by removing a proton from the alcohol group. Sodium methoxide ($NaOCH_3$) is considered the best catalyst from a commercial point of view. The effluent from the reaction vessel is a mixture of glycerol, biodiesel, and unreacted triglycerides. This stream is either centrifuged with water or extracted with ether to separate the glycerol and the biodiesel. It is then desired to purify the biodiesel. However, since the remaining triglycerides are in a basic state, they are soaps and act as emulsifying agents. To achieve a good separation, the biodiesel stream is washed with water which has been acidified to a pH of approximately 4. This returns the triglycerides to their neutral configuration, which allows them to be extracted in the water stream. The biodiesel is then dried to meet fuel standards.

To include algae in the mathematical model, it was necessary to compute each of the relevant sets of coefficients: stoichiometric, utility consumption, utility generation, capital, and operating costs. Stoichiometric coefficients were computed in two stages: one for algae production and one for transesterification. Values for the amount of CO_2 required for algae production was found in recent research. Values for transesterification were easily computed from the chemical equation. For the other four sets, a SuperPro simulation for the transesterification of soybean oil was adapted for algal oil. The coefficients were then computed from the simulation results. The methods used were identical to those used previously for other processes.

Mathematical Model

GAMS/CPLEX was used to optimize the select processes and design parameters within the biorefinery to maximize the net present value.

Set	Name
i,k	Processes
j,jj	Chemicals
t,tt	Time Periods
m	Market Locations
n	Raw Material Locations
p	Plant Locations
u	Utilities

The objective function maximized the net present value (maxNPV). This function summed the proceeds returned to the investors each year (P_t) and adjusted this value to the current time period by using the interest rate. The capital investment (capinv) was then subtracted from this sum.

$$maxNPV = \sum_t \frac{P_t}{(1+interest)^{year_t}} - capinv \tag{1}$$

Economic Equations

The cash on hand for each year is equal to the previous year's cash plus the total revenue from all processes minus the money returned to the investors all costs, including transportation costs, operating costs, and fixed costs. In the first year, the capital investment is added to the cash.

$$cash_t = cash_{t-1} + \sum_j revenue_{j,t} - transport_t - totalopcost_t - FC_t - tax_t - P_t \tag{2}$$

The tax equation is equal to the tax rate times the cash flow, not including depreciation.

$$tax_t = taxrate(cash_t - deprate \times \sum_{tt} FC) \tag{3}$$

There is also a stipulation that the cash on hand for each year must be larger than a certain value for contingencies. In this case, the contingency money is 1% of the capital investment.

$$cash_t \geq 0.01 \times capinv \tag{4}$$

The capital investment for this program is defined as the sum of the fixed costs and material costs for all years adjusted to the current time period.

$$capinv = \sum_t \frac{FC_t + materialcost_t}{(1+interest)^{year_t}} \tag{5}$$

An additional constraint was added to ensure that the capital investment is less than the maximum available investment, which was set in advance.

$$capinv \leq investment \tag{6}$$

The fixed cost for each year is the sum of the initial fixed costs, expansion fixed costs, and utilities fixed costs for all the processes or utilities.

$$FC_t = \sum_i FCinitial_{i,t} + \sum_i FCexpansion_{i,t} + \sum_u FCUtilities_{u,t} \tag{7}$$

The initial fixed capital investment for each process was modeled as a linear function with a minimum cost to build the process ($alpha_i$) and an incremental cost ($beta_i$) associated with the capacity of the process initially. $isBuilt_{i,t}$ is a binary variable that is equal to 1 in the year the process is built and is equal to 0 for all other years.

$$FCinitial_{i,t} = alpha_i \times isBuilt_{i,t} + beta_i \times initialcapacity_{i,t} \tag{8}$$

The expansion is similarly based on a minimum cost ($alpha2_i$) and an incremental cost ($beta2_i$). The coefficients alpha2 and beta2 are 71% of alpha and beta, respectively. This percentage is based on the price to expand a process with the infrastructure already built versus building a grassroots plant. Similar to $isBuilt_{i,t}$, $isExpanded_{i,t}$ is also a binary variable, though it indicates whether or not a process is expanded in the year indicated.

$$FCexpansion_{i,t} = alpha2_i \times isExpanded_{i,t} + beta2_i \times expansion_{i,t} \tag{9}$$

The fixed costs for the utilities closely resemble the cost equations for the chemical processes above.

