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A techno-economic analysis of syngas fermentation for the production of hydrogen and polyhydroxyalkanoate

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ABSTRACT

This thesis is an exploration into the technical and economic issues related to a syngas fermenting biorefinery producing 50 metric tons per day of hydrogen gas and 12 metric tons per day of PHA, a biodegradable plastic. In addition, an optimization study on the bioreactor is performed by varying reactor diameter and stirring speed.

The analysis assumed switchgrass costing $55/Mg as feedstock, and the bacterium *Rhodospirillum rubrum* to ferment the syngas. With a hydrogen market value of $1.90/kg assumed, 95% pure PHA was determined producible for approximately $2.05/kg. Grassroots capital for the biorefinery was estimated to be $55 million, with annual operating costs at $8.3 million. For a constant volumetric mass transfer coefficient of 0.05 s^{-1} the optimum reactor size was a 14.8 m diameter being stirred at 0.6 rev/s. Producing PHA by this method was found to be less expensive than processes using sugar fermentation.

INTRODUCTION

MOTIVATION

In recent years, crude oil prices have fluctuated greatly. Since crude oil is a feedstock for many products such as plastics, as well as being used as a transportation fuel, its price fluctuations have disruptive effects on several different parts of the economy. Finding alternative feedstocks to replace all or part of the petroleum used would help to reduce the economic disruptions caused by crude oil supply variability. Biomass offers a potential alternative to crude oil, but requires new and innovative processing methods than those traditionally used in the petroleum industry. One alternative method for processing biomass is gasification followed by syngas fermentation. This thesis is an exploration into the technical and economic issues related to a syngas fermenting biorefinery producing 50 Mg per day of hydrogen gas and 12 Mg per day of polyhydroxyalkanoate (PHA), a biodegradable plastic.

The term "biorefinery" has been used to describe the chemical refining of many different processes. The common theme, however, is that the feedstock is organic material from recent biological origin. The modifier of "recent" differentiates biorefineries from traditional chemical refineries which use a fossil organic material, such as petroleum or coal [1].

Gasification is a thermochemical conversion process which offers an alternative to biological processes. Rather than using biologically active molecules to assist in the breakdown of the resilient compounds found in biomass, thermochemical conversion uses heat to convert biomass into a flammable gaseous mixture. If the gasifier is oxygen blown and operated at temperatures above 900°C, the mixture is mostly hydrogen (H_2), carbon monoxide (CO), and carbon dioxide (CO_2), which is known as syngas. If the gasifier is air-blown and operated between 700 and 900°C, the mixture also includes substantial nitrogen (from the air) and small amounts of hydrocarbons, which is known as producer gas [2]. Either oxidizing gas is suitable for biocatalytic synthesis, so the term syngas fermentation is applied whether the gas comes from an oxygen-blown or air-blown gasifier.

BACKGROUND

GASIFICATION BASICS

The term “gasification” actually refers to a multi-step process in which solid biomass is broken down into simpler gaseous molecules and some remaining solids in three main steps [1]. The first step, drying, drives moisture from the biomass and gives way for pyrolysis, the next step. Pyrolysis is the physical breakdown of the solid molecules in biomass into gases, vaporized liquids such as tars, and the remaining solids of char and ash. Char is mainly carbon, while ash consists mostly of non-combustible minerals such as sodium, potassium, calcium or silicon. The third and final step is also called gasification, because it refers to the partial oxidation of the pyrolysed biomass into hydrogen, carbon monoxide, and carbon dioxide. Partial oxidation means that not enough air or oxygen is provided to completely combust the biomass. The gas, vapor and char produced during pyrolysis can all be partially oxidized during this phase [2]. Not all the pyrolysed biomass is converted, however, and contaminants such as vaporized tar, solid char and ash will have to be removed or otherwise converted downstream from the gasifier. This will be discussed in a later section. Gasification is overall an endothermic process and requires either an external heat source to maintain the reactions, or that some of the gas produced be combusted to provide the necessary heat [3, 4]. If the latter is implemented, enough additional oxidizer is added to the gasifier vessel to allow some gas to combust and thus provide heat to the reaction.

GASIFICATION TECHNOLOGY

Gasifiers are typically split into two main categories: “fixed bed” and “fluidized bed”. The terms describe very well their differentiating features but require some explanation. The “bed” refers to whatever structure is used inside the gasification vessel to support the biomass during the process. In a fixed bed gasifier this is typically a grate, while in a fluidized bed this is sand or some other inert material. The grate of a fixed bed allows gas to flow through while preventing large pieces of unreacted biomass from passing. In a fixed bed gasifier the biomass is typically fed from the top of the reactor vessel and the oxidizer flows through the biomass from above, below, or the side. Oxidizer flowing from above in a fixed bed makes a downdraft gasifier, and if it comes from below is called an updraft gasifier. Logically then, oxidizer from the side creates a cross flow gasifier [3]. There are other variations on the fixed bed design, but the three

described here are the most common [2]. Downdraft gasifiers typically produce gas with low tar, but a high particulate content. Because the gas exiting a downdraft gasifier is typically at the same temperature as within the reactor, its thermal efficiency is low compared to an updraft gasifier [3]. Updraft gasifiers are typically the opposite and produce gas with a high tar content, low particulate content, and high thermal efficiency.

A fluidized bed gasifier is more complex than a fixed bed in that the "bed" is made up of inert material through which the biomass moves. The mass of sand in the vessel rests on what is called a "distributor plate" which prevents the sand from falling further down in the vessel, but also has small holes in it to allow gas to pass through. Below the distributor plate, the oxidizer is blown into the vessel, flows through the distributor plate, and then upward through the sand causing it to bubble or "fluidize". While the bed is fluidized, biomass is fed into the vessel just above the distributor plate and flows upward through the sand, gasifying as it goes. The gas produced exits through the top of the gasifier vessel. Some char and ash solids also exit with the gas [2].

Depending on the flow rate of oxidizing gas, a fluidized bed can be either a bubbling fluid bed reactor (BFBR) or a circulating fluid bed reactor (CFBR). In a BFBR, the gas flow rate through the sand is low such that the bed is dense, and large solids separate easily from the gas. There is typically a large enough headspace (known as "freeboard") above the bed in the gasifier vessel to allow this gas-solid separation. The bed in a CFBR moves more vigorously, due to a higher gas flow rate, and the bed material is distributed almost evenly throughout the gasifier vessel. As a result of this design, inert bed solids exit the vessel, which is known as "elutriation" [2]. In addition to the char and ash produced, these exiting solids include some of the bed material which must be returned to the gasifier vessel. A cyclone separator is typically used to remove the elutriated solids for recirculation to the gasifier. Small particles still escape the cyclone, however, and must be removed downstream.

Compared to fixed bed reactors, fluidized bed reactors are more complex and have higher capital costs to construct. However, fluidized beds have an advantage over fixed beds in their greater control over temperatures, increased tolerance to fuel quality, and ease of scale-up to large capacities [2].

Another type of gasifier sometimes categorized with fluidized beds is the entrained flow reactor. This variation does not use an inert bed of sand but instead, fuel is fed along with oxidizer at one end of the reactor [5]. While reacting, they flow concurrently to the opposite end of the vessel [6] and exit, where a cyclone is typically used to recycle large unreacted solids. This type of gasifier is more commonly used with

coal as a fuel source than biomass, because of the need for finely ground fuel [2]. Maintaining adequate control of the gasifier is another reason that entrained flow reactors are less commonly used with biomass [3].

GAS CLEANUP TECHNOLOGY

After the gasification of biomass, contaminants must be removed before the syngas can be sent to the bioreactor. The bacteria used as biocatalysts are capable of tolerating a wider range of contaminants compared to traditional metal-based catalysts. However, cleanup of the syngas is still necessary to prevent bacteria die-off from poisoning. The two main contaminants that must be removed are solid particulates and vaporized tars [7]. Solids are typically removed from the syngas stream before the tars, and to prevent the tars from condensing must be performed at temperatures above 500°C [3].

SOLID PARTICULATE REMOVAL

This category is typically divided into two sections: cyclonic filters and barrier filters [8]. Cyclone filters remove solids by swirling the gas and causing the heavier solids to fall out of the stream due to their inertia causing them to impact the cyclone walls. Downstream from the gasifier, the first stage cleanup is usually high-efficiency cyclones, which are capable of removing solids above 5 to 10 μm and can operate at high temperatures [6]. Below this size barrier filters must be used [3], such as ceramic candle filters or fabric filters. Barrier filters are capable of particulate capture within the 0.5 to 100 μm range, with removal efficiencies approaching 100% [8].

A ceramic candle filter is a long hollow cylinder made of porous ceramic which is open at one end and capped at the other. An array of these filters is usually hung inside a larger steel vessel through which the syngas flows. Dirty gas moves through the filter from the outside to the inside with the solid contaminants being trapped on the surface. This layer of dust, known as the “filter cake”, is periodically blown off with compressed air blown from the inside of the filter [9]. Candle filters have been tested at 850°C [10] and above [11] without degradation, but are fragile and prone to cracking from thermal stresses [2, 8].

Fabric bag filters are similar in arrangement to ceramic candle filters in that an array of filter bags is hung inside a vessel and dirty gas is forced through the bags.

Likewise, the bags are periodically cleaned by pulsing air through the bags to blow off the filter cake. The fabrics used for these bags must be capable of withstanding temperatures of at least 500°C. Various composites using ceramics and fiberglass have been developed. Temperature as high as 850 to 1,100°C are possible [6, 11].

GAS REFORMING

The tars formed during gasification come from biomass that has not completely reacted [12] and must be removed or reformed before the syngas passes to the bioreactor. Removal of these high molecular weight hydrocarbons typically requires cooling of the gas stream and scrubbing it with water or oil. However, this process is expensive and generates a new stream of contaminated water or oil which must be handled [2, 8].

Reforming of tars involves breaking the long chain molecules into hydrogen, carbon monoxide, and carbon dioxide using some combination of heat, steam, and catalysts [12]. Catalytic destruction of tars is typically performed between 800 and 900°C using catalysts such as dolomite, nickel, or olivine [2, 3]. Thermal destruction of tars does not use catalysts and consequently requires the reforming vessel to operate at higher temperatures, anywhere between 900 and 1,100°C [3, 12]. Both catalytic and thermal tar destruction require additional water in the process to provide hydrogen and oxygen to combine with the cracked molecules.

SYNGAS FERMENTATION

Syngas fermentation uses bacteria to consume a portion of the syngas, such as the carbon monoxide or hydrogen, in order to produce a variety of chemicals, including methane, acetic acid, butyric acid, ethanol, and butanol [13]. These bacteria serve as biocatalysts, which offer several advantages over traditional mineral-based catalysts. First, biological catalysts can operate at temperatures and pressures which are closer to standard conditions compared to traditional catalysts which often require high temperatures and pressures. Second, the output of biological catalysts is less sensitive to the ratio of carbon monoxide to hydrogen in syngas compared to traditional catalysts that typically require a specific ratio of CO to H_2 in order to produce their desired chemicals. Finally, biological catalysts are less sensitive to contaminants in the syngas such as char, tar, ash, chlorine and sulfur [14].

