Utility-Integrated Biorefineries and Capacity Planning

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Abstract

This report describes how capacity planning models can be used to plan investments in biorefineries. For this, we have considered several processes belonging to a chemical supply chain that can be fed by a raw material, such as switchgrass, and used to produce valuable commodities. To build our model we have considered 58 possible processes to choose from, part of which are 12 chemicals chosen by the U.S. Department of Energy for production of value-added chemicals from biomass. The model maximizes net present value, considers budgeting conditions to self-finance expansions and determines what process ought to be constructed in the biorefinery, initial process capacity, as well as construction time and the timing and size of future expansions. Projected raw material availability, market projected demand and prices, as well as transportation costs are included. Among other results, the model is also able to provide the location of the refinery based on market demand and proximity to feed. All these features notwithstanding, integration of centralized utilities was analyzed to determine the optimal value added chain of processes, a feature that has not been considered in any previous models.

Introduction

A biorefinery processes biomass to yield industrial chemical products including commodity chemicals, specialty chemicals and biofuels. A refinery is simply a large grouping of processes or plants into one facility which results in savings on transportation and operating costs. A biorefinery operates with similar principles to a petroleum-based refinery, but with biomass as a feedstock instead of crude. Biomass is material derived from organic sources, especially plants. Popular biomass feedstocks include corn, wood, and switchgrass. All sources of biomass are being researched as possible replacements for fossil fuels. Corn is touted by many as the new hope for biofuels, but cellulosic biomass holds many advantages over corn. Cellulosic biomass grows naturally in every one of the 48 contiguous states. More importantly, unlike corn, cellulosic biomass is not a major food source since cellulose is not readily digested by humans. Also, innovative bio-based technology sometimes produces chemicals for less than current industrial practices. For example, Massachusetts-based Biofine, Inc. has revolutionized the production of levulinic acid from paper mill biomass sludge that costs a tenth of current petroleum-based techniques. [1] A large sector of biomass proponents

**Undergraduate Capstone Students*

*** Chemical Engineering Capstone Professor* are those who believe that biorefining can stimulate rural economies by promoting large-scale harvest of natural crops. The booming economies create so-called green-collar jobs. Rural communities also hope to benefit from government incentives attached to green development. A biorefinery is an attractive innovation in the chemicals industry due to environmental issues surrounding fossil fuel dependence. A biorefinery utilizes renewable resources, exhibits decreased waste and offsets CO_2 emissions by planting new crops. The utilization of renewable resources has been touted for years as a possible solution to global warming and fossil fuel shortage but it has never been more feasible or necessary than now. In the past, research groups have developed capacity planning models to plan investments in biorefineries. Some of the limitations of these models include the number of processes considered for the biorefinery as well as the method for choosing optimal plant location. The following paper details our progress in advancing the capacity planning model to include a substantially greater number of processes and to consider many plant locations, switchgrass farm locations, and market locations for sale of products. In addition, we have added in the consideration of centralization of utilities to show the potential cost savings associated and the benefits to profitability of the biorefinery.

Background

The relevance of biomass-derived fuels and chemicals is increasing greatly, causing a so-called "Green Boom." The central concern regarding the environment is global climate change, specifically global warming. Global warming threatens many ecosystems across the planet and is projected to cause devastating problems in the near future. Global warming has been linked to carbon dioxide emissions from both consumer and industrial sources. Decreasing industrial carbon dioxide emissions could potentially have a great effect on global warming rates. The burning of fossil fuels emits significantly more CO_2 than the biomass-based biofuels being researched and produced in biorefineries. Aside from pollution and greenhouse gas emission, petroleum consumption depletes natural resources. The search for a fully-renewable feedstock is a continuing objective in biofuel and bio-based chemicals research. Switchgrass has presented itself as having great potential in this area. Due to the dire concerns involving the environment, federal governments have taken action. The Energy Independence and Security Act of 2007 predicates that 8 billion gallons of alternative fuels be produced during 2008. This bill also projects that by 2022, 36 billion gallons per year of alternative fuels be produced, 21 billion of which will be advanced biofuels, such as the ones produced in a biorefinery. [2] However, a challenge in biorefinery operation is achieving efficiency and production rates comparable to petroleum-based refineries. Higher efficiency and cost-

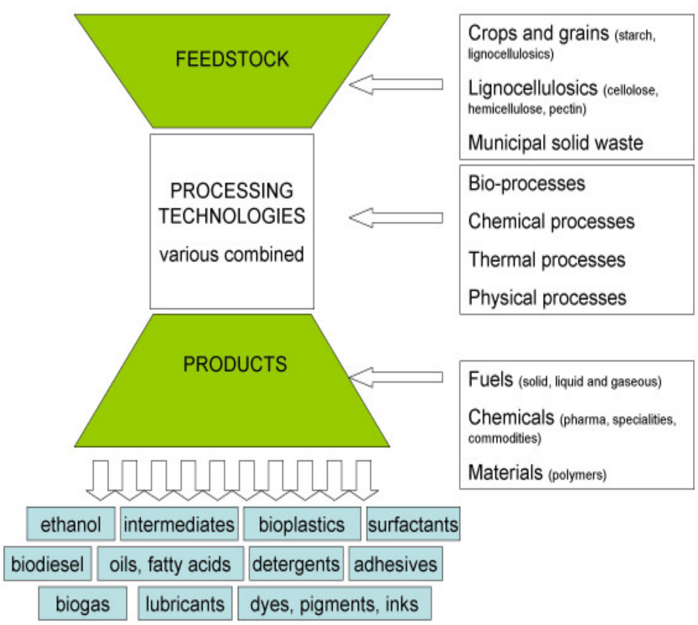

Figure 1- Biorefinery Basics,
http://www.microbialcellfactories.com/content/6/1/9/figure/F1

effectiveness can be achieved through utility integration, wherein all processes are connected minimizing waste.

Efficient biorefinery design is integral to the future of industry across the board as environmental issues become more prevalent in society. The operation of a biorefinery is similar to that of a petroleum refinery in that the biomass feedstock is analogous to crude oil and must be processed to transform it into a product that can be used or sold. The basic operations and objectives of a biorefinery are shown in Figure 1. One of the objectives of this investigation was to increase the efficiency and profitability of the biorefinery by incorporating centralized utilities and comparing them with traditional utilities. Since biorefineries are based on principles of sustainability, it is integral to run all processes at efficient rates with little waste. Fully integrating processes helps to decrease utility costs. Integration between processes is possible where a reaction produces a by-product that is used as a reactant in another process.

Centralized utilities involve sharing of utility streams across all plants of the biorefinery instead of having individual utility facilities for each process in the biorefinery. The main utilities analyzed for centralization were process, cooling, and treatment water, steam, and air. Cooling towers, boiler plants, and water treatment plants were also analyzed. Figure 2 shows a schematic depicting an example centralized utility model.