$$FCUtilities_{u,t} = FCUinitial_{u,t} + FCUexpansion_{u,t} \tag{10}$$

$$FCUinitial_{u,t} = a_u \times isBuiltUtil_{u,t} + bb_u \times intitalutilitycapacity_{u,t} \tag{11}$$

$$FCUexpansion_{u,t} = a2_u \times isExpandedUtil_{u,t} + bb2_u \times utilityexpansion_{u,t} \tag{12}$$

The total operating cost is equal to the sum of the operating costs for all processes and utilities.

$$totalopcost_t = \sum_i operatingcost_{i,t} + \sum_u utilitycosts_{u,t} \tag{13}$$

The operating cost is based on a linear model, similar to the model for fixed costs.

$$operatingcost_{i,t} = delta_i \times \sum_{tt} isBuilt_{i,tt} + epsilon_i \times \sum_j output_{i,j,t} \tag{14}$$

$$utilitycosts_{u,t} = d_u \times \sum_{tt} isBuiltUtil_{u,tt} + e_u \times makeup_{u,t} \tag{15}$$

The revenue for each chemical is the sum of all the chemicals sold to markets at the price that can be obtained from that market.

$$revenue_{j,t} = \sum_p \sum_m prodsell_{p,j,m,t} \times price_{j,m,t} \tag{16}$$

The cost associated with the raw materials is equal to the sum of raw material bought at each field times the raw material price for that location.

$$materialcost_t = \sum_n \sum_p raw\_price_{n,t} \times rawbuy_{n,p,t} \tag{17}$$

The transportation cost for any year is the sum of the cost of transporting raw materials from their fields and the cost to move products to their markets.

$$Transport_t = rawTransport_t + salesTransport_t \tag{18}$$

The product and raw material transport costs are equal to the amount of material moved multiplied by the distance traveled and the cost to move the material per kilogram per mile.

$$salesTransport_t = \sum_{p,j,m} prodsell_{p,j,m,t} \times salesdistance_{p,m} \times salesfreight \tag{19}$$

$$rawTransport_t = \sum_n \sum_p rawbuy_{n,p,t} \times rawdistance_{n,p} \times rawfreightcost \tag{20}$$

Constraints and Material Balances

These equations ensure that mass is not created or destroyed and that the model does not violate common sense. Equation 21 ensures that any one process is only built once.

$$\sum_t isBuilt_{i,t} \leq 1 \tag{21}$$

The following equation makes sure that the process cannot be expanded and built in the same year.

$$isBuilt_{i,t} + isExpanded_{i,t} \leq 1 \tag{22}$$

The next equation sums the time periods, tt, up to the present year. Its purpose is to keep the process from being expanded until it is built.

$$isExpanded_{i,t} \leq \sum_{tt} isBuilt_{i,tt} \tag{23}$$

The utility building and expansion equations are essentially the same as those for the chemical processes above.

$$\sum_{t} isBuiltUtil_{u,t} \leq 1 \tag{24}$$

$$isBuiltUtil_{u,t} + isExpandedUtil_{u,t} \leq 1 \tag{25}$$

$$isExpandedUtil_{u,t} \leq \sum_{tt} isBuiltUtil_{u,tt} \tag{26}$$

The capacity for each process is equal to the initial capacity that year (the initial capacity is zero in years the process is not built) plus the capacity from the year before plus any expansions that occurred this year.

$$capacity_{i,t} = initialcapacity_{i,t} + capcity_{i,(t-1)} + expansion_{i,t} \qquad (25)$$

The following equation causes the process capacity to be larger than the sum of its products.

$$capacity_{i,t} \geq \sum_{j} output_{i,j,t} \qquad (26)$$

The initial capacity must be zero for all years except the one in which the process is built, and in that year, the initial capacity must be larger than the minimum capacity.

$$initialcapacity_{i,t} \geq isBuilt_{i,t} \times mincapacity_{i,t} \tag{27}$$

Similarly, the initial capacity in the year the process is built must be less than the maximum allowable capacity.

$$initialcapacity_{i,t} \leq isBuilt_{i,t} \times maxcapacity_{i,t} \tag{28}$$

Similar equations exist for the process expansion term.