Datar *et al.* [14] produced ethanol from a novel clostridial bacterium grown on "artificial" producer gas in a bubble column reactor. This "artificial" producer gas was a mixture of pure nitrogen, hydrogen, carbon monoxide and carbon dioxide. However, when the bacteria were given "real" producer gas from a gasifier using switchgrass the bacterial growth stopped. The researchers concluded that a possible cause was trace contaminants in the "real" producer gas that inhibited one or more of the metabolic pathways in the bacterium.

Acetate, another possible product of syngas fermentation, was produced by Vega *et al*. [15] using *Peptostreptococcus productus* grown from a mix of pure carbon monoxide, methane, and carbon dioxide. The experiment was performed in a continuously stirred tank reactor (CSTR) at both steady and non-steady state conditions. A key finding of this research is that a mass-transfer controlled operating condition is likely the most economical operating point for gaseous substrate fermentations performed in a CSTR, because at this point the dissolved concentration of gas in the liquid is approximately zero and conversion of the gas by the bacteria is highest.

Another bacterium used for syngas fermentation is *Rhodospirillum rubrum*, and Klasson *et al*. [16] used this for the production of hydrogen in a CSTR. The bacteria culture was fed a gas mixture containing pure hydrogen, argon, carbon monoxide, and carbon dioxide. The carbon source for this experiment was the carbon monoxide, and the bacteria also consumed water to produce hydrogen through the water-gas shift reaction:

Equation 1: Water-gas shift reaction

$$CO + H_2O \rightarrow H_2 + CO_2$$

The experimenters found that production of hydrogen was inhibited by an excess amount of carbon dioxide in the liquid.

Maness and Weaver [17] used a novel bacterium identified as *Rhodobacter* sp. CBS, which is capable of both producing hydrogen gas and also creating PHA as an energy storage medium within the cell. The bacteria were grown on a mixture of pure hydrogen, carbon monoxide, and nitrogen gases in anaerobic tubes. Since this particular bacterium was photosynthetic, incandescent lamps were also used as a light source. A key finding of their research was that in both the light as in the dark, the bacteria converted carbon monoxide to hydrogen gas at nearly the same rate. However, during growth in the light phase the bacterium re-consumed all the hydrogen gas it produced.

METHODOLOGY

Four major steps were taken in the techno-economic analysis for this biorefinery. First, the material and energy flows were determined by simulating the biorefinery with computer software. Next, an optimization was performed on the bioreactors to determine their most cost effective configuration. Then, the capital and operating costs for the biorefinery were determined and the PHA product cost was estimated. Finally, the sensitivity of the PHA product cost to several input variables was calculated.

MODELING THE BIOREFINERY

In order to properly determine the size of the equipment used in the biorefinery, as well as to estimate material and energy flows, a material and energy balance was performed. The main work for the mass and energy balance was done using Aspen Plus, a flow sheet simulation software package from Aspen Technologies [18]. In addition to Aspen Plus, a bioreactor model was made using Microsoft Excel to optimize the size of the bioreactor used and its stirring speed. The optimization process will be described in a later section. One of the first steps in producing a simulation using Aspen Plus is to lay out the flow sheet, which consists of choosing function blocks and creating streams for mass and energy flows (Figure 1).

FUEL & AIR DELIVERY

The biomass feedstock entering the biorefinery was assumed to be switchgrass with a 0.6 to 1 m length. The grinder (GRINDER, Figure 2) reduced the size of the switchgrass to 0.03 m based on research by Lysenko [19]. Power consumed by the grinder was 180 kW, based on the motor size of the unit specified and quoted by Pesco Incorporated. The grinder was modeled as a dual roll hammer mill.

As described earlier, the proximate and ultimate analysis of the switchgrass was specified in the Aspen Plus model, however it was not used by the software. This was mainly because the software was not used to calculate the energy change in the gasifier. Due to the challenge of modeling the kinetics of various reactions which occur in the gasifier, only the component mass yields of the gasifier were specified, based on experimental research performed by Lysenko [19]. To produce 50 Mg of hydrogen gas per day, the grinder was required to process 708 Mg of switchgrass or approximately 30 Mg/hour. The grinder size quoted by Pesco Incorporated reflected this.

The blower (AIRCOMP), which was used to supply air to the gasifier, took air at 20°C and 1.01 bar and raised the pressure to 2 bar. Power consumed by the blower was calculated by Aspen Plus, but also by the Aspen Icarus Process Evaluator (IPE) software, to be described later. For contingency purposes, the Aspen IPE power consumption was used for the cost estimation because it was higher. After the blower, the air was preheated by a heat exchanger before moving to the gasifier. This will be discussed in detail in the section describing the heat exchanger network.

GASIFICATION

The gasifier (GASIFIER, Figure 2) chosen for this techno-economic analysis was a bubbling fluidized bed reactor (BFBR). It was necessary to choose this type of gasifier because the outlet gas composition used in the simulation was based on previous experimental work by Lysenko on a BFBR [19]. Future work could compare other types of gasifiers for this biorefinery.

The BFBR was sized with assistance from Jerod Smeenk at Frontline Bioenergy [20]. For a BFBR using 708 Mg/day of biomass, an approximately 41 m^2 bed area is required. Assuming a cylindrical reactor the diameter of the bed is then 7.25 m. Also based on correspondence with Smeenk, the length of the reactor was assumed to be 10 m, and the bed depth to be 1 m. For costing purposes, the bed material was assumed to be 40 m^3 of crushed limestone. In addition, the gasifier vessel was cost estimated with a refractory brick lining of a 90% alumina firebrick, backed by an insulating firebrick lining. Area of both linings was assumed to be 300 m^2. Adjustment to the steel vessel diameter from the brick lining thickness was not performed. Future cost estimates can include this.

Operating temperature of the gasifier was 730°C, and the pressure was 2 bar. The gasifier pressure was assumed from the blower outlet pressure, and the temperature was based in work performed by Lysenko [19]. The mass composition of the outlet syngas was also based on his work (Table 1). As mentioned earlier, only a mass balance was performed on the gasifier.

For the purposes of hot gas cleanup, a particle size distribution (PSD) of the char and ash exiting the gasifier was based on research done by Ritzert [21]. The particle size distribution of the char and ash was tabulated and graphed (Figure 3).

PARTICULATE REMOVAL

In the simulation, syngas exiting the gasifier was cleaned by two stages of cyclones (CYCLONE1, CYCLONE2, Figure 2) followed by a fabric filter bag house (BAGHOUSE, Figure 2). The cyclones were modeled in Aspen Plus as high efficiency units using Leith-Licht correlations [22]. Based on those correlations, it was determined that five parallel cyclones of 1.5 m in diameter were needed for each stage. For costing purposes, the cyclones were assumed to have gunned monolithic refractory linings of 90% alumina because of the high temperatures of the syngas. Area of the coating was assumed to be 15 m^2 per cyclone. For the fabric filter bag house, it was necessary in the Aspen Plus software to specify the filter area, pressure drop, and dust resistance coefficient [23]. The total filter area was calculated to be 1,600 m^2 with a pressure drop of 250 N/m^2. The dust resistance coefficient used for this simulation was 60,000 $Pa/[(kg/m^2)\cdot(m/s)]$, based on a mean particle size of 55 μm [23].

Initially it was planned to cost a candle filter system for this analysis. Difficulty in getting estimates led to the costing of a fabric bag house using Aspen IPE. From research performed by Nelson [11], high-temperature fabrics are available that are capable of withstanding the temperatures typically found in hot gas cleaning conditions. However, these fabrics are not available within the Aspen IPE software. Thus, future work should include an accurate accounting of either high-temperature fabrics for bag houses, or a candle filter system. Filter area for the bag house was estimated at 1,600 m^2, based on requirements given in the IPE software, and volumetric flow rate of the syngas.

Estimation of particulate removal efficiency was performed by the Aspen Plus software, and the simulation results were simulated to be below 10 mg/m^3, which gives a char particle loading of 10 parts per million (ppm) in the syngas at standard temperature and pressure. For this analysis, no use was made of the char and ash after its removal from the syngas stream. Future work could analyze the value of recovering the heat from these streams, as well as the use of the char and ash for further combustion and/or nutrient recycling.

GAS & TAR REFORMING

After removing most solid particulate matter from the syngas, it was necessary to eliminate methane and other hydrocarbons. As mentioned earlier, the gas composition for this analysis was based on prior work performed by Lysenko [19] which found

methane, ethylene, ethane, and tar as contaminants in the syngas. For the Aspen Plus simulation the tar was modeled as $C_{20}H_{42}$, also known as n-eicosane.

For this analysis, a high temperature steam reforming vessel (GASREFRM, Figure 4) was modeled with 100% conversion of all contaminants assumed. The complete conversion of all hydrocarbons in the gas reformer is idealized, and future work could assume a number based off experimental values. Reactions are as follows:

Equation 2: Hydrocarbon shift reactions

Methane: $CH_4 + H_2O \rightarrow CO + 3H_2$

Ethylene: $C_2H_4 + 2H_2O \rightarrow 2CO + 4H_2$

Ethane: $C_2H_6 + 2H_2O \rightarrow 2CO + 5H_2$

Tar: $C_{20}H_{42} + 20H_2O \rightarrow 41H_2 + 20CO$

Three times the stoichiometric amount of steam was provided to the reformer [12], and the vessel operated at a temperature of 750°4C and a pressure of 1.5 bar [24]. Based on work reported in Spath *et al*. [25], the gas reformer was modeled as a fluidized bed reactor of the same size as the gasifier, with the same specifications except for bed material. Instead of crushed limestone, the catalyst described by Spath *et al*. was used for cost estimations. The reactions taking place in the gas reformer require heat, and this was modeled as coming from a stream of syngas split off from the main stream before the gas reformer. Aspen Plus calculated the LHV of the wet syngas to be 4,400 kJ/kg. The combustion of the syngas was modeled in a reactor block to give the effects of a furnace (FURNACE1, Figure 4) and provide the heat necessary for the gas reformer.

HEAT EXCHANGER NETWORK

In this simulation four stages of heat exchangers (Figure 5) were used to cool the syngas from the gas reformer prior to entering the bioreactors, from 750°C to 25°C. The heat energy contained in the syngas was enough to preheat the gasifier air, gas reformer water, and bioreactor water. First, the hot syngas was used to pre-heat air for the gasifier (HEATX1), and then it was used to pre-heat water entering the gas reformer (HEATX2). Next, more process water had to be heated a few degrees before entering the bioreactors (HEATX3). Finally, the remaining heat in the syngas was removed with cooling water (HEATX4). In the Aspen Plus software, the heat exchangers were modeled in a shortcut method where exchanger geometry is not specified. Only the desired cold stream outlet

temperature needed to given and the software calculated the necessary heat exchanger area. The calculated areas were 2,240, 824, 3.34, and 3,060 m^2 respectively. The overall heat transfer coefficients used were 60 $W/m^2 \cdot K$ for HEATX1, and 230 $W/m^2 \cdot K$ for the rest [23]. To find the cost of the exchangers, the data was imported into Aspen IPE and they were specified to be floating head tube and shell exchangers. The software then determined the capital, labor, and material costs.