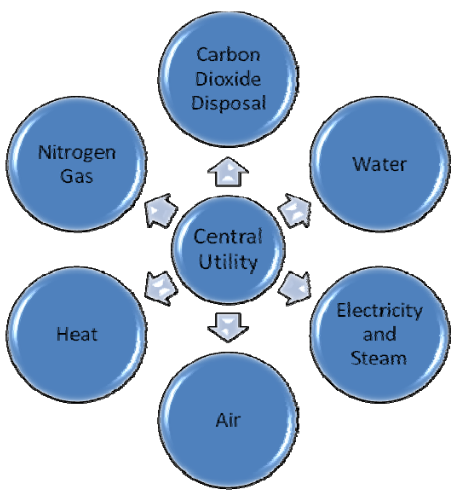

Figure 2 – Sample Centralized Utility Facility

Biorefineries can operate at a variety of capacities with any number of products. The most common type of biorefinery produces ethanol or biodiesel from corn. The biorefinery designed in this article produces value-added chemicals from switchgrass, a type of lignocellulosic biomass. The switchgrass is pretreated to separate it into its cellulosic components and lignin. Typical biomass is 30% lignin by weight and 70% cellulosic material. A popular biomass conversion process is biomass fractionation. The fractionation employs a countercurrent extraction technique which separates the lignin as a liquid, leaving behind solid cellulose fibers. This technology exhibits most efficient separations at high temperature and pressure. The lignin can be further processed or burned for energy. Lignin pyrolysis yields about 17 kJ/kg of energy. Cellulose is a polysaccharide consisting of repeating units of glucose and can be broken down enzymatically. The resulting glucose is then either fermented or reacted to yield the building-block molecules of the chemicals that will eventually be sold. Anaerobic fermentation of glucose by the bacteria solventogenic clostridia produces ten useful compounds. Solventogenic clostridia is ideal for biorefining since it can produce such a wide variety of products from glucose. It also results in a high yield of desired products. Yields for some desired chemicals from fermentation of glucose by Solventogenic clostridia are shown in Table 1.[4]

Process	Reaction	Yield, g/g
P4	Glucose → Ethanol	0.48
P12	Glucose→ Lactic Acid	0.90
P29	Glucose → 3-Hydroxypropionic Acid	0.90
P33	Glucose → Glucaric Acid	0.64
P37	Glucose→ Pyruvate	0.75

Table 1 – Solventogenic clostridia fermentation yields for selected processes

Fermentation is a complex process and requires specific operating conditions to effectively yield desired products. The main factors that affect fermentation are pH and temperature. Further optimization of fermentation broth conditions should be examined in future work. Glucose is also transformed into five additional chemicals through other processes, including hydrogenation and decomposition.

Problem Statement

An integrated biorefinery incorporates a variety of chemical processes and pathways to yield both bulk and value added chemicals. This biorefinery was structured to include all researched pathways where chemicals were produced from cellulosic biomass. In 2004, the Department of Energy conducted a study of value added chemicals to maximize profitability while taking into account feasibility.[3] They concluded that twelve chemical pathways were most profitable out of hundreds. A list of these chemicals is shown in Table 2. These processes occur via multiple pathways including but not limited to the following: fermentation, oxidation, and hydrolysis. Further research yielded even more information, specifically regarding bulk chemicals such as ethanol, methanol, acetone and butanol.

12 Building	Blocks
1,4 succinic, fumaric and malic acids	3-hydroxybutyrolactone
2,5 furan dicarboxylic acid	itaconic acid
3 hydroxy propionic acid	levulinic acid
aspartic acid	glycerol
glucaric acid	sorbitol
glutamic acid	xylitol/arabinitol

Table 2 – 12 Building Block Chemicals chosen by US DOE

The following projected product tree seen in Figure 3. depicts the cumulative findings from the DOE and other outside research. The tree is structured with boxes and arrows. The boxes symbolize the individual processes. The products formed in each process are inside the box. The products from the processes may either be sold for profit or converted into another chemical via another box or process. For example, levulinic acid may either be sold for a profit or converted into tetrahydrofuran, succinic acid, or gamma-butyrlactone. The product tree shows all of the potential options for the 58 processes in the figure below. Processes were divided into three categories: lignin-based processes which are orange in the flow chart below, glucose fermentation based processes, in blue, and other processes, represented in purple. The “other” processes include hydrogenation, decomposition, fungal fermentation, and oxidation of glucose.

There are 58 different processes with the potential to either sell products or use them to form different chemicals. Fifty-eight processes with approximately two options for each process results in trillions of options to sell, continue with, or completely neglect a chemical. As processes are eliminated, the number of possibilities decreases greatly. Profitability is the limiting factor within the product tree. It is necessary to investigate the characteristics and profitability factors for each process for each year in the economic lifetime. The economic lifetime of this project is assumed to be twenty years based on projections by the DOE. Further analysis of the individual processes includes the following: raw material purchase price, chemical selling price, reaction stoichiometry, product demand and market size, and operating costs. For example, the demand for ethanol as a fuel is extremely high, but it may not be more profitable than a higher-priced chemical such as vinyl acetate monomer which is produced from ethanol derivatives. It is vital to combine all of the profitability factors for each process and determine the most profitable setup for the integrated biorefinery. The most effective way of achieving this all-inclusive equation is via mathematical modeling.