$$expansion_{i,t} \geq isExpanded_{i,t} \times minexpansion_{i,t} \tag{29}$$

$$expansion_{i,t} \leq isExpanded_{i,t} \times maxexpansion_{i,t} \tag{30}$$

This equation allows for setting a maximum allowable number of expansions.

$$\sum_t isExpanded_{i,t} \leq nexp_i \tag{31}$$

The utility capacity is the sum of the initial capacity for utilities, the capacity last year, and the expansion for that year.

$$utilitycapacity_{u,t} = initialutilitycap_{u,t} + utilitycap_{u,(t-1)} + utilityexp_{u,t} \tag{32}$$

The makeup term will be explained later in the Utility Integration subsection. It is essentially the amount utility that the process requires. This equation ensures that the utility capacity is equal to or larger than the required utility.

$$utilitycapacity_{u,t} \geq makeup_{u,t} \tag{33}$$

These equations closely resemble Equations 27-31 above.

$$initialutilitycapacity_{u,t} \geq isBuiltUtil_{u,t} \times minutilitycapacity_{u,t} \tag{34}$$

$$initialutilitycapacity_{u,t} \leq isBuiltUtil_{u,t} \times maxutilitycapacity_{u,t} \tag{35}$$

$$utilityexpansion_{u,t} \geq isExpandedUtil_{u,t} \times minutilityexpansion_{u,t} \tag{36}$$

$$utilityexpansion_{u,t} \leq isExpandedUtil_{u,t} \times maxutilityexpansion_{u,t} \tag{37}$$

$$\sum_t isExpandedUtil_{u,t} \leq nuexp_u \tag{38}$$

Q_p is a binary variable which is set to 1 if the biorefinery is to be built at this location or zero if it is not. This equation ensures that the biorefinery is only located at one optimal location.

$$\sum_p Q_p = 1 \tag{39}$$

The following equation makes sure that the amount of raw material purchased from any one field does not exceed the maximum amount of raw material that field can produce.

$$rawbuy_{n,p,t} \leq maxRawPerField \times Q_p \tag{40}$$

The sum of the raw materials needed for all the processes must equal the amount of raw materials purchased.

$$\sum_i \sum_j raw_{i,j,t} = \sum_n \sum_p rawbuy_{n,p,t} \tag{41}$$

The input to any process is equal to the raw materials coming from other processes plus the amount of raw materials purchased for this process from raw material producers.

$$input_{k,j,t} = raw_{k,j,t} + \sum_i flow_{i,k,j,t} \tag{42}$$

The input into a process is defined as a fraction of the total input into that process. The value of this fraction is $f_{i,j}$ for each process and chemical.

$$input_{i,j,t} = f_{i,j} \times \sum_{jj} input_{i,jj,t} \tag{43}$$

This is the primary mass balance which states that the sum of all the inputs into a process must equal the sum of all the outputs from the process.

$$\sum_j input_{i,j,t} = \sum_j output_{i,j,t} \tag{44}$$

The output from the process must be greater than or equal to the minimum capacity of the process, if the process has been built.

$$\sum_j output_{i,j,t} \geq \sum_{tt} isBuilt_{i,tt} \times mincapacity_i \tag{45}$$

The flow of a chemical from this process to another cannot exceed the output of this chemical from this process. Gamma is a binary parameter which is equal to one if the process can transfer this chemical to another process and is equal to zero if the process cannot.

$$flow_{i,k,j,t} \leq gamma_{i,j,k} \times output_{i,j,t} \tag{46}$$

The output from a process is defined as a stoichiometric fraction of the total output from that process. The fraction of the output for each chemical is $g_{i,j}$.

$$output_{i,j,t} = g_{i,j} \times \sum_{jj} output_{i,jj,t} \tag{47}$$

The output of the process is equal to the amount to be sold plus the amount of product that is transferred to use in other processes.

$$output_{i,j,t} = sales_{i,j,t} + \sum_{k} flow_{i,k,j,t} \tag{48}$$

The amount of chemicals from all the processes to be sold is equal to the amount of chemicals sold at markets from the plant.

$$\sum_{i} sales_{i,j,t} = \sum_{p} \sum_{m} prodsell_{p,j,m,t} \tag{49}$$

The amount of chemical to be sold cannot exceed the demand for that chemical.

$$\sum_{i} sales_{i,j,t} \leq demand_{j,t} \tag{50}$$

The amount of product sold to one market cannot exceed a predetermined limit per year.

$$prodsell_{p,j,m,t} \leq maxPerCityPerYear \times Q_{p} \tag{51}$$

The amount of product sold to one market cannot exceed a certain number for the sum of all years the chemical is sold.

$$prodsell_{p,j,m,t} \leq maxPerCityTotal \times Q_{p} \tag{52}$$

Intermediate Processes

Some of the processes considered do not use switchgrass as a raw material, but instead use a chemical that must be processed from switchgrass as a feedstock. This equation is set up to ensure that these secondary processes cannot be built unless the intermediate chemical is being produced from another process in the biorefinery.