BIOREACTORS

The bioreactors (BIOREACT, Figure 6) were modeled first using a Microsoft Excel spreadsheet. The purpose of this spreadsheet was to determine the optimal size and stirring speed of the bioreactors needed based on several process variables. While this process will not be described in this section, the volumetric flow rates of syngas as well as the volumetric mass transfer coefficient of carbon monoxide were two important variables in the process. For the economic analysis, the optimal configuration of one reactor 6.6 m in diameter was used for the baseline analysis. For comparison, the costs of a configuration with a 14.8 m diameter bioreactor were also estimated. The reactors were cost estimated as enclosed, fully jacketed, agitated tank reactors with a shell of 304 stainless steel [26] and a jacket of low carbon steel [27]. Design pressure was 3.45 bar and design temperature was 125°C. Operating temperature and pressure, however, were modeled as 1.1 bar and 25°C. The bioreactors were also cost estimated with variable frequency drives on the agitator motors because of the need to adjust agitation speed for optimum gas dispersion. Excess heat from the exothermic bacterial reactions was used to preheat the make up water entering the bioreactor at 20°C, and also to maintain the bioreactor at the necessary 25°C (Figure 7).

BACTERIAL REACTIONS

In addition to modeling the physical geometry of the bioreactors, the chemical reactions taking place inside them had to be simulated as well. The reactions were based on those performed by *Rhodospirillum rubrum*, which is a gram-negative bacterium that consumes carbon monoxide and water to produce hydrogen, as well as PHA. The PHA is used as an energy storage medium within the cell [7]. Of the carbon monoxide consumed by the cell, 80% of it is used for the water gas shift reaction:

Equation 3: Water-gas shift reaction

$$CO + H_2O \rightarrow H_2 + CO_2$$

The remaining 20% of the carbon monoxide is used to make the cell biomass, of which 40% is PHA. For this analysis, the PHA was assumed to be poly-3-hydroxybutyrate (P3HB), with a monomer of $C_4H_6O_2$. The reaction to produce P3HB is:

Equation 4: PHA production reaction

$$9CO + 3H_2O \rightarrow C_4H_6O_2 + 5CO_2$$

All non-PHA biomass was assumed to be dextrose ($C_6H_{12}O_6$), with a production reaction of:

Equation 5: Cellular biomass production reaction

$$12CO + 6H_2O \rightarrow C_6H_{12}O_6 + 6CO_2$$

In the P3HB and dextrose reactions, only the energy needed to form the monomers was accounted for; polymerization and its associated energy were not calculated. Based on work by Do [7] the outlet dry cell weight concentration from the bioreactor for this simulation was assumed to be 1.9 g/L, or 0.19% total solids. A later section will detail the optimization process and the modeling of the bioreactors.

STREAM MIXERS & SPLITTERS IN FLOW SHEET

It can be seen on the process flow sheet (Figure 1) that after the bioreactors there is another vessel named GASLIQ. It should be noted that this vessel exists only in the Aspen Plus simulation and was not used for the economic analysis. It is not an actual piece of equipment but a modeling convenience. The block used to model the bioreactors only allowed one exit, and therefore it was necessary to use a second vessel which allowed the gases and liquids to separate from each other in the process stream. Several other stream mixers and splitters exist in the simulation that were not cost estimated due to their minimal effects on overall system cost.

HYDROGEN PSA

Separation and purification of the hydrogen gas (H2PSA, Figure 6) was modeled as a pressure swing adsorption (PSA) unit [28]. This process uses a mineral with a high surface area called a zeolite. These minerals are capable of adsorbing gases to their surface. The adsorptive ability is a function of pressure, so pressure is increased to 20 bar or more until most of the undesired gases are adsorbed to the surface of the zeolites. Then, a small drop is used to remove the unadsorbed hydrogen [28]. Pressure swing adsorption is a batch process by design, but with multiple pressure vessels filled with zeolites and a valve manifold capable of switching between vessels it can be made into a continuous process.

In this analysis, the Aspen Plus flow sheet modeled the PSA unit as a separation, and the hydrogen component was assumed to be separated from the other gases with 100% purity and 100% recovery. All costs for the equipment (equipment, materials, and labor) are taken directly from a previous analysis performed by Lysenko [19]. Since that analysis also estimated equipment for 50 Mg/day of hydrogen, no re-sizing of the equipment was required. A real-world PSA unit would be capable of hydrogen purity of 99.999%, so the 100% purity assumption is accurate [28]. Recovery of the hydrogen would likely be less than 100%, however.

PHA SEPARATION PROCESS

Separating biopolymers from their parent cell material is typically one of the most costly parts of production [27]. Energy, water, and chemicals can be consumed in large quantities to accomplish this, and many different processes have been developed [29].

This analysis draws heavily on a surfactant/hypochlorite treatment presented by Choi and Lee, and their published paper which details the economics of a batch system which uses this process [29]. Surfactant is first used to break down the cell wall, and then a solution of sodium hypochlorite further solublizes the cell material. Centrifugation and washing steps are then used to separate the PHA granules from the remaining cell biomass and water solution.

While the Choi and Lee paper was useful for a source of the overall process steps and chemical costs, sizing of the equipment had to be based on needs specific to the *R. rubrum* bacteria. Because other equipment in the biorefinery operates optimally in a continuous manner, the material flow in the Choi and Lee process was switched from batch to continuous. Re-sizing of the centrifuges was especially important. For example,

the Choi and Lee process assumed production based on *E. coli* bacteria which give a final cell density of 110 g dry cell weight (DCW) per liter of growth medium, or 11% total solids. The *R. rubrum* simulated in this analysis has an optimal cell density of 1.9 g DCW per liter, or 0.19% total solids. This requires significant de-watering before the bacteria can be treated with the surfactant and hypochlorite solutions.

CENTRIFUGE 1

The first stage of centrifugation (CENTRIF1, Figure 8) takes the material from the bioreactors at 0.19% solids and increases the solids content to 4%. Water removed is recycled back to the bioreactor after adding make up water and nutrients and heating the mixture to 25°C in order to match the bioreactor conditions. For this stage, the economic analysis assumes an array of four centrifuges operating in parallel, modeled as solid bowl centrifuges with bowl diameters of 0.92 m and a length of 3.35 m. The dimensions were based on product information from Flottweg Corporation [30]. The total solids at the outlet were also based on product information from Flottweg. It was assumed that 99% of the solids (cell material) entering the centrifuge are captured and the remainder are recycled back to the bioreactors.

SURFACTANT BLENDING TANK

After the first set of centrifuges, the chemical surfactant is mixed with the slurry to begin breaking down the cell walls (BLNDTNK2, Figure 8). For the economic analysis, this was assumed to be a stirred tank made of 304 type stainless steel with a volume of 75 m^3. The capacity was chosen by scaling up the blending tank used in the Choi and Lee analysis [29]. The rate of surfactant added to the process stream was 0.15 g surfactant per gram of 95% pure PHA, the same ratio as used in the Choi and Lee analysis.

HYPOCHLORITE MIXING

The next step in the process was the hypochlorite mixing, to further break down the cell biomass (MIX3, Figure 8). In the Choi and Lee paper, this was simply a mixing valve, so it was also modeled this way in the Aspen Plus simulation but its cost was not estimated in the economic analysis. The hypochlorite solution was assumed to be a 5%

solution of sodium hypochlorite in water, and the ratio of solution to 95% pure PHA was 2.8 g/g. This also came from the Choi and Lee analysis.

CENTRIFUGE 2

After treatment with hypochlorite, a second centrifugation pass (CENTRIF2, Figure 8) was performed to remove the cell biomass dissolved by the chemical treatment. This stage increased total solids from approximately 3.5% to 25%. It was assumed that 90% of the dextrose-based cell biomass left the process in the wastewater stream. Also, the hypochlorite solution was assumed to leave the process completely in this waste stream. It should be noted here that the simulation differs from what can be achieved in actual practice. The economic analysis calculated the cost of treating this stream based on assumed wastewater treatment costs. In reality, though, some of the hypochlorite will stay with the main process stream and end up being removed in the spray dryer. Future work can include a wastewater treatment analysis. Details on the centrifuge came again from the Flottweg Corporation website as described above. For cost estimating purposes, a single solid bowl centrifuge was used for this stage.

BLEND TANK 3

This step is similar to the previous surfactant blending step in that an agitated tank was used to mix two streams together (BLNDTNK3, Figure 8). However, in this step only water was assumed to enter the main process stream to help wash any additional cell biomass from the PHA granules. Water was added to bring the process stream down from 25% to 4% solids to wash out the remaining chemicals and cell material. The volume was assumed to be 4.7 m^3, calculated by scaling up the vessel used in the Choi and Lee process.

CENTRIFUGE 3

The third stage of centrifugation (CENTRIF3, Figure 8) brings the solids content up from 4% to 25% solids. Also, the remaining dextrose is sent to the wastewater stream until the main process stream is 95% pure PHA. This centrifuge stage is identical to the second centrifuge stage.

SPRAY DRYER

To dry the 95% pure PHA granules a continuous spray drying system was used (SPRAYDRY, Figure 8). The heat source for this system was modeled to come from a syngas stream split off from the main stream prior to the gas reformer, similar to the heat source used for the gas reformer. The heat required for drying was estimated to be the latent heat of vaporization for water to be removed, plus an extra 50% to account for losses and additional sensible heat needs [1]. From the entering slurry mixture of water and 25% solids, 34 Mg/day of water was assumed to be removed, leaving the exiting PHA stream with 10% moisture content.

COMPONENT SPECIFICATION

After the flow sheet was created and the blocks defined, the components used in the simulation were specified (Table 2) as follows: hydrogen, oxygen, nitrogen, carbon monoxide, carbon dioxide, methane, ethylene, acetylene, ethane, propane, water, "CHARASH", n-eicosane ($C_{20}H_{42}$), "SWGRASS", "P3HB", dextrose, carbon, and sodium hypochlorite.

Of these components, "SWGRASS" and "CHARASH" were modeled as "non-conventional" components. This means that the physical properties of the component are not defined based on information from the software's databanks. Instead, empirical properties such as ultimate, proximate, and sulfur analyses are used to define the component. Data for both these components came from previous work by Lysenko [19].