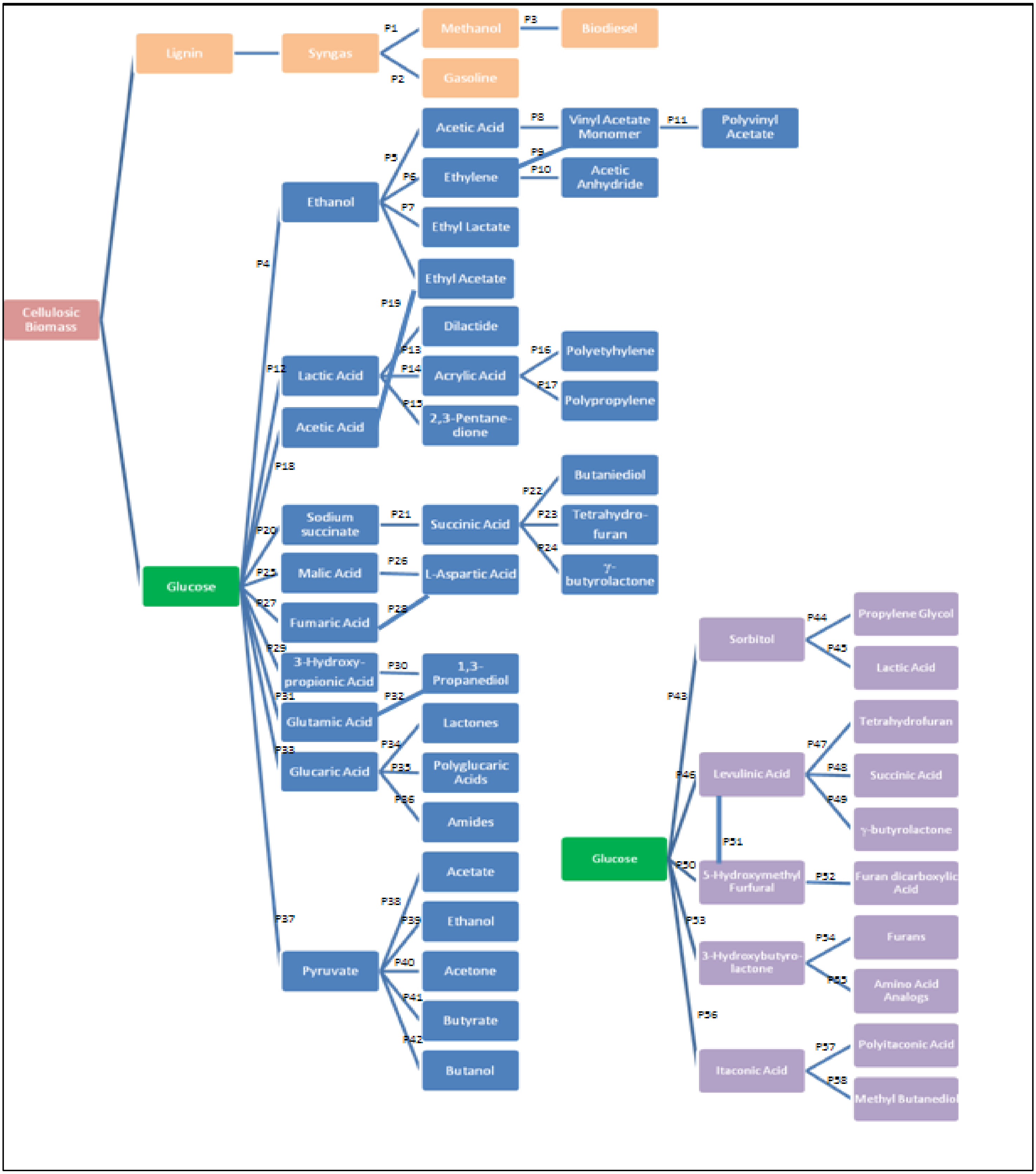

Figure 3-Final Process Flow Chart

Mathematical Model

The sets used are the following: (i) *I*, processes; (ii) *J*, chemicals; (iii) *T*, time periods; (iv) *M*, selling market locations; (v) *N*, raw material (feedstock) locations; (vi) *P*, plant locations; (vii) *U*, utilities. Parameters and variables are described in detail in the following mathematical model.

Objective Function. The core focus of the mathematical model is to maximize the profitability of an integrated biorefinery by maximizing its net present value. NPV is determined by the money returned to investors in time period *t* (R_t) minus the capital investment (capinv).

$$\max NPV = \sum_t \frac{1}{(1+orate)^t} R_t - capinv \tag{1}$$

Constraints. Mass Balances. The input for process *i* for chemical *j* in period *t* ($input_{i,j,t}$) is equal to the raw materials purchased for process *i* for chemical *j* in period *t* ($raw_{i,j,t}$) plus intermediate materials from all previous processes *k* flowing to all new processes *i*for chemical *j* in period t ($flow_{i,k,j,t}$).

$$input_{i,j,t} = raw_{i,j,t} + \sum_k flow(i,k,j,t) \tag{2}$$

Input is equal to the stoichiometry coefficient for the reactants *j* for process *i*, which is a given parameter ($f_{i,j}$), times the sum of the previously defined input.

$$input_{i,j,t} = f_{i,j} \sum_{j'} input(i,j',t) \tag{3}$$

The output for process *i* for chemical *j* in period *t* ($output_{i,j,t}$) is equal to the materials to be sold for process *i* for chemical *j* in period *t* ($sales_{i,j,t}$) plus intermediate materials flowing to the new processes *i*.

$$output_{i,j,t} = sales_{i,j,t} + \sum_k flow_{i,k,j,t} \tag{4}$$

Output is equal to the stoichiometry coefficient for the products *j* for process *i*, which is a given parameter ($g_{i,j}$) times the sum of the output.

$$output_{i,j,t} = g_{i,j} \sum_{j'} output_{i,j',t} \tag{5}$$

The mass balance around each process is defined as the sum of the output for process *i* for period *t* for all chemicals *j* is equal to the input for process *i* for period *t* for all chemicals *j*.

$$\sum_j output_{i,j,t} = \sum_j input_{i,j,t} \qquad (6)$$

The chemical flow must be less than products transferred from process *i* for chemical *j* in period *t* (parameter $gamma_{i,j,k}$) times output.

$$flow_{i,j,k,t} \le gamma_{i,j,k} \cdot output_{i,j,t} \qquad (7)$$

Capacity &Expansions. Constraints. The capacity for process *i* in period *t* ($cap_{i,t}$) is equal to capacity for process *i* in the previous year *t-1* ($cap_{i,t-1}$) plus the expansion for process *i* in period *t* ($exp_{i,t}$) plus the initial capacity for process *I* in period *t* ($initcap_{i,t}$).

$$cap_{i,t} = cap_{i,t-1} + exp_{i,t} + initcap_{i,t} \qquad (8)$$

The initial capacity minus the minimum capacity for process *i* ($mincap_i$) which is controlled by the binary variable indicating the first installation, $Y_{i,t}$ must be greater than or equal to zero.

$$initcap_{i,t} - Y_{i,t} mincap_i \ge 0 \qquad (9)$$

The initial capacity must be less than or equal to the maximum capacity for process *i* ($maxcap_i$).

$$initcap_{i,t} - Y_{i,t} maxcap_i \le 0 \qquad (10)$$

For all chemicals *j* the sum of the output for process *i* and period *t* is less than or equal to the capacity of the process and is greater than the sum of the minimum capacity for all years prior to time *t*.

$$\sum_j output_{i,j,t} \le cap_{i,t} \qquad (11)$$

$$\sum_j output_{i,j,t} \ge \sum_{t} Y_{i,t} mincap_i \qquad (12)$$

The expansion for process *i* in period *t* ($exp_{i,t}$) minus the minimum expansion for process *i* which is controlled by a binary variable indicating expansion, $X_{i,t,}$ must be greater than or equal to zero.

$$exp_{i,t} - X_{i,t} minexp_i \geq 0 \tag{13}$$

The initial expansion must be greater than or equal to the maximum expansion for process *i* ($maxexp_i$).

$$exp_{i,t} - X_{i,t} maxexp_i \geq 0 \tag{14}$$

The total number of expansions throughout the entire life of the project must be less than or equal to the maximum number of expansions for process *i* ($nexp_i$).

$$\sum_{t} X_{i,t} \leq nexp_i \tag{15}$$

Process *i* is built once or never.

$$\sum_{t} Y_{i,t} \leq 1 \tag{16}$$

A process cannot be built and expanded in the same year.

$$X_{i,t} + Y_{i,t} \leq 1 \tag{17}$$

A process must be built before it is expanded.

$$X_{i,t} \leq \sum_{t'}^{t-1} Y_{i,t'} \tag{18}$$

Utility Balances. Constraints. The utilities *u* generated for process *i* in period *t* ($ugen_{i,u,t}$) when process generation, a parameter, is equal to 1 ($PG_{i,u}$) is equal to the utility coefficient for process *i* and utility *u* ($ucoeff_{i,u}$) times the sum of the input for all chemicals*j*.

$$ugen_{i,u,t} = ucoeff_{i,u} \sum_{j} input_{i,j,t} \quad (PG_{i,u} = 1) \tag{19}$$

No utilities are generated when the process generation is 0.

$$ucon_{i,u,t} = ucoeff_{i,u} \sum_{j} input_{i,j,t} \qquad (PG_{i,u} = 0) \tag{20}$$

The utilities *u* consumed for process *i* in period *t* ($ucon_{i,u,t}$) when process consumption, a parameter, is equal to 1 ($PC_{i,u}$) is equal to the utility coefficient for process *i* and utility *u* ($ucoeff_{i,u}$) times the sum of the output for all chemicals*j*.

$$ucon_{i,u,t} = ucoeff_{i,u} \sum_{j} output_{i,j,t} \qquad (PC_{i,u} = 1) \tag{21}$$

No utilities are consumed when the process consumption is 0.

$$ucon_{i,u,t} = ucoeff_{i,u} \sum_{j} output_{i,j,t} \qquad (PC_{i,u} = 0) \tag{22}$$