$Prereq_{i,k}$ is a binary parameter that is set to one if the process requires a feedstock other than switchgrass and zero if the process uses switchgrass.

$$isBuilt_{i,t} \leq \sum_k prereq_{i,k} \times isBuilt_{k,t} \tag{53}$$

The following equation is only applicable if the process requires an intermediate feedstock. This equation makes sure that the input to the secondary process does not exceed the amount of chemical the process producing its feedstock can produce.

$$input_{k,j,t} \leq \sum_i input_{i,j,t} \tag{54}$$

Utility Integration

The idea of utility integration allows for utilities being created in one process to be used in another. If a process creates a utility, the utility generation variable is equal to a coefficient times the total input into the process.

$$utilitygeneration_{i,u,t} = utilitycoeff1_{i,u} \times \sum_j input_{i,j,t} \tag{55}$$

Similarly, the amount of utility consumed by a process is equal to a coefficient times the total input into the process

$$utilityconsumption_{i,u,t} = utilitycoeff2_{i,u} \times \sum_j input_{i,j,t} \tag{56}$$

The $makeup_{u,t}$ variable is the amount of utility that is required beyond what is created in all the processes. If a process generates enough utility for all the processes that are built, then the makeup is not needed and no fixed capital will be spent on creating that utility.

$$makeup_{u,t} \geq \sum_i utilityconsumption_{i,u,t} - \sum_i utilitygeneration_{i,u,t} \quad (57)$$

Results

Baseline Results

After narrowing the list of processes to be incorporated to thirteen, the final screening was run. The major variables that were included in the model were the processes built (including biofuels), the capacity of each process, the capacity of expansions, the location of the biorefinery, the markets for buying and selling, and the possible utility schemes. As mentioned before, the objective of the model was to maximize the net present value of the refinery. The model was initially based on a maximum capital investment of \$2.5 billion. The current available government tax credit of \$1 per gallon of biofuel produced was included by adding it directly to the sales price of the biofuels. For example, the original sales price of biodiesel was set at \$1.23 per kilogram but the sales price incorporated into the model was \$1.56 per kilogram after accounting for the \$1 per gallon tax credit. The results of the baseline (initial) optimization are organized in the included table.

Baseline Results		
Location:	**Processes:**	**Capacity (kg/yr)**
Lexington, KY	Biofuels	1,440,000,000
	3-HPA	6,500,000
	Levulinic Acid	57,600,000
	Tetrahydrofuran	40,000,000
TCI ($)	**NPV ($)**	**ROI**
176,000,000	687,000,000	24.5%

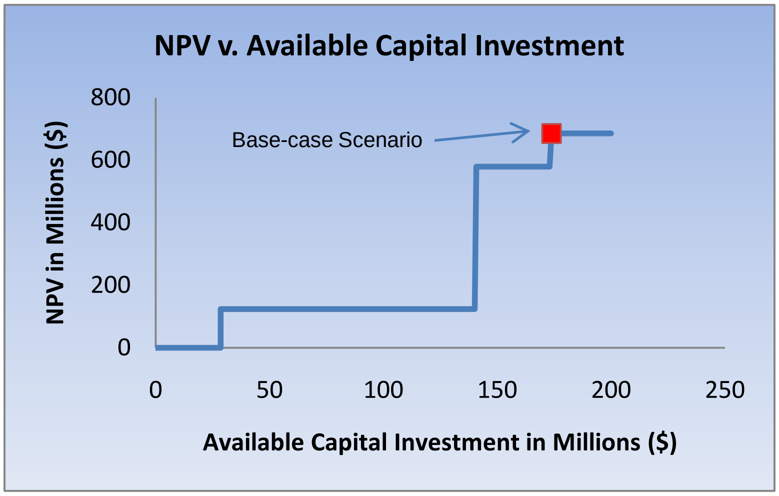
With the current demands of each process and sales prices in the United States the profitable processes to incorporate in the biorefinery are the production of biofuels, 3-hydroxypropionic acid, levulinic acid, and tetrahydrofuran. The raw materials, specifically the switchgrass are supplied from across the state of Kentucky. The biofuels are sold in Louisville, KY while the chemical commodities are sold in various locations ranging from Missouri to Florida. Initially only enough levulinic acid is produced to be used as the building block for tetrahydrofuran production, but after the second year expansion levulinic acid is also sold.