The component "P3HB" was modeled in yet another way. This component was used to represent the PHA created by the bacteria, and thus it was necessary for a particular molecule to be specified. In this case the molecule was defined as $C_4H_6O_2$, and the molecular structure and weight were specified within the software, which was then used to estimate other material properties such as energy of formation. As mentioned earlier, only the monomer of PHA was used, and the simulation did not account for polymerization energy. Future work could include this energy in the simulation.

Finally, it should be noted that dextrose was assumed to make up all the other cell biomass within the bacteria. Again, this was also modeled as a monomer, with no polymerization energy accounted for. After all the above components were specified, it was then possible to define the details of the components used in the flow sheet.

BIOREACTOR OPTIMIZATION

Previous research [7] has determined that the rate limiting step in syngas fermentation by *Rhodospirillum rubrum* bacteria is the mass transfer of carbon monoxide from the syngas to the cell culture medium in the bioreactor. Therefore, particular attention was given to this area of the bioreactor system. Although the cell culture medium contained various nutrients in trace amounts, it was mostly water [7]. For the bioreactor optimization model, then, it was assumed that the working fluid was only water, and all of water's associated physical properties were used.

In the biorefinery analyzed here, bioreactor equipment makes up a large part of the plant, both physically and financially. This requires special attention to be paid to the estimation of the size of the equipment in order to minimize both capital and operating costs. To minimize costs, an optimization was performed on the bioreactor section of the biorefinery which took into account the capital costs of various sizes of CSTRs and their associated operating costs.

Two variables were controlled in order to find the optimal point in this analysis. First, the diameter of the bioreactors was varied from 1 m to 25 m. Second, the bioreactor stirring speed was varied from 0 to 5 revolutions per second (rps). Since carbon monoxide is the molecule consumed in the bacterial reactions, the parameter optimized was chosen to be dollars per kilograms of CO absorbed ($/kg CO). The optimization was performed by gathering all necessary coefficients and correlations to model stirred tank reactors and entering the information into an Excel spreadsheet, where the optimal reactor size could be seen graphically.

VOLUMETRIC MASS TRANSFER COEFFICIENT & TANK GEOMETRY

The mass transfer of carbon monoxide is described by the volumetric mass transfer coefficient, $k_L a$. This coefficient has units of inverse time and the transfer process can be modeled as a first-order reaction of the form [31]:

Equation 6: First-order mass transfer

$$\frac{dC}{dt} = k_L a\left(C_i - C\right)$$

where C is the concentration of CO dissolved in the water at time t, and C_i is the concentration of CO in the entering syngas.

For this techno-economic analysis two different values of k_La were used for estimating PHA product cost. One method assumed a constant volumetric mass transfer coefficient while the other assumed a varying k_La. For the varying k_La model, the value was calculated based on a correlation developed by Kapic, Jones, and Heindel [32], who analyzed several different correlation methods in CSTRs before presenting their own size independent correlation as:

Equation 7: Volumetric mass transfer coefficient correlation

$$\frac{k_L a}{U_g^{1.155}} = 19.15\left(\frac{N}{N_{CD}}\right)^{1.650}\left(\frac{T}{D}\right)^{-0.415}$$

where k_La is in s^{-1} and U_g is the superficial gas velocity in m/s. This value is equal to the volumetric flow rate of syngas divided by the reactor cross sectional area. The other two ratios will be described later in this section.

In addition to using this correlation to develop the volumetric mass transfer coefficient, the constant value of 0.05 s^{-1} from Kapic *et al*. was used for a comparison analysis, based on the median of their 0.02 to 0.08 s^{-1} range. To check the value of the correlated k_La, it was also compared to the k_La values found by Klasson *et al*. [33] of 101.1 and 28.1 hr^{-1} (0.028 and 0.0078 s^{-1}) for CO mass transfer. Finally, the correlation value was compared to the range for CSTRs given in the Handbook of Industrial Mixing of 0.02 to 0.5 s^{-1} for gas dispersion [34].

Because the bioreactor optimization for this paper was built on their work, it was also necessary to scale up the biorefinery reactors from their laboratory scale reactor. This required the bioreactors to be geometrically similar stirred tank reactors (Figure 9).

The scale up from a laboratory size reactor to an industrial scale requires maintaining similarity between the two sizes of vessels [32]. First, geometric similarity must be maintained, which means the industrial scale vessel must be proportionate to the laboratory reactor. For gas to liquid mass transfer using stirred tanks, the majority of the research has focused on a very specific geometry for the vessel and agitator. This includes the use of a cylindrical vessel with a slightly dished bottom, and a six bladed “Rushton” impeller. The vessel is filled with water to a height (H) equal to the diameter (T) of the vessel. The agitator has a diameter (D) which is 0.33 of the tank diameter. Baffles are used in the vessel to prevent swirling, and four of them are placed evenly around the tank with a thickness of 10% of the vessel diameter T [34]. After making sure

that physical dimensions for the industrial scale are correct, the hydrodynamic similarity must be maintained [35]. This requires the flow regime in the larger tank to match that of the smaller tank, and is typically controlled by adjusting the impeller speed.

BIOREACTOR MODEL EQUATIONS

After fixing the geometry and volumetric mass transfer coefficient for the bioreactors, it was necessary to define some key variables used in the bioreactor model. The first of these was the volumetric flow rate of the syngas entering the bioreactors. From the Aspen Plus simulation, the molar flow rate of the syngas was available. However, it was necessary to translate this from a molar to a volumetric value for use in the bioreactor model. This was based off a rate form of the Ideal Gas Law:

Equation 8: Ideal Gas Law

$$pQ_g = \dot{n}R\theta$$

where (p) is the pressure of the entering syngas, (Q_g) and ($\dot{n}$) are the respective volumetric and molar flow rates, (R) is the universal gas constant, and (θ) is the temperature of the syngas. For the bioreactor model, the system temperature for the reactors as well as the entering syngas was assumed to be 25°C. The pressure of the entering syngas, however, was assumed to vary with the depth of each bioreactor being modeled:

Equation 9: Pressure of syngas entering bioreactor

$$p = \rho g H + p_{atm}$$

where (ρ) is the water density, (g) is acceleration due to gravity, (H) is the water depth in the vessel, and (p_{atm}) is the atmospheric pressure assumed to be 1.01 bars. The next important variable needed for the bioreactor model was the mean residence time (τ_R) of the syngas in the bioreactor [36]:

Equation 10: Syngas mean residence time

$$\tau_R = \frac{V_L}{Q_g}$$

where (V_L) is the volume of liquid in each bioreactor, and (Q_g) is the volumetric flow rate of syngas entering each bioreactor. It should again be noted that the bioreactor was assumed to be a perfectly mixed tank reactor, also known as a CSTR. Along with the volumetric mass transfer coefficient, the residence time was used to calculate the CO conversion (X_{CO}) by each bioreactor using the equation [36]:

Equation 11: Carbon Monoxide conversion

$$X_{CO} = \frac{k_L a \tau_R}{1 + (k_L a \tau_R)}$$

which assumes a perfectly mixed CSTR with the gas to liquid mass transfer as the rate limiting step of the process. Essential to the optimization process is accounting for the capital and operating costs for the bioreactor system. The capital costs were determined by using Aspen IPE version 2004.0.6, which has a cost base from first quarter 2004 in its database. For the final economic analysis these numbers were adjusted for inflation, but for the optimization they were used directly. Thus possessing the direct equipment costs, the annual capital charges (C_{CC}) were calculated using [1]:

Equation 12: Annual capital charges

$$C_{CC} = \frac{C_D i (1+i)^n}{\left[(1+i)^n - 1\right]}$$

where (C_D) is the total direct cost for the bioreactors, (i) is the annual interest rate of the loan, and (n) is the life of the loan. For this analysis, interest rate was assumed to be 10% and life of loan to be 20 years.

In addition to finding the annual capital charges associated with the bioreactors, the annual operating costs also required calculation. Since each reactor vessel is continuously agitated, the electric cost for this stirring was used to determine annual operating costs for the bioreactors. Because the chemical reactions performed by the bacteria are overall exothermic, the reactors also needed to be cooled. However, this was not considered for the optimization because the bioreactor cooling needed varied by a small amount relative to other bioreactor costs. The heat generated by the bacteria was only a function of the amount of carbon monoxide flowing into the bioreactor and being converted by the bacteria, thus cooling load did not vary significantly with reactor size. Bioreactor cooling was included in the overall biorefinery analysis, and as mentioned

earlier the heat from the bioreactor was used to preheat some of the make up water entering the bioreactor (Figure 7).

When calculating stirring costs, the first variable which needed to be specified was the impeller speed. Before impeller speed could be determined, though, three dimensionless variables had to be calculated which related to stirred tanks: Reynolds, Froude, and gas flow numbers. The first of these, the Reynolds number, is defined by:

Equation 13: Reynolds number

$$\mathrm{Re} = \frac{\rho N D^2}{\mu}$$

where (N) is the impeller speed and (μ) is the water dynamic viscosity. The Reynolds number represents the ratio of the inertial stirring forces to the viscous forces. For stirred vessels it has been found that the Reynolds number must be greater than ~10,000 for adequate mixing [34].

The next dimensionless variable, the Froude number, is defined by:

Equation 14: Froude number

$$Fr = \frac{N^2 D}{g}$$

which represents the ratio of inertial stirring forces to gravitational forces. It has been determined by Warmoeskerken [37] that the Froude number must be above 0.045 for large cavities to form. The term “large cavities” refers to the gas-filled cavities behind each impeller blade as the reactor is being stirred, which is the sign of a reactor being adequately loaded with gas. For a given reactor size, a Froude value of 0.045 was considered by Warmoeskerken to be the minimum speed the reactor must be stirred to begin dispersing gas [37].

Finally, the third dimensionless variable used in estimating the impeller speed is the gas flow number:

Equation 15: Gas flow number

$$Fl_g = \frac{Q_g}{N D^3}$$

which incorporates the gassing rate of the stirred vessel as well as the impeller speed and diameter. The value of the gas flow number is very useful in characterizing the various flow regimes possible in gas-dispersing stirred tank reactors [38].

As mentioned earlier, bioreactor stirring speed was one of the two variables controlled for this optimization, and varied from 0 to 5 rps. However, a constraint was imposed on the stirring speed to ensure adequate dispersion of gas within the reactor. A correlation was developed by Nienow to describe the condition of "flooding" in a stirred tank reactor [34]:

Equation 16: CSTR flooding correlation

$$\left(Fl_g\right)_F = 30\left(Fr\right)_F\left(\frac{T}{D}\right)^{-3.5}$$

where the subscript (*F*) denotes gas flow and Froude numbers at the flooded condition. The ratio of tank diameter to impeller diameter (*T/D*) was assumed to be 3 for this optimization. Substituting the dimensionless variables defined above and solving for impeller speed yields:

Equation 17: CSTR flooding correlation solved for impeller speed

$$N_F = \left[\left(\frac{T}{D}\right)^{3.5}\frac{gQ_g}{30D^4}\right]^{1/3}$$

The condition of "flooding" is such that the flow rate of gas fed into the stirred tank reactor is so high as to overwhelm the impeller, preventing it from dispersing the gas properly. For a given reactor size, flooding can be eliminated by either increasing the stirring speed or decreasing the gas flow. For this optimization impeller speeds that fell below the flooded impeller speed (N_F) were ignored.