The utility capacity for utilities *u* and period *t* ($ucap_{u,t}$) is equal to the initial utility capacity for utility *u* and period *t* ($initucap_{u,t}$) plus the utility capacity from the previous year plus the capacity gained from utility *u* expansions in period *t* ($ucapexp_{u,t}$).

$$ucap_{u,t} = initucap_{u,t} + ucap_{u,t-1} + ucapexp_{u,t} \tag{23}$$

The initial utility capacity minus the minimum utility capacity for utility *u* ($minucap_u$), which is controlled by the binary variable indicating the first installation, $V_{u,t}$ must be greater than or equal to zero.

$$initucap_{u,t} - V_{u,t} minucap_u \geq 0 \tag{24}$$

The initial utility capacity must be less than or equal to the maximum utility capacity for utility *u* ($maxucap_u$).

$$initucap_{u,t} - V_{u,t} maxucap_u \leq 0 \tag{25}$$

The utility expansion for utility *u* in period *t* ($ucapexp_{u,t}$) minus the minimum utility expansion for utility*u* which is controlled by a binary variable indicating utility expansion, $W_{u,t}$, must be greater than or equal to zero.

$$ucapexp_{u,t} - W_{u,t} minuexp_u \geq 0 \tag{26}$$

The utility expansion must be greater than or equal to the maximum utility expansion for utility*u* ($maxuexp_u$).

$$ucapexp_{u,t} - W_{u,t} maxuexp_u \geq 0 \tag{27}$$

The total number of utility expansions must be less than or equal to the maximum number of expansions for utility *u* ($nuexp_u$).

$$\sum_t W_{u,t} \le nuexp_u \tag{28}$$

Utility *u* is built once or never.

$$\sum_t V_{u,t} \le 1 \tag{29}$$

A utility cannot be built and expanded in the same year.

$$V_{u,t} + W_{u,t} \le 1 \tag{30}$$

A utility facility must be built before it is expanded.

$$W_{u,t} \le \sum_{t}^{t-1} V_{u,t} \tag{31}$$

Integrated Utilities. The difference in the sum of the utilities generated and the utilities consumed for all processes *i* for chemical *j* and time period *t* is equal to the total amount of extra utilities *u* for period *t* ($makeup_{u,t}$) needed to satisfy the utility requirements of the process.

$$\sum ugen_{i,u,t} + makeup_{u,t} = \sum ucons_{i,u,t} \tag{32}$$

The utility capacity must be greater than or equal to the extra makeup utilities required.

$$ucap_{u,t} \ge makeup_{u,t} \tag{33}$$

Non-Integrated Utilities. The utility capacity must be greater than or equal to the utilities consumed for all processes.

$$ucap_{u,t} \ge \sum_i ucons_{i,u,t} \tag{34}$$

Location Equations. The sum of the raw materials needed for all processes *i* and chemicals *j* over period *t* ($raw_{i,j,t}$) is equal to the sum of the raw materials purchased from all feedstock locations *n* for plants *p* over time period *t* ($rawbuy_{n,p,t}$).

$$\sum_{i} raw_{j,t} = \sum_{n,p} rawbuy_{n,p,t} \tag{35}$$

The limit to the amount of raw materials that may be purchased from a feedstock location for a specific plant in a time periodis controlled by the binary variable indicating the installation of the plant in location *p* (Q_p).

$$rawbuy_{n,p,t} \leq C_1 * Q_p \tag{36}$$

The total raw transportation cost for period *t* ($rawTR_t$) is equal to the sum of the purchased raw materials times the distance from all feedstock locations *n* to plant locations *p* ($rawdist_{n,p}$) times the freight cost for the raw materials (rawfreight).

$$rawTR_t = \sum_{n,p} \left(rawbuy_{n,p,t}\, rawdist_{n,p}\, rawfreight \right) \tag{37}$$

The sum of sales for all processes *i* for chemical *j* in time period *t* is equal to the total products sold for plants *p* in markets *m* for process *i* and chemical *j*.

$$\sum sales_{j,t} = \sum_{p,m} prodsell_{j,p,m,t} \tag{38}$$

The limit to the total products sold must be less than or equal to a coefficient, C_2, times binary variable, Q_p.

$$prodsell_{j,p,m,t} \leq C_2 * Q_p \tag{39}$$

Total sales transportation cost for period *t* ($salesTR_t$) is equal to the sum of the sold products times the distance from all plant locations *p* to market locations *m* ($salesdist_{p,m}$) times the freight cost for the products (salesfreight).

$$salesTR_t = \sum_{p,j,m} \left(prodsell_{j,p,m,t}\, salesdist_{p,m}\, salesfreight \right) \tag{40}$$

The total transportation costs for period *t* (TR_t) are equal to the sum of raw material and product transportation costs.

$$TR_t = rawTR_t + salesTR_t \tag{41}$$

The plant will only be built in one location.

$$\sum_{p} Q_p = 1 \tag{42}$$

Fixed & Operating Costs. Total material cost for period *t* ($matcost_t$) is equal to the sum of the rawprice for all feedstock locations*n* for period *t* ($rawprice_{n,t}$)and times the amount of raw materials purchased from all feedstock locations *n* for all plant locations *p* in period *t*.

$$matcost_t = \sum_{n,p}\left(rawprice_{n,t} \, rawbuy_{n,p,t}\right) \tag{43}$$

*Integrated Utilities.*The utility costs for utility *u* in period *t* ($ucost_{u,t}$) is equal to fixed utility operating costs (parameter d_u) for built utility facilities all years before time *t* plus the incremental utility operating costs (parameter e_u) times the utilities purchased from outside the plant.

$$ucost_{u,t} = d_u \sum_{t'}^{t} Y_{u,t'} + e_u \, makeup_{u,t} \tag{44}$$

Non-Integrated Utilities. The utility cost is equal to the fixed utility operating costs for built utility facilities in all periods before time *t* plus the incremental utility operating cost for the total amount of utilities consumed in the plant.

$$ucost_{u,t} = d_u \sum_{t'}^{t} Y_{u,t'} + e_u \sum_{i} ucon_{i,u,t} \tag{45}$$

The operating cost for the plant (excluding utilities) for process *i* in period *t* is equal to the minimum operating cost to build process *i* (parameter $delta_i$) in all years prior to period *t* plus the incremental operating cost for process *I* (parameter $epsilon_i$) times the sum of the output of all chemicals for process *i* and period *t*.

$$opcost_{i,t} = delta_i \sum_{t'}^{t} Y_{i,t'} + epsilon_i \sum_{c} output_{i,c,t} \tag{46}$$

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

$$totalcost_t = \sum_{i} opcost_{i,t} + \sum_{u} ucost_{u,t} \tag{47}$$

Integrated Utilities. The initial fixed capital for utilities *u* in period *t*($FCUinitial_{u,t}$) is equal to the fixed utility investment costs (parameter a_u) plus the incremental utility investment costs (parameter bb_u) times the initial utility *u* capacity for period *t* ($initucap_{u,t}$).

$$FCUinitial_{u,t} = Y_{u,t} a_u + bb_u initucap_{u,t} \tag{48}$$

The fixed capital investment for utility *u* expansions in period *t* is equal to the fixed utility investment costs plus the incremental utility investment costs times the utility *u* capacity for expansions in period *t* ($ucapexp_{u,t}$).

$$FCUexp_{u,t} = W_{u,t} a_u + bb_u ucapexp_{u,t} \tag{49}$$

Non-Integrated Utilities. The initial fixed capital for utilities *u* in period *t* ($FCUinitial_{u,t}$) is equal to the sum of the fixed utility investment costs for all processes *i* (parameter $aa_{i,u}$) plus the sum of the incremental utility investment costs for all processes *i* (parameter $cc_{i,u}$) times the initial utility *u* capacity for period *t* ($initucap_{u,t}$).