The chemical commodities to be produced in the biorefinery have a variety of applications. 3-hydroxypropionic acid, or 3-HPA is used as a building block for a variety of chemicals including acrylics, malonic acid, 1,3-propanediol, EEP, and some polymers. Tetrahydrofuran, also known as THF, is used primarily as a solvent for industrial resins. It is also used to coat PVC and cellophane, and is used in paint manufacture while levulinic acid has a wide variety of uses from the production of synthetic rubber and pharmaceuticals to cigarettes.

Therefore from the base-case results it can be concluded that the mathematical model supports the hypothesis that the combination of multiple processes in a single biorefinery from a common feedstock is an optimal investment. The results also support the inclusion of biofuel production in a biorefinery setting as a profitable choice. The results from the initial model will be used in a stochastic analysis which will determine the uncertainty of the results and find an optimal design given uncertainty.

Available Capital Investment

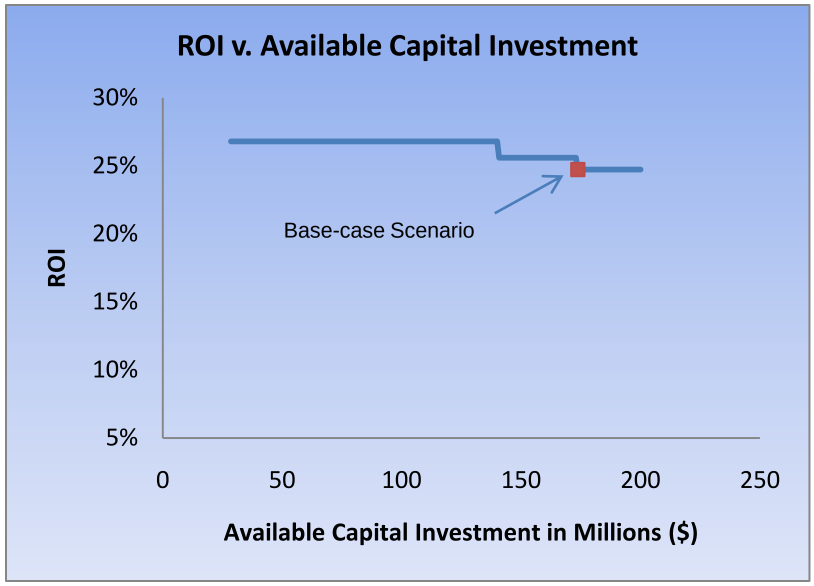
After examining the base-scenario and the effect of uncertainty on the results it was important to study the different profitable scenarios under varying ranges of available capital investment. For this study the amount of available capital investment was ranged from $10 million to $2.5 billion. A graph of the results comparing available capital to net present value can be seen here.



From a maximum investment of $10 million to $28.5 million it is not profitable to build any single or combination of processes. From $28.5 million to $140 million the optimal net present value corresponds to a tetrahydrofuran plant built in Lafayette, LA. Over the range of $140 million to $176 million in available capital the highest net present value is found by the building of a biofuels plant in Lexington, KY, the same location as the base-case scenario. Finally from $176 million to $2.5 billion the highest net present value is associated with the base-case scenario discussed earlier, a biorefinery including biofuels, 3-HPA, levulinic acid, and tetrahydrofuran production in Lexington, KY. This is not to say that these three scenarios are the only possibilities that yield a positive net present value just that they are the most profitable decision when optimizing net present value, when considering the available capital. The next analysis performed using the mathematical model was to compare the return on investment (ROI) for a varying range of available capital investments. The same range of available capital was used that was examined for the available capital investment versus net present value study. It is important at this time to comment on the definition of return on investment that was used for this study. There are varying definitions of ROI depending on their application and the focuses of the study. The ROI equation used for this study is shown below.