ESTIMATING GASSED POWER CONSUMPTION

Two kinds of power consumption can be calculated: ungassed power (P_u) and gassed power (P_g). The term "ungassed power" refers to the stirring power needed for the bioreactor when syngas is not flowing through the fermentation broth, while "gassed power" is the stirring power needed when syngas is flowing through the broth. Ungassed

power demand is a single straightforward calculation, but calculating gassed power is more complex.

UNGASSED POWER CONSUMPTION

The standard correlation for gassed power consumption is based on the cube of impeller speed and the fifth power of impeller diameter [34]:

Equation 18: Ungassed power consumption correlation

$$P_u = P_O \rho N^3 D^5$$

where (P_O) is the dimensionless impeller power number. For 6 bladed Rushton impellers this is typically somewhere between 4.75 and 5.5 [39]. Tatterson [40] shows that for a well-stirred reactor the impeller power number reaches a value around five, which is used in this analysis.

GASSED TO UNGASSED POWER RATIO

Many different researchers have developed correlations for the gassed power of stirred tank reactors in terms of ungassed power and various dimensionless parameters [41]. Development of a single equation to match experimental data is difficult, because the "S" shape of the curve when plotted (Figure 10) versus gas flow number [37].

An analysis of the different correlations was performed by Warmoeskerken, who concluded that the best approximation of the curve required three separate equations, depending on the gas flow number [37]. The correlations developed by Warmoeskerken are:

Equation 19: Power ratio correlations separated by flow regime

Regime I: $$\frac{P_g}{P_u} = A = 1 - 16.7(Fl)(Fr)^{0.35} \qquad (0 < Fl < Fl_{3\text{-}3})$$

Regime II: $$\frac{P_g}{P_u} = B - \frac{0.1(A-B)}{Fl_{3-3} - 0.1} + \frac{(A-B)Fl}{Fl_{3-3} - 0.1} \qquad (Fl_{3\text{-}3} < Fl < 0.1)$$

Regime III: $$\frac{P_g}{P_u} = B = 0.27 + 0.022(Fr)^{-1} \qquad (Fl > 0.1)$$

where (P_g/P_u) is the ratio of gassed to ungassed power. It can be seen that the middle flow regime (II) is made up of a linear interpolation between the ends of flow regime I and III, and includes the large cavity gas flow number ($Fl_{3\text{-}3}$) defined by:

Equation 20: Large cavity gas flow number correlation

$$(Fl)_{3-3} = 0.0038\left[\frac{(\mathrm{Re})_{3-3}^{2}}{(Fr)_{3-3}}\right]^{0.067}\left(\frac{T}{D}\right)^{0.5}$$

which gives the gas flow number at which large cavities begin to form behind the impeller [37].

Although Warmoeskerken's use of three different equations to define the gassed to ungassed power ratio implies greater accuracy, the correlation has its shortcomings. A discontinuity occurs in Regime II of the correlation, and the ratio (P_g/P_u) becomes negative (Figure 11).

Another power ratio was developed by Reuss in 1980 [34]. This correlation uses the Froude, Reynolds, and gas flow number along with the impeller to tank diameter ratio which gives:

Equation 21: Power ratio correlation

$$\frac{P_g}{P_u} = 0.0312(Fr)^{-0.16}(\mathrm{Re})^{0.064}(Fl_g)^{-0.38}\left(\frac{T}{D}\right)^{0.8}$$

Unlike the Warmoekerken power ratio, the Reuss power ratio offers a good approximation in the middle range of gas flow numbers encountered. However this correlation also has its shortcomings. At extremely low gas flow numbers the Reuss correlation goes toward infinity and at high gas flow numbers goes to zero (Figure 11).

This analysis combined the best aspects of both Warmoeskerken and Reuss in order to overcome the shortcomings of both these correlations. Logic was incorporated into the optimization spreadsheet such that the Warmoeskerken correlation was used at gas flow numbers above 0.3, and the Reuss correlation at gas flow numbers below 0.3. In addition, as the gas flow number reached zero the Reuss correlation was stopped so that (P_g/P_u) never became greater than 1.0 (Figure 11).

PROJECT COST ESTIMATION

INDIVIDUAL COMPONENTS

After results for the mass and energy flows in the biorefinery were achieved, an analysis of the biorefinery economics was performed. Individual components for the biorefinery were estimated first for their free-on-board (f.o.b.) equipment costs (C_P), and then for the costs of labor to install the components (C_L) and the costs of the associated material used for the installation (C_M). The term "free-on-board" refers to the cost the vendor charges to place a particular piece of equipment on a shipping truck or railcar at the fabrication plant [42]. This f.o.b. cost, then, does not include any additional expenses for shipping, setting, or installation. Those additional costs are covered by (C_L) and (C_M).

The majority of these costs came from Aspen IPE. Several items, however, were estimated from other sources. The equipment cost for the hydrogen PSA unit, as well as costs of labor and materials came directly from a previous economic analysis performed by Lysenko [19]. The grinder equipment cost was given by Pesco Incorporated, a dry material handling vendor, and the labor and installation material costs were given by IPE. The reasoning behind this was that all the grinder costs available in IPE were for equipment used mostly to process coal and other dense feedstocks. Cost estimations within the software for grinders were performed on a mass flow rate basis. Since a biomass grinder requires a large volumetric feed rate but low mass flow, this would give unsuitably low equipment costs if estimated in IPE. Pesco Incorporated, a vendor familiar with processing biomass was able to give an accurate equipment cost, and the IPE software was used to give labor and material for installation costs.

In a similar manner, the catalyst estimated for the gas reformer was assumed to cost $4.67/lb in 1994 dollars [25] and have a specific gravity of 2.711 [23], the same as limestone. All costs were adjusted to be in 2005 US dollars, as shall be described later.

CO-PRODUCT VALUE

For accounting purposes, the hydrogen produced by the biorefinery was considered to be a co-product with a market value of $1.90/kg. This value was calculated from target hydrogen market prices from the U.S. Department of Energy [43], which gives a goal hydrogen market price of $2 to $3 per gallon of gasoline equivalent (GGE). A hydrogen market value of $1.90/kg is equivalent to $1.90/GGE [44, 45]. The main

product was assumed to be PHA, and the techno-economic analysis estimated the cost of this using all other inputs.

MATERIAL INPUTS

For material input flows, the most expensive input into the biorefinery was the switchgrass raw material used as the feedstock. This was assumed to cost $55/Mg delivered to the plant gate. Water was assumed to cost $0.0012/kg. This value was reached by calculating the cost of water assumed in Choi and Lee [29] and adjusting for inflation so that the value would be in 2005 US dollars. The sodium hypochlorite solution was also from the Choi and Lee paper and found to be $0.12/kg. The surfactant solution was similarly determined to be $1.85/kg in 2005 US dollars. Nutrient costs for the bacteria culture were considered to negligible and ignored, as they were in economic analyses performed by Choi and Lee [29] and van Wegen et al. [46].

ELECTRICITY & WASTEWATER TREATMENT

For energy inputs into the biorefinery, electricity was assumed to be $0.0425/kWh, based on 2005 data from the Energy Information Administration for the state of Iowa [47]. The cost of wastewater treatment was assumed to be $0.0006/kg. This value came from a table in Peters, Timmerhaus, and West [48]. Both values were adjusted for inflation.

LABOR INPUTS

Operator labor input was assumed to be $25/man·hour, based on Lysenko's work [19]. The number of operators needed to run the biorefinery was based on equipment requirements presented in Brown [1], Peters & Timmerhaus [48], and Ulrich [42]. For the baseline biorefinery, the number of operators was calculated to be 7.4 per shift.

INFLATION ADJUSTMENT

As mentioned earlier, cost estimations came from various sources with different base years. These numbers had to be brought into the same year before they could be used. The adjustment was made using a formula from Brown [1]:

Equation 22: Inflation adjustment

$$C_{CY} = C_{PY}\left(\frac{I_{CY}}{I_{PY}}\right)$$

where C_{CY} and C_{PY} are the costs from the current and previous years, respectively. Inside the brackets I_{CY} and I_{PY} correspond to the inflation index for current and previous years. Values for the inflation indexes were the Chemical Engineering Plant Cost Index (CEPCI) from Chemical Engineering magazine [49].

DIRECT PROJECT EXPENSES

For the overall biorefinery, the methodology used was adapted from Brown [1] which will be summarized here. After gathering all equipment, material, and labor costs and adjusting for inflation, the total equipment (C_P), material (C_M) and labor (C_L) costs were calculated by summing each individual component's costs. The total direct cost (C_D) was then calculated as:

Equation 23: Direct project expenses

$$C_D = C_P + C_M + C_L$$

where all variables now refer to the total rather than individual costs. These total costs were used to calculate all other capital needs for the construction of a new biorefinery.

INDIRECT PROJECT EXPENSES

These types of expenses refer to the less tangible costs of building a new biorefinery such as the taxes, insurance, and engineering expenses. Estimation of indirect costs for this analysis was done by assuming them to be a percentage of the direct project expenses. The first of these types of expenses was for freight, insurance, and taxes (C_{FIT}):

Equation 24: Freight, insurance, and taxes

$$C_{FIT} = 0.08C_P$$

where it can be seen that (C_{FIT}) was assumed to be 8% of total equipment costs. The next expense, construction overhead (C_O), covers various payroll costs for hired labor as well as equipment and tool rental:

Equation 25: Construction overhead

$$C_O = 0.70C_L$$

and was assumed to be 70% of the cost of the labor for installing all equipment. The third and final indirect expense estimated for the biorefinery capital costs was engineering expenses (C_E):

Equation 26: Engineering expenses

$$C_E = 0.15(C_P + C_M)$$

which was assumed to be 15% of the sum of equipment and material costs, and used to cover the costs of hiring design and project engineers for the project of constructing a biorefinery. These three indirect expense estimates were summed up to produce:

Equation 27: Total indirect expenses

$$C_{ID} = C_{FIT} + C_O + C_E$$

which is called the total indirect expense (C_{ID}). This completed the estimation of the indirect project expenses for the capital estimation of the biorefinery.