$$FCUinitial_{u,t} = Y_{u,t} \sum_i aa_{i,u} + initucap_{u,t} \sum_i cc_{i,u} \tag{50}$$

The fixed capital investment for utility *u* expansions in period *t* is equal to the sum of the fixed utility investment costs for all processes plus the sum of the incremental utility investment costs for all processes times the utility *u* capacity for expansions in period *t* ($ucapexp_{u,t}$).

$$FCUexp_{u,t} = W_{u,t} \sum_i aa_{i,u} + ucapexp_{u,t} \sum_i cc_{i,u} \tag{51}$$

The total fixed capital for utilities *u* in period *t*($FCU_{u,t}$) is equal to the initial fixed investment for utilities plus the fixed investment for utility expansions.

$$FCU_{u,t} = FCUinitial_{u,t} + FCUexp_{u,t} \tag{52}$$

The initial fixed capital (excluding utilities) for process *i*in period *t*($FCinit_{i,t}$) is equal to the minimal cost to build a process *i* (parameter $alpha_i$) plus the initial capacity for process *i* in period *t* times the incremental capacity cost ($beta_i$).

$$FCinit_{i,t} = Y_{i,t} alpha_i + initcap_{i,t} beta_i \tag{53}$$

The fixed capital for expansions (excluding utilities) for process *i* in period *t*($FCexp_{i,t}$) is equal to the minimal cost to build a process plus the capacity of the expansion for process *i* in period *t* times the incremental capacity cost ($beta_i$).

$$FCexp_{i,t} = X_{i,t} alpha_i + exp_{i,t} beta_i \tag{54}$$

The total fixed capital for period *t* (FCI_t) is equal to the sum of the initial fixed capital for all processes plus the sum of the expansion fixed capital for all processes plus the sum of the utility fixed capital for all utilities.

$$FCI_t = \sum FCinit_{i,t} + \sum_i FCexp_{i,t} + \sum_u FCU_{u,t} \tag{55}$$

The capital investment (capinv) is equal to the sum of the total fixed capital over all periods plus the material costs over all periods divided by annually compounded interest (rate).

$$capinv = \sum_t \left(\frac{FCI_t + matcost_t}{(1 + rate)^t} \right) \tag{56}$$

The capital investment must be less than or equal to the total available investment.

$$capinv \le available\ investment \tag{57}$$

Profits. The sales from all processes for a chemical in a time period must be less than the demand for the same chemical in that time period.

$$\sum sales_{j,m,t} \le demand_{t} \tag{58}$$

The revenue for chemical *j* in period *t* is equal to the sum of the products sold in all plants to all markets times the price of the chemical *j* in all markets *m* in period *t* (parameter $price_{j,m,t}$).

$$revenue_{j,t} = \sum_{i,m} \left(prodsell_{i,j,m,t}\, price_{j,m,t} \right) \tag{59}$$

The cash generated in the plant over period *t* ($cash_t$) is equal to the sum of the revenue for all chemicals minus transportation costs minus total costs minus fixed capital minus material cost all in period t divided by the annual interest rate.

$$cash_t = \frac{\sum_j revenue_{j,t} - TR_t - totalcost_t - FCI_t - costoed_t}{rate^t} \qquad (60)$$

Budgeting Equations. Taxes in period *t* (tax_t) are equal to the taxrate times the cash in period *t* minus the depreciation rate times the sum of the fixed capital for all processes from all previous time periods.

$$tax_t = taxrate\left(cash_t - deprate\sum_{t} FCI_t\right) \qquad (61)$$

The net profit after taxes in period *t* ($NPAT_t$) is the difference in cash and taxes from that period.

$$NPAT_t = cash_t - tax_t \qquad (62)$$

The budget at time *t* (B_t) is equal to the budget from the previous time period (B_{t-1}) plus the net profit after taxes and reduced by the money returned to investors (R_t). All capital is invested while no money is returned to investors in year 1.

$$B_t = B_{t-1} + NPAT_t - R_t \qquad (63)$$

$$B_1 = NPAT + caplev \qquad (64)$$

Using the above model, processes were systematically eliminated from the initial 58 processes through systematic screening involving costs within the biorefinery. The first screening involved the assumption that all costs were zero. This essentially eliminates all processes that will never be profitable under any circumstances. Eliminating these processes based on price alone allows for resources within the biorefinery being concentrated on more profitable processes. The second screening added in capital costs with operating costs and utilities still assumed to be zero. The screening further refined the flow chart. The next screening added in operating costs. The final screening simulated realistic facility operating with capital costs, operating costs and utilities. The final screening gives the best combination of processes to maximize the profitability of the biorefinery. This screening process is shown in Figure 4. After initial screening with zero total costs, 23 processes were eliminated based solely on revenues generated from sales of products, yielding the flow chart in Figure 5.