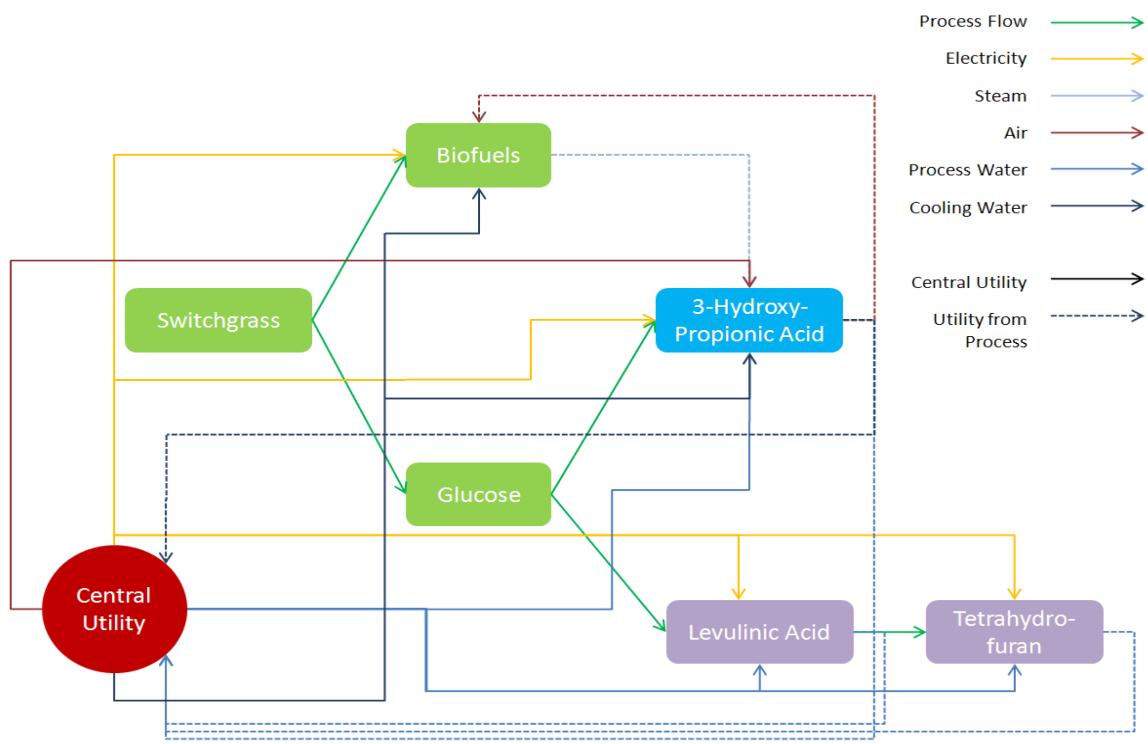
$$ROI = \frac{\sum_t \frac{P_t}{(1+i)^t}}{N \cdot capinv}$$

In this equation P_t refers to proceeds as defined in the mathematical model section. This definition of ROI was used because it takes into account the time-value of money while also giving equal weight to each year in 20 year economic life of the biorefinery. The results of this analysis are organized in the following graph. From this analysis, an optimal capital investment based on ROI was found. While the optimal ROI of 26.8% corresponding to a capital investment of $28.5 million in a tetrahydrofuran production plant in Lafayette, LA there is not much change in the ROI over the entire range of the study. The lowest ROI of the study at 24.5% was actually associated with the base-case scenario; however there is only a 2.3% difference in ROI between the two cases which is not significant enough to discourage the base-case scenario. While it is thought that ROI is a more appropriate measure of profitability because net present value does not take into account the lower return on capital used to maximize the net present value, ROI is a non-linear relationship. Due to the constraints of the model net present value, a linear profitability equation must be used as the objective function.



Integrated Utilities

The diagram below shows the integration of utilities in the base-case scenario.



Although the base-line scenario included integrated utilities, the same model was run excluding integrated utilities to examine the difference. The difference between the two scenarios is two fold. First non-integrated utilities does not allow for transfer of excess utilities from one process to another or the recycling of utilities. At the same time individual utility infrastructures must be built for each process as opposed to a single infrastructure for the refinery. The results of the comparison are included in the table below.