OTHER PROJECT EXPENSES

Several other costs were calculated in the process of estimating capital costs for this biorefinery. The first is called the bare module cost (C_{BM}), and sums the direct and indirect expenses:

Equation 28: Bare module cost

$$C_{BM} = C_D + C_{ID}$$

which reflects the minimum cost of designing and building the biorefinery. This bare module cost was then used to calculate the contingency and fee cost:

Equation 29: Contingency and fee cost

$$C_{CF} = 0.18C_{BM}$$

This value was used to account for unplanned issues and delays in the construction of the project. Here it was assumed that (C_{CF}) be 18% of the bare module cost. For a design and build firm which would undertake the biorefinery project, the contingency and fees cost represents the firm's profit. A project which comes in on time and within budget means the firm gets to keep all the (C_{CF}) to itself. The next cost calculated was the total module cost (C_{TM}) which sums the bare module and contingency and fees costs:

Equation 30: Total module cost

$$C_{TM} = C_{BM} + C_{CF}$$

Another, optional cost to add when calculating the project capital costs is the auxiliary facilities cost (C_{AF}). This cost represents any additional buildings such as administrative offices or warehouse which might have to be built to support the biorefinery. For this analysis, the construction of auxiliary facilities were included and assumed to be 30% of the total module cost:

Equation 31: Auxiliary facilities cost

$$C_{AF} = 0.30C_{TM}$$

Finally, the grassroots capital (C_{GR}) for the project was calculated. This cost represents the total capital which would have to be raised to complete this biorefinery project and is a sum of the total module cost and the auxiliary facilities cost:

Equation 32: Grassroots capital cost

$$C_{GR} = C_{TM} + C_{AF}$$

The grassroots capital cost is also called the fixed capital cost (C_{FC}). After calculating all the necessary capital costs to complete the biorefinery project, the operating costs for the facility had to be determined. The next section will describe this process.

OPERATING COST ESTIMATION

The costs of operating the biorefinery include such expenses as labor, raw materials, and taxes, and are typically calculated on an annual basis of dollars per year. Some of the operating costs are based on the estimated capital costs, while others come from the material and energy flows into the biorefinery. The first cost calculated was the working capital:

Equation 33: Working capital cost

$$C_{WC} = 0.13C_{FC}$$

and it is seen here assumed to be 13% of the fixed capital cost. Anywhere from 10% to 20% is used, and this cost represents money tied up in the inventory of raw materials and finished product. This amount is added to the fixed capital to create a total capital cost (C_{TC}) represented by:

Equation 34: Total capital cost

$$C_{TC} = C_{FC} + C_{WC}$$

which is used to calculate annual capital charges (C_{CC}) as described earlier in the bioreactor optimization section. The equation presented earlier for calculating capital charges is:

Equation 35: Annual capital charges

$$C_{CC} = \frac{C_D i(1+i)^n}{\left[(1+i)^n - 1\right]}$$

with an interest rate (i) of 10% and a loan life (n) of 20 years.

An important factor used in the estimation of plant operating costs is the plant capacity factor, (f_0). This defines the percentage of each year that the plant operates, and allows a calculation of the annual hours of production. For this analysis, a plant capacity factor of 90% was used, which gave 7,889.4 hours of annual operation assuming 365.25 days each year.

DIRECT OPERATING COSTS

Direct costs are mainly raw material, energy, and labor costs, but include other expenses such as laboratory charges as well. Raw material costs (C_R) are all calculated in the same way. The hourly mass flow rate of the material ($\dot{m}$) is multiplied by its cost on a mass basis (C_B) and by the annual hours of operation (A_H):

Equation 36: Raw material costs

$$C_R = C_B \times \dot{m} \times A_H$$

For this analysis, all raw material costs including switchgrass, water, surfactant, and hypochlorite solution were calculated in this way. The credits from the production of co-products such as the hydrogen produced (C_{CP}) were also calculated with this formula, but they of course were treated as a credit instead of a cost. In addition, the cost of the labor needed to operate the biorefinery (C_{OL}) was calculated using this formula, except the value of 6.8 operators replaced the mass flow rate ($\dot{m}$) in the formula, and hourly wage of $25 replaced the material cost (C_B). Finally, the utilities (electricity and wastewater treatment) were calculated in a similar way. The unit cost of the utility was multiplied by its usage rate and then multiplied by the annual hours of operation.

Based on the methodology in Brown [1], supervisory labor (C_{SL}) was calculated to be a percentage of operating labor, and 15% was used for this analysis. Typical values range from 10% to 20%. Similarly, the cost for maintenance and repairs (C_{MR}) was assumed to be 6% of total fixed capital (C_{FC}), the median value of a typical 2% to 10% range. This cost accounts for work needed to keep the biorefinery operational. Closely associated with the maintenance and repair cost is the operating supplies cost (C_{OS}), calculated to be from 10% to 20% of (C_{MR}). This analysis assumed (C_{OS}) to be 15% of (C_{MR}). Another direct cost is laboratory expenses (C_{LE}), which covers costs for quality control of raw materials and products. Based on a range of 10% to 20% of operating labor (C_{OL}), this analysis assumed a 15% median value. The final direct cost calculated was for patents and royalties (C_{PR}), needed to cover the use of licensed technologies. This cost was assumed to be 3% of all other direct operating costs combined, from raw materials to laboratory expenses:

Equation 37: Patents and royalties cost

$$C_{PR} = 0.30 \times (C_R + C_{OL} + C_{SL} + C_{MR} + C_{OS} + C_{LE})$$

where (C_R) represents raw material and utility costs only. Finally, all directs were added together to create the total direct operating expenses (C_{DE}):

Equation 38: Direct operating expenses

$$C_{DE} = C_R + C_{OL} + C_{SL} + C_{MR} + C_{OS} + C_{LE} + C_{PR}$$

INDIRECT OPERATING COSTS

After calculating all the direct operating costs, it was necessary to find the indirect operating costs. Indirect costs include expenses such as insurance, taxes, and administrative costs. The first expense in this category calculated was overhead (C_{OH}), which accounts for the additional expenses of hiring employees such Social Security taxes and retirement funds. This was assumed to be a percentage of the operating labor (C_{OL}), supervisory labor (C_{SL}), and maintenance and repair (C_{MR}):

Equation 39: Overhead cost

$$C_{OH} = 0.60 \times (C_{OL} + C_{SL} + C_{MR})$$

with a typical range of 50% to 70%, and for which this analysis assumed to be a 60% median value. Next, the cost of paying local taxes was calculated (C_{LT}) and assumed to be 1.5% of fixed capital (C_{FC}), with 1% to 2% being the typical range. In the same way, insurance for the biorefinery (C_{IN}) was calculated at 0.7% of (C_{FC}), which has a range of 0.4% to 1%. The final two indirect costs fall under the category of "General Expenses." Administrative Expenses (C_{AE}) is the first which was taken as 15% of operating labor (C_{OL}). The second General Expense is the distribution and marketing cost (C_{DM}), taken as 5% to 10% of total direct operating expenses (C_{DE}). This analysis assumed 7.5% as the value. Finally, all indirect expenses were summed up to find the total indirect operating expense (C_{IE}):

Equation 40: Total indirect operating expenses

$$C_{IE} = C_{LT} + C_{IN} + C_{AE} + C_{DM}$$

ANNUAL OPERATING COST AND PRODUCT COST

The annual cost of operating the biorefinery (C_{OC}) is a sum of all the annual costs, including capital charges, co-product credits, and both direct and indirect operating expenses:

Equation 41: Annual biorefinery operating cost

$$C_{OC} = C_{CC} + C_{CP} + C_{DE} + C_{IE}$$

The cost of producing the biorefinery main product (C_{PHA}), which in this case is PHA, is a matter of dividing the annual operating cost by the annual output of PHA (A_{PHA}):

Equation 42: PHA product cost

$$C_{PHA} = \frac{C_{OC}}{A_{PHA}}$$

A similar formula was used in the bioreactor optimization to determine the carbon monoxide conversion cost (C_{CO}). The annual operating cost of operating the bioreactor was divided by the annual mass of carbon monoxide converted to give:

Equation 43: Carbon Monoxide conversion cost

$$C_{CO} = \frac{(C_{OC})_{bioreactor}}{A_{CO}}$$

where (C_{OC}) is the annual bioreactor operating cost and A_{CO} is the annual amount of carbon monoxide converted.

SENSITIVITY ANALYSIS

To check the response of PHA cost to change in various process variables, several sensitivity analyses were performed.
Holding

all other process variables constant, the value of the variable in question was changed by a percentage and the change in the unit cost of PHA was checked. Results were then

placed into a table and graphed. Specifically, the switchgrass cost, hydrogen market value, operating labor cost, and electricity cost were varied to check PHA cost sensitivity.

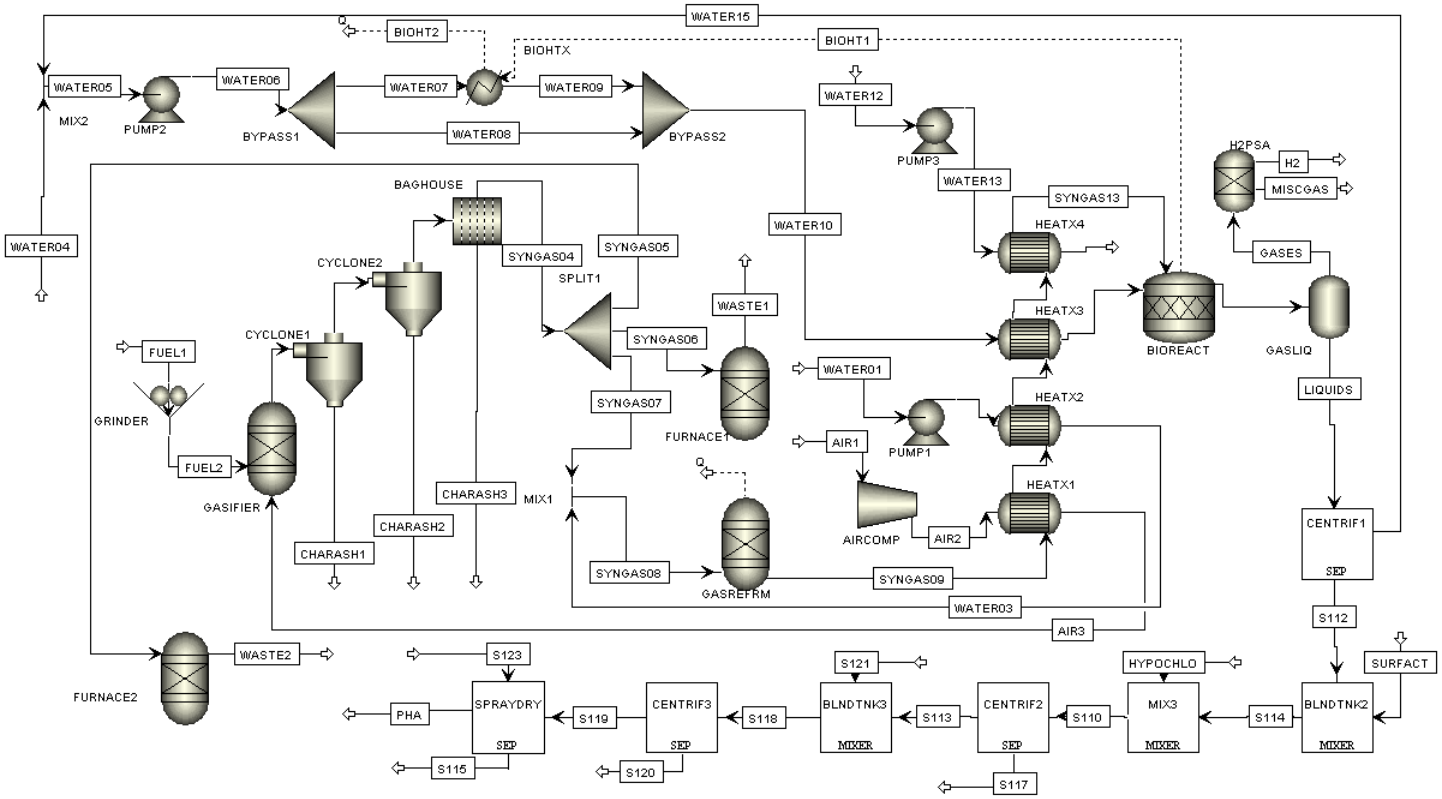

Figure 1. Flow sheet of the biorefinery created in Aspen Plus. Further detail of specific areas can be seen in figures to follow.