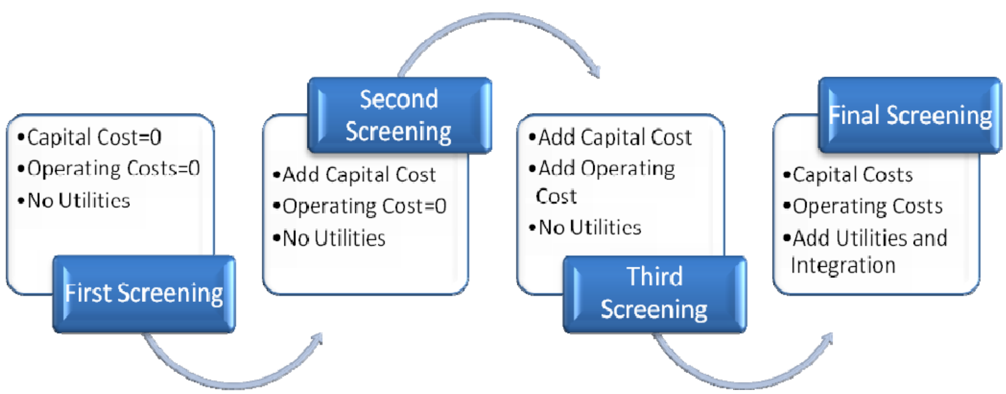

Figure 4- Process Elimination Screening

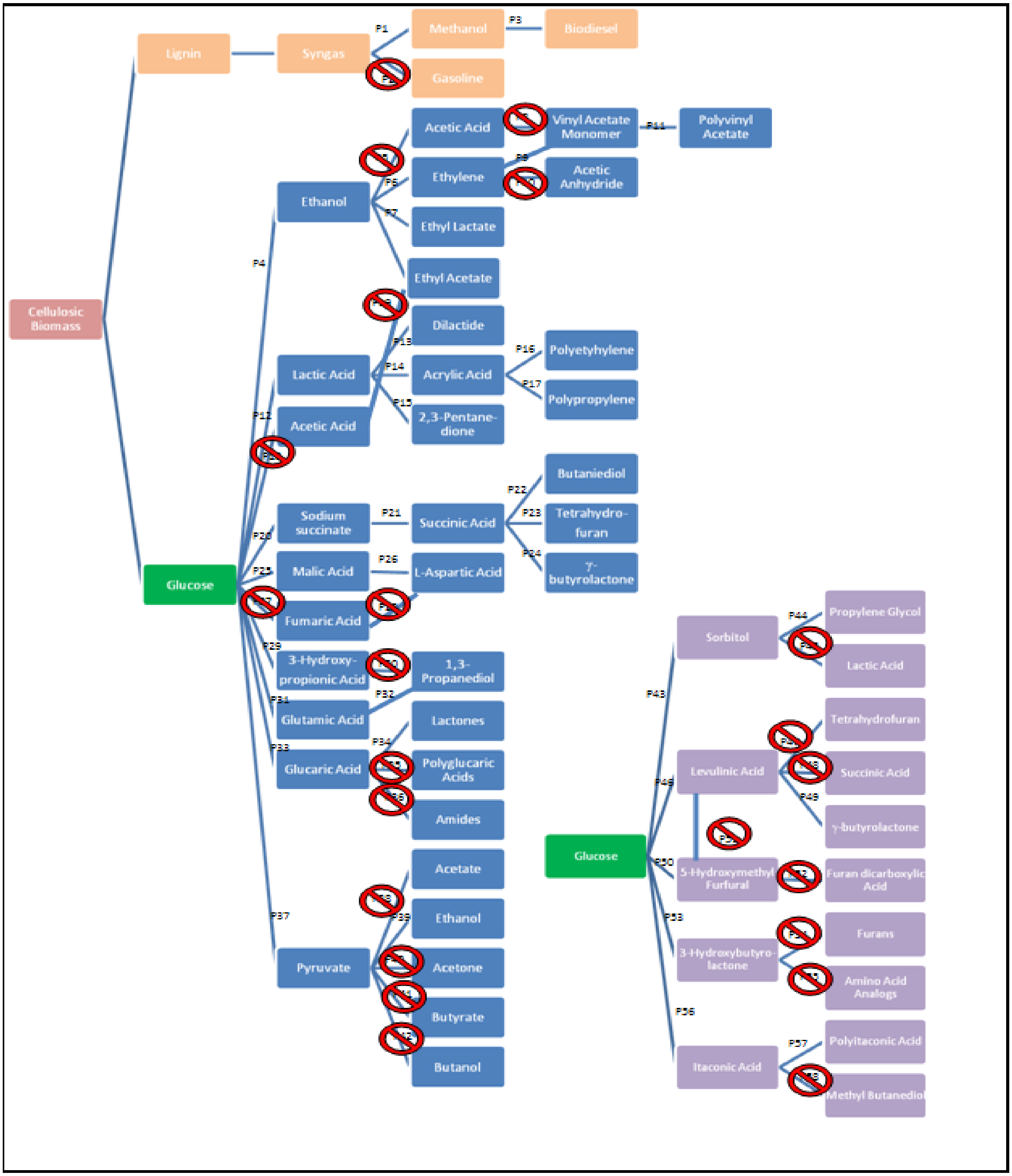

Figure 5 – Process flow chart with elimination after initial screening

Centralization of Utilities

In adding utilities costs into the model, one important result sought was an estimate of the cost savings associated with having centralized utilities for multiple processes as opposed to individual service facilities for each process as would be the case for individual plants. For the case of centralized utilities, a single utilities facility is used for the entire biorefinery. The facility includes all the units necessary to supply utilities to the entire biorefinery. This differs from non-centralized utilities, where each process has its own service facilities (steam generation, water treatment, etc). The difference is represented in Figure 6 below:

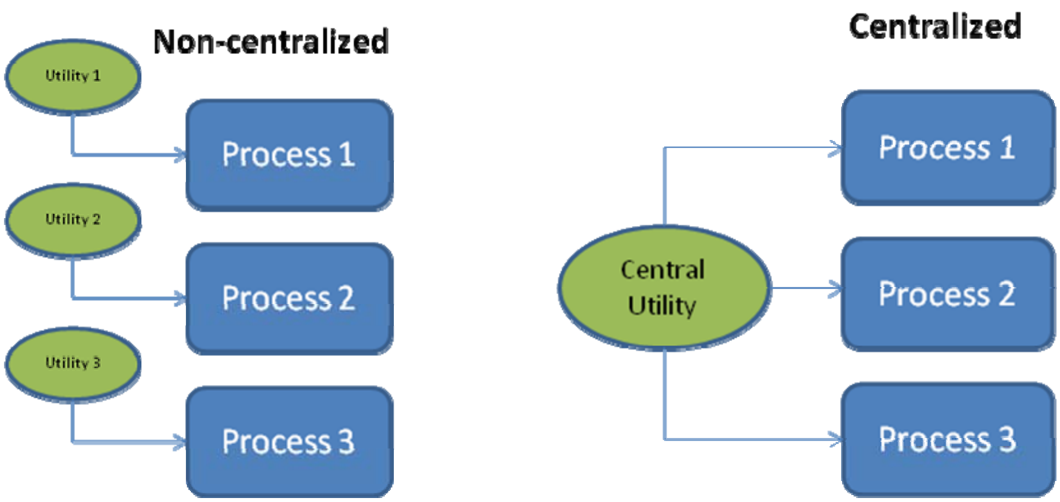

Figure 6 –Utilties Comparison

We chose to consider four major utilities, based on the processes incorporated into the model. These utilities include the following:

1. Electricity - which would be produced from a steam turbine
2. Steam – for heating and for sterilization
3. Air – for aeration in fermentation reactions
4. Water – including process water, treatment water, and cooling water

The major service facilities necessary for production of the preceding utilities include a boiler plant, a compressor plant, two water treatment plants (one for process water and another for treatment water), and a cooling tower. Costs for these facilities can be estimated from figures in Appendix B of Peters and Timmerhaus [6] which give the cost for the facilities based on some capacity and also from Table 6-8 in the same book which gives the typical range of fixed-capital investment for various service facilities.

The amount of electricity, steam, air, and water that would be required for each process was estimated based on simulations of similar processes in the process modeling software SuperPro Designer as well as on cost data given in Bioseparations Science and Engineering [5]. From this information, we were able to determine typical utilities needs based on the quantity of reactants and products. This degree of accuracy is acceptable for our purpose of showing a contrast in the cost of centralized utilities versus non-centralized utilizes and for demonstrating that these costs can be effectively incorporated into the model to maximize net present value.

In order to incorporate the utilities costs into the model for the cases of centralized and non-centralized utilities, these costs were determined as a function of capacity. For the non-centralized utilities case, the model calculates both fixed and incremental utilities costs for each process. The fixed cost is the minimum capital cost for the service facilities based on a very small capacity. The incremental cost is the capacity-dependent part of the cost. Thus an equation for utilities costs is in the form of y=mx + b where y=total utility costs, m=incremental utility costs, b=fixed utility costs, and x is the capacity in units of amount/time. Therefore, for the non-centralized utilities case, there is a utilities cost calculated for each process in the model. For the case of centralized utilities, on the other hand, the utilities cost is calculated for the entire biorefinery, not for individual processes. This utilities cost is calculated in the same way as for the non-centralized case, but is based on the total utilities requirements for all the processes in the biorefinery, not on the utilities requirements for each process separately. Having centralized utilities means that only one boiler, one compressor plant, etc. is required for the entire biorefinery, instead of one for each separate process. Thus, the fixed capital portion of the utilities cost is substantially reduced by having a centralized utilities facility. The reason for the cost reduction has to do with economies of scale. If you increase the size of a piece of equipment by a factor of 2, its cost generally increases by a smaller factor. The scaling law for process equipment is commonly given by $Cost_2 = \cos t_1 \left(\frac{size_2}{size_1} \right)^a$ where a has an average value of around 0.6. By application of this rule, when the size of a piece of equipment doubles, its cost will increase by a factor of $(2/1)^{0.6}$ which is about 52%. Thus it becomes apparent that using one piece of equipment at a larger capacity saves money over using multiple pieces of equipment at a lower capacity. This is the major benefit of using centralized utilities.