	Integrated	Non-integrated
Net Present Value	\$687,000,000	\$665,000,000
Capital Investment	\$176,000,000	\$185,000,000
Return on Investment	24.5 %	22.9 %

From the economic comparison it is clear that integrated utilities increases the profitability of a biorefinery. There is a 5.2% savings in capital investment when comparing the two scenarios. More significantly, the inclusion of integrated utilities accounts for a $22 million increase in the net present value of the biorefinery over the 20 year economic lifetime. While the integration of utilities does not affect the overall feasibility of the biorefinery it does significantly improve profitability as expected

Algae Results

To determine how the inclusion of algae would affect the results, the baseline scenario was run again with algae included. The results were very similar, as shown in the table below; the same processes were built with the same capacities as the run without the algae.

	Results w/o Algae	**Results w/ Algae**
Location	Lexington, KY	Lexington, KY
Processes	Biofuel 3-HPA Levulinic Acid Tetrahydrofuran	Biofuel 3-HPA Levulinic Acid Tetrahydrofuran Algae
Capacities (kg/yr)	1,440,000,000 (Biofuel) 6,500,000 (3-HPA) 57,600,000 (LA) 40,000,000 (THF)	1,440,000,000 (Biofuel) 6,500,000 (3-HPA) 57,600,000 (LA) 40,000,000 (THF) 200,000,000 (Algae)
TCI	$176,000,000	$277,000,000
NPV	$687,000,000	$642,000,000
ROI	24.5%	14.8%
CO_2 Emissions (kg/yr)	592,000,000	451,000,000
Emissions Reduction	–	24.8%

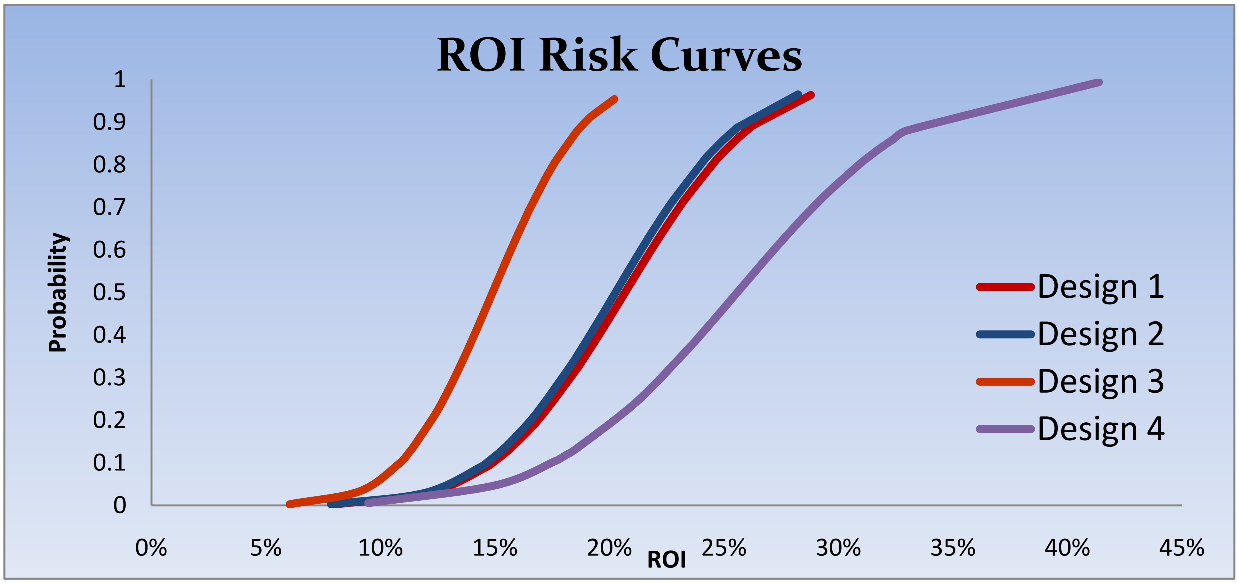
The major difference was that instead of emitting the CO_2 produced by the processes; it was fed to the algae first, resulting in a substantial decrease in emissions. Compared to the baseline results, the algae results were economically comparable. The NPV was 642 million dollars, 6.6%

lower than the baseline. At the same time, the FCI was 19% higher, resulting in a slightly lower ROI (14.8% vs. 24.5%). The most significant result was the massive reduction in CO_2 emissions. The inclusion of algae cut emissions from 592 million kilograms per year to 451 million, a reduction of 25%. Given the closeness of the economic results, the clear environmental advantage of including algae makes including it an easy decision.