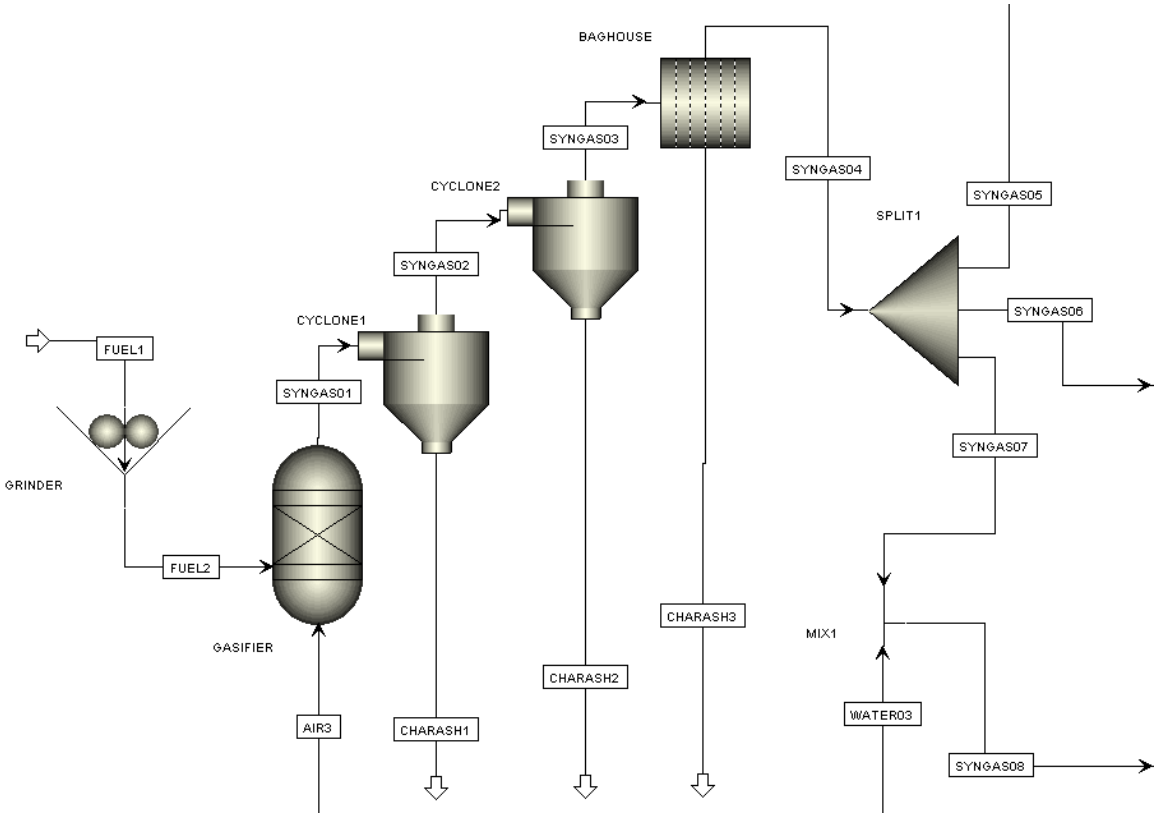

Figure 2. Section of biorefinery flowsheet showing the grinder, gasifier, particulate removal system, and stream splitter.

Table 1. Gasifier component mass fractions used in simulation. Based on Lysenko, 2006.

Component	Mass Fraction
H2	0.0046
O2	0.0002
N2	0.4761
CO	0.1290
CO2	0.2561
CH4	0.0206
C2H4	0.0180
C2H2	0.0000
C2H6	0.0024
C3H8	0.0000
H2O	0.0630
Char	0.0202
Tar	0.0098
Total Output:	**1.0000**

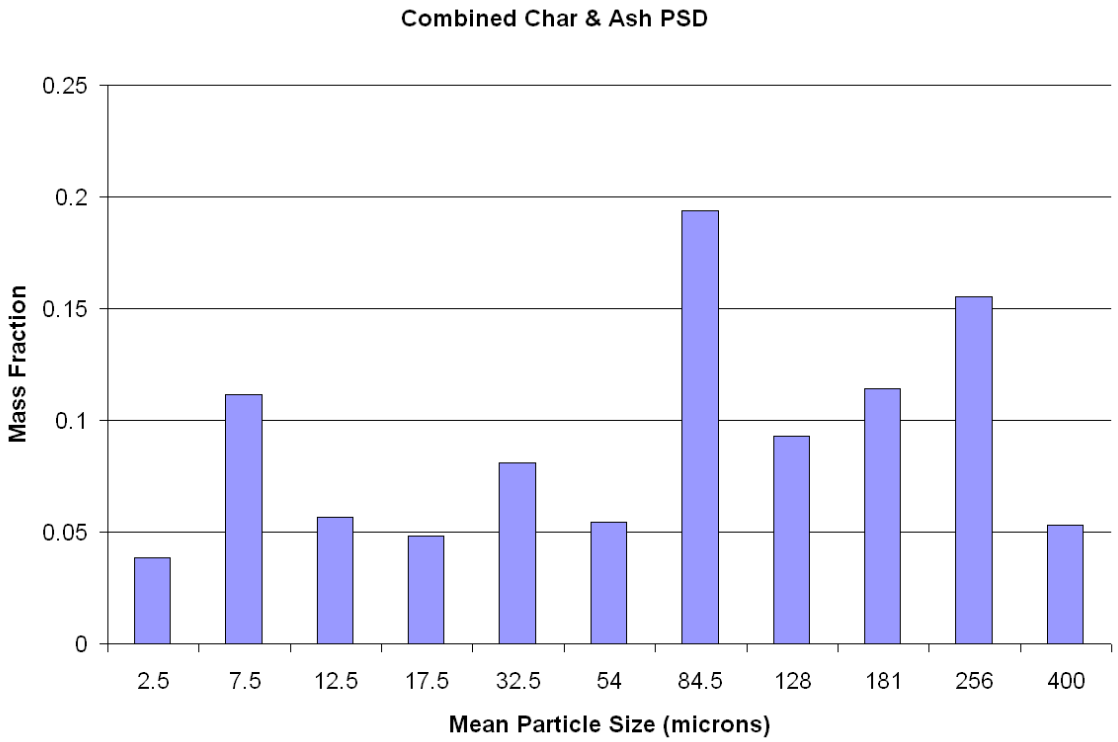

Figure 3. Particle size distribution used for char and ash. Based on Ritzert (2004).

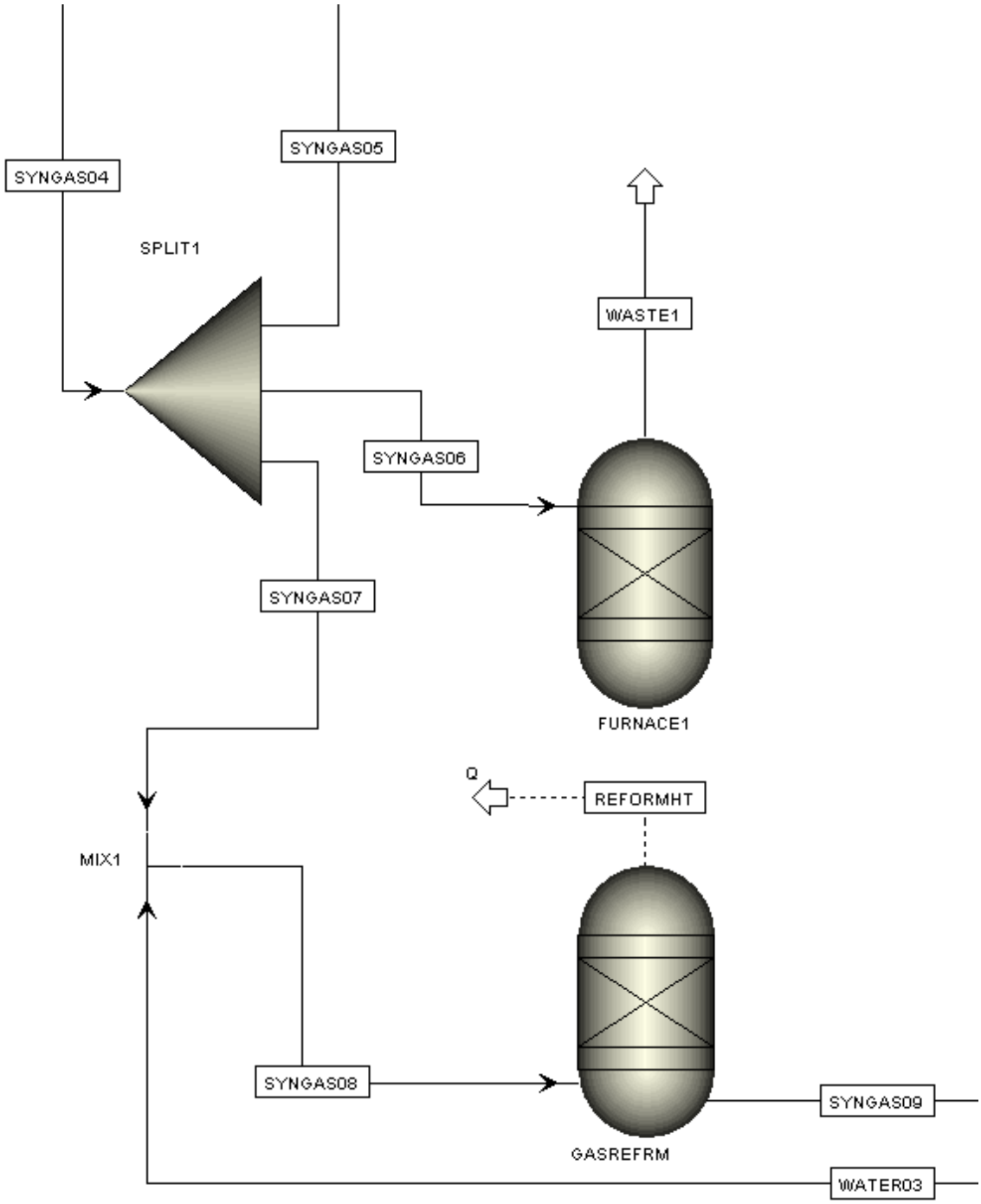

Figure 4. Section of biorefinery flowsheet showing the syngas stream splitter, gas reformer, and furnace.