Location

The model possesses capability to optimize the location of the biorefinery through a combination of binary variables and parameters. The optimal locations for purchase of raw materials and markets for sales of final products were also examined within the model. The 34 potential plant locations were chosen based upon current biorefinery development, corporate growth of the area, local taxes and rent, and proximity to crops and chemical markets. The markets were chosen based on large cities with formidable chemical industries. The biorefinery locations and potential markets are shown in the map in Figure 7. The model also chose a region from which to purchase the switchgrass feedstock. The farm locations were chosen based upon labor costs, length of harvest season, local farmgate price, and availability of switchgrass. The farmgate price is the raw price paid directly to the farmer without taking transportation into account. Local rent and availability are considered in this price, however. Shown below, respectively, are the local farmgate prices in $/ton for the 25 farm locations and a map detailing the locations.

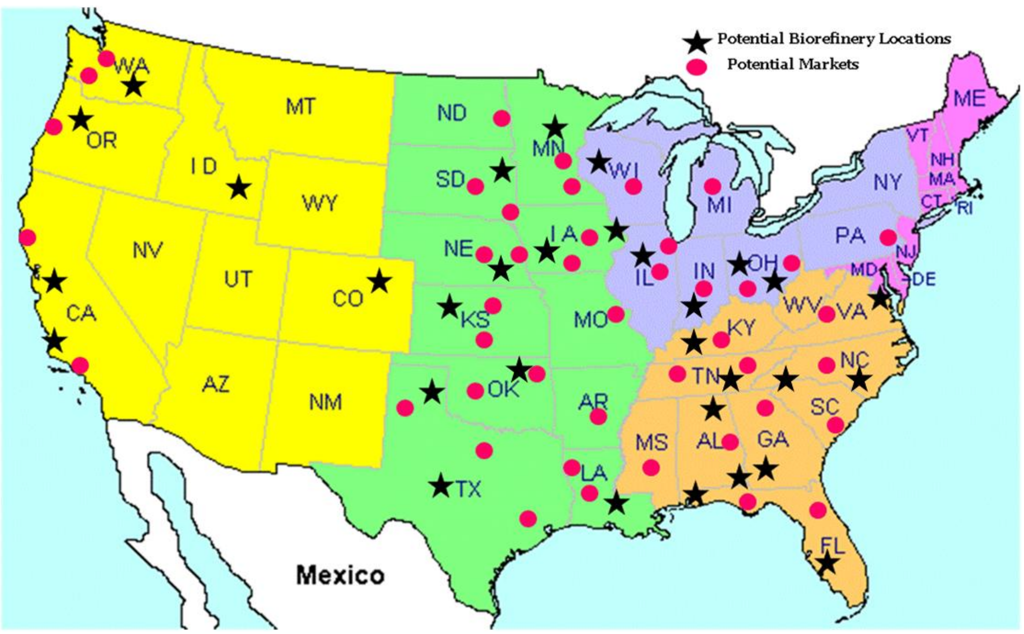

Figure 7 – Potential locations for biorefinery construction and potential markets for sales of products

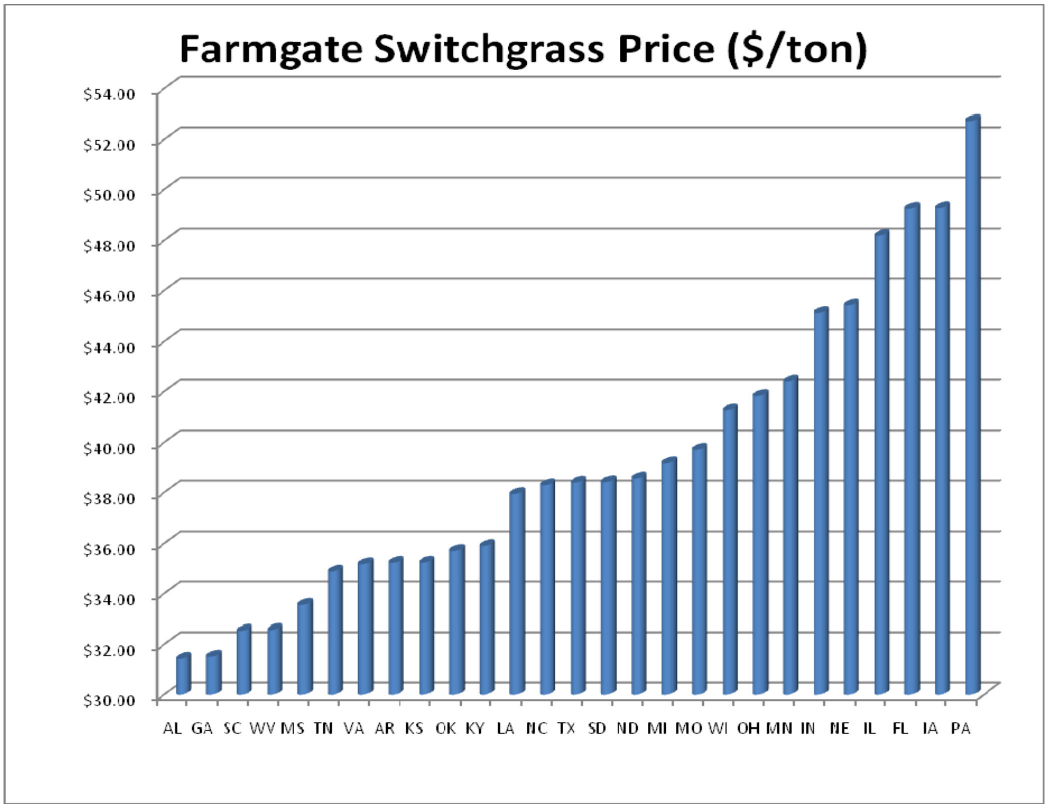

Figure 8 – Farmgate switchgrass price per state [7]