Uncertainty Results

The base-case is built on values and trends in parameters that were assumed. Because the future is unknown, some of these parameters may be different than the assumed values. In order to correct for this, an uncertainty analysis was performed. This analysis, built into the model, automatically chooses different designs and then optimizes the design based on a series of scenarios. For this case, a design is a set of here-and-now decisions which must be made prior to constructing the plant. These include which processes to build, the initial capacities of each of the processes, and the location of the biorefinery. A scenario is one set of parameters which corresponds to one possible way the varied parameters could change in the future. Thirty scenarios were considered for each design. The parameters which were varied for the scenarios include the raw material price, the product price, the transportation costs, the operating costs, and the demand for each chemical. To vary these parameters, random values were chosen based on a normal curve for each parameter varied around a chosen mean and standard deviation.

The results from this analysis were a series of risk curves generated from the output of each design, taking into account the probability of each scenario occurring. The results are visualized in the figure below. The average return on investment for each of the designs is given by the value with a probability of 0.5. Therefore, the curve that is the furthest to the right on the graph has the largest average return. In this analysis, Design 4 has the largest expected return on investment. The steepness of the slope indicates the amount of variance in the expected return. So, although Design 4 has the maximum expected profit, it shows the most variance. It is still the best choice for the design because it shows a higher return even at low probabilities.



The here-and-now decisions for Design 4 are summarized in the table below. The results were similar to the base-case design, but two processes were added and a few of the initial capacities changed. The added processes produce glucaric acid and 5-hydroxymethylfurfural. The tetrahydrofuran and 3-hydroxypropionic acid processes were slightly smaller than the base-case and the levulinic acid capacity was slightly larger. The location of the biorefinery for this case is the same as the base-case in Lexington, KY. This uncertainty analysis provided criteria for making the best decision now for unknown events that could occur in the future.

Process	Initial Capacity (kg/yr)
Biofuels	800,000,000
3-HPA	5,870,000
Glucaric Acid	1,000,000
Levulinic Acid	61,000,000
THF	37,800,000
5-HMF	59,800,000

Further Study

As mentioned throughout the report, there is further study to be done in order to refine the model and create more meaningful and accurate results. The most significant improvements that will need to be made are in the area of cost estimation. Specifically, the modeling of capital and operating costs for the CSTR based processes is overly simplified and better simulations of these processes will need to be used. For both the CSTR based processes and the biofuels process, the amounts of utilities needed are significantly lower than for the fermentation processes. It will be important to reassess and refine this estimation to increase the feasibility and reliability of the model's results.

There is also much more study needed in the area of government incentives. While the available incentives have been researched thoroughly, only the federal and state tax credits for biofuels are currently incorporated in the model. Not only should the rest of the available incentives be incorporated into the model, but it is also possible to use the model to provide values for necessary further incentives in the area of biofuels.

While a single biorefinery may be the optimal design solution, it is also possible that building multiple, smaller biorefineries is more profitable. Currently the model only considers a single biorefinery. With further study, it could be possible to consider multiple biorefineries, locations, and combinations of processes.

The area of CO_2 emissions and the environmental impact of the biorefinery is another aspect of the report that can be examined more thoroughly. Currently CO_2 production is only addressed with respect to its incorporation into biofuels production from algae. While the current mathematical model is optimizing the biorefinery design and producing useful results, there is still work to be done. Once these additions and alterations have been made to the model and incorporated into the analysis of the resulting biorefinery design, the resulting report will be more complete and relevant.

Conclusion

The mathematical model showed that a switchgrass biorefinery can be extremely profitable. The baseline results had a net present value of $687,000,000 over the 20 year economic lifetime while producing both commodity chemicals and biofuels. While this value may be inflated, it is still a convincing validation of the potential of biorefineries. When stochastic analysis was applied, the model showed significant resistance to market changes. The optimal solution determined by the stochastic analysis showed less than a 2% change in ROI compared to the baseline solution. This indicates that the model is viable over a broad range of real world situations. The inclusion of algae biofuel production in the model showed significant potential from an environmental perspective. Although the ROI fell by approximately 10%, from 24.5% to 14.8%, CO_2 emissions were reduced by 25%. The integration of these exciting new technologies shows significant promise for a renewable and environmentally friendly future.

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