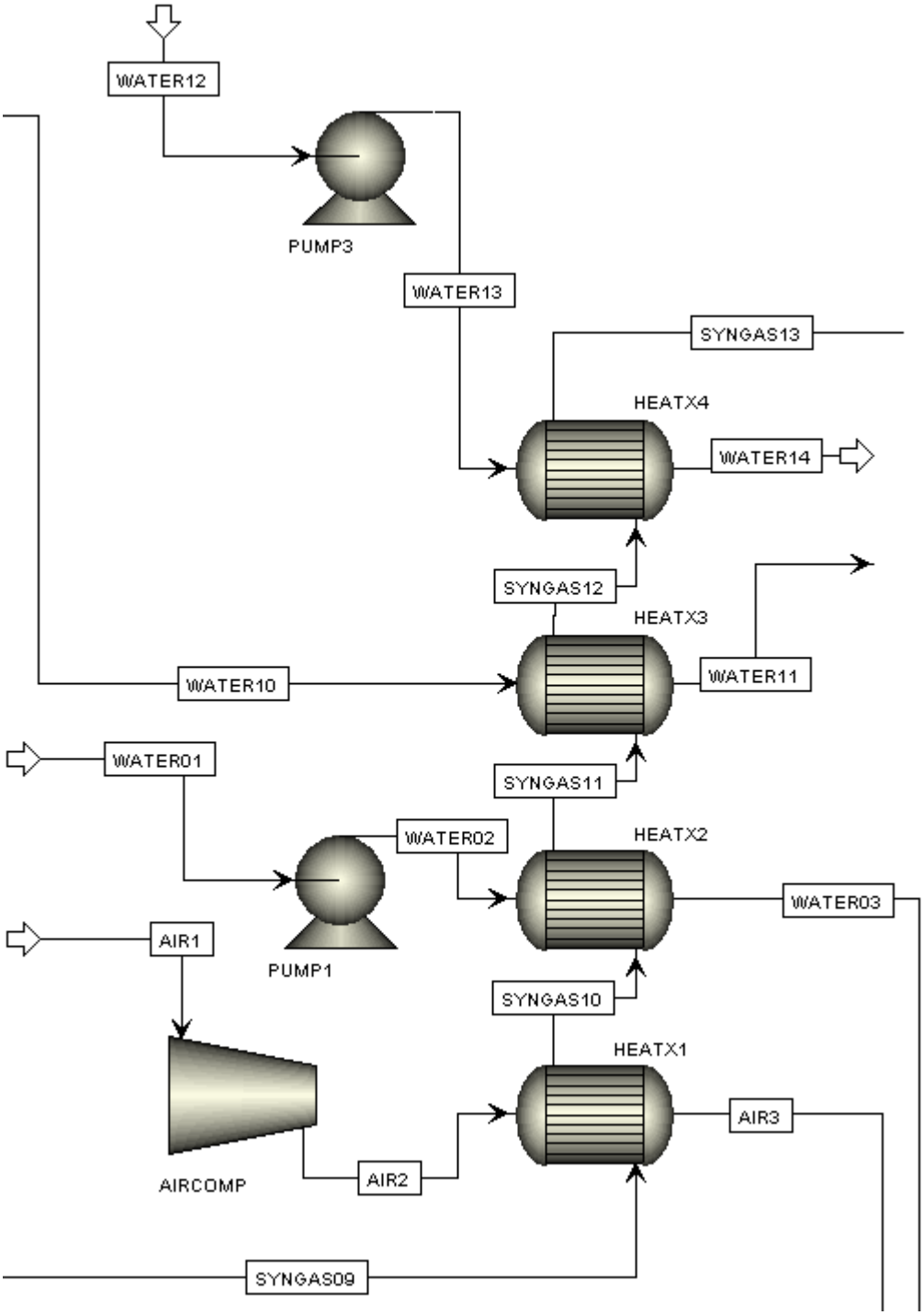

Figure 5. Section of biorefinery flowsheet showing the heat exchanger network.

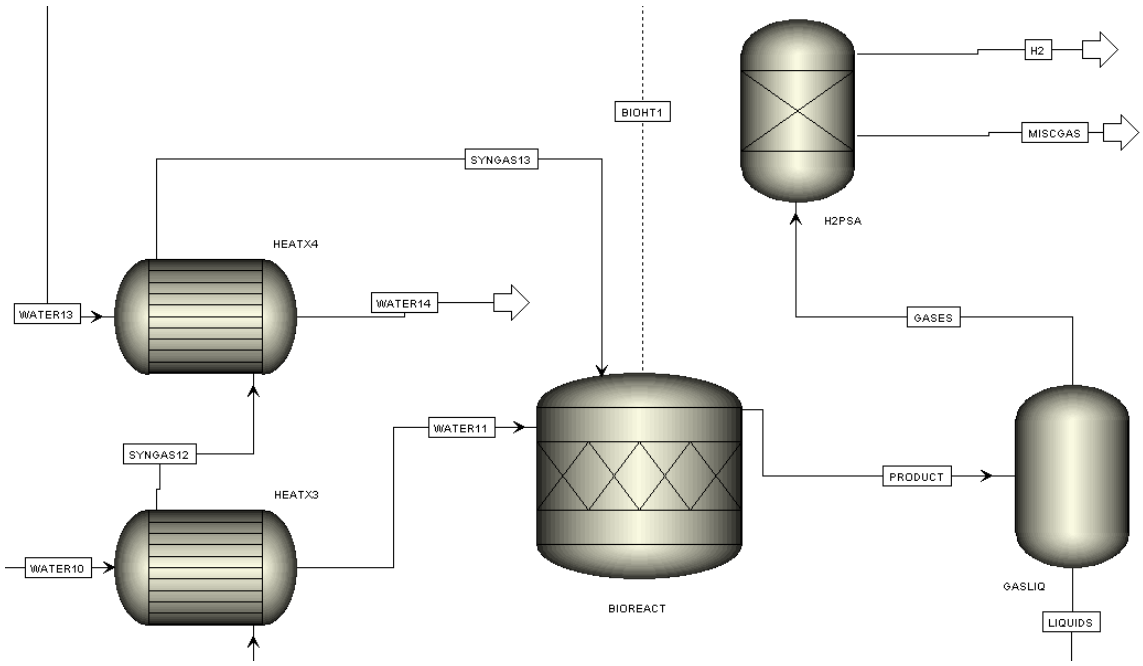

Figure 6. Section of the biorefinery flowsheet showing the bioreactor, gas separation unit, and two heat exchangers.

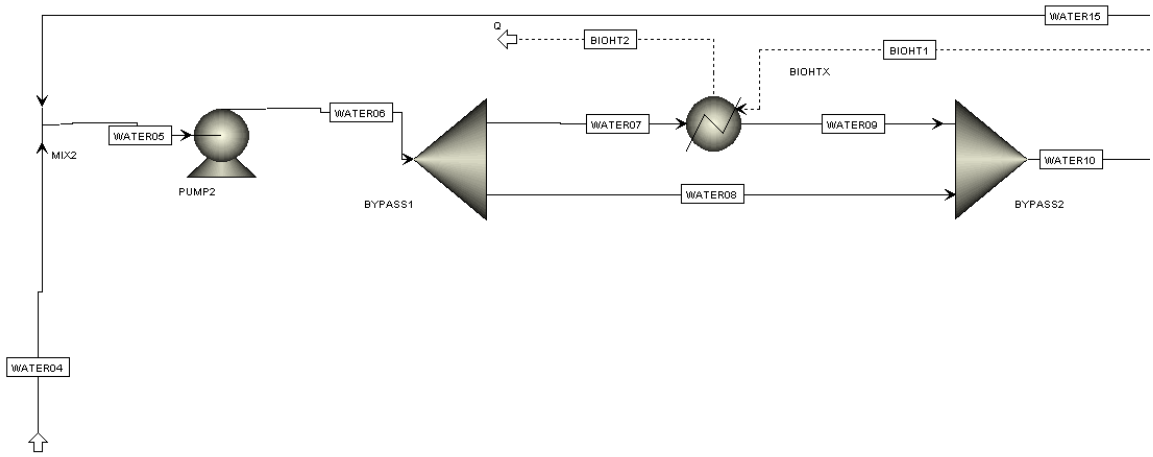

Figure 7. Section of the biorefinery showing how excess bioreactor heat is used to preheat make up water flowing into the bioreactor.

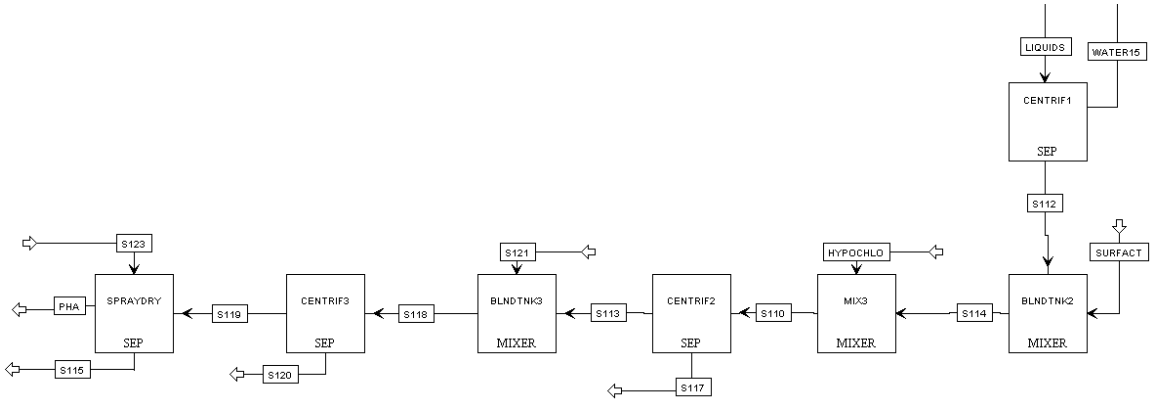

Figure 8. Section of the biorefinery showing the PHA separation line. Adapted from Choi & Lee (1997).

Table 2. Components used in the Aspen Plus biorefinery simulation.

Component ID	Type	Component name	Formula
H2	CONV	HYDROGEN	H2
O2	CONV	OXYGEN	