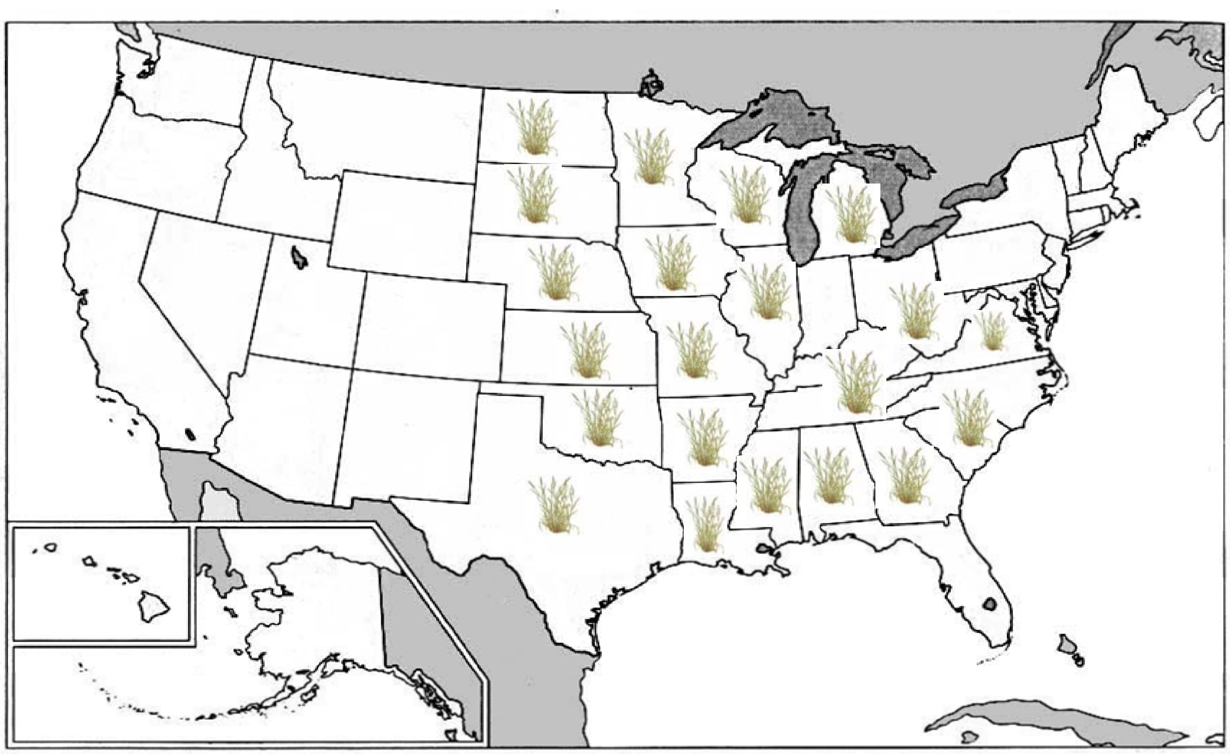

Figure 9 – Potential switchgrass farm locations for purchase of raw materials

Results

After running the mathematical model under various conditions and conducting all steps of the screening process, only the most profitable combination of processes remained. The final process flow chart included only three processes, each of which produces a high-priced value added chemical. The final process flow chart is seen in Figure 10. Out of the three processes, two are fermentation-based, producing 3-Hydroxypropionic acid and Glucaric Acid. The third process produces 5-hydroxymethyl furfural through decomposition of glucose. The model also determined the best time to build and expand these processes. Under the current conditions, the model determined that all processes should be built immediately with no expansions during the twenty year lifetime. These processes were chosen not only on the basis of final product selling cost, but also on the lower operating costs compared with other processes. The capacities of these processes were varied within the model. The model also determined the minimum capital investment required to carry out the start-up from a given amount of available money for investment. Assuming $250 million investment available, the results for centralized and non-centralized utilities differ significantly. Table 4 summarizes the important results.

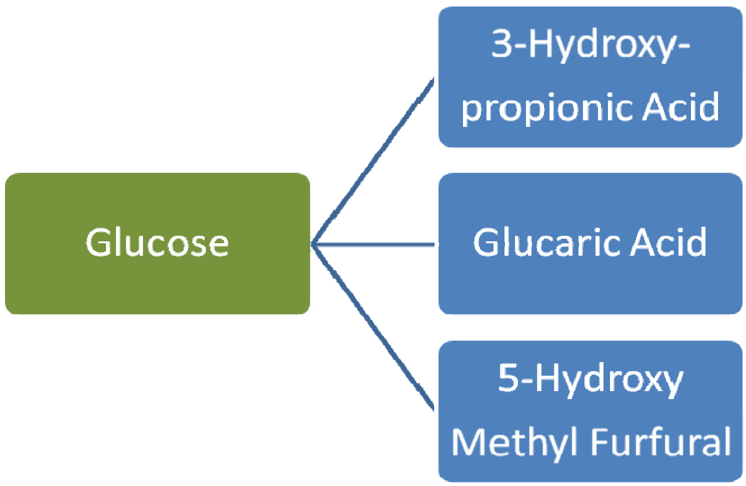

Figure 10 – Final process flow chart after full screening

	Centralized	Non-centralized
Capital investment	$221 million	$221 million
Net present value	$621 million	$151 million
Return on investment	14%	3%

Table 3 – Summary of economic results from mathematical model

With the same capital investment of $221 million, we see that the profitability of the biorefinery is significantly affected by the centralization of utilities. The difference in return on investment when employing centralized utilities is substantial and could mean the difference in whether or not the project is considered profitable to investors.

Finally, the model chose the biorefinery location as well as locations to sell the final products and buy the raw materials. This was done by minimizing costs associated with the various locations through transportation costs, taxes and other parameters. Distances from farm to biorefinery and from biorefinery to markets had the greatest impact on location choice, however. The model determined that the final three-process biorefinery was best located in Huntsville, Alabama. The feedstock to the facility was purchased from Alabama as well. The final products are sold in Houston, TX and Chicago, IL. Alabama was chosen as the best state from which to purchase switchgrass due to its low farmgate switchgrass price of $31.44 compared with the national average of $39.26. Alabama also boasts a high average switchgrass yield of 6.2 tons/acre/year compared with a national rate of 5.4 tons/acre/year. [7]

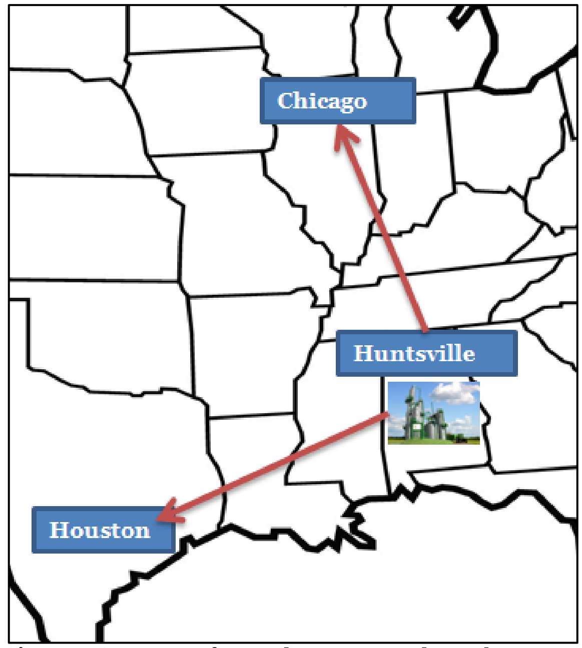

Figure 6 – Biorefinery location and markets

Conclusion

The model developed for biorefinery capacity planning effectively maximizes net present value while taking into account the simultaneous effects of plant location, switchgrass farm location, and location of markets for sale of products. Many locations across the United States were considered, an expansion on past research on this subject. In addition, the model incorporates centralization of utilities, a feature distinct from other biorefinery capacity planning models. It also includes budgeting considerations, following the cash flow over the life of the project. The results from the model show that centralization of utilities leads to substantial cost savings and a higher net present value for the project.

Recommendations

Biorefinery design is complex and the design procedures presented in this report have potential for expansion. Work that was beyond the scope of this project includes separation considerations, risk analysis, accurate market predictions, more detailed fermentation information, and uncertainty analysis. Also, cost estimates could be improved with more detailed equipment estimates. Many final products in processes must undergo rigorous separations to prepare them for sale and these processes may add considerable costs. In addition, purity required for sales of the products will be investigated. Since a facility such as an integrated biorefinery requires not only a large capital investment, but also continuous re-investment of revenues to ensure continuous successful operation, risk analysis and uncertainty over the lifetime may be considered. The current mathematical model may be refined and updated for accuracy regarding these concerns. Future work will determine optimal fermentation broth conditions such as temperature and pH to maximize yield.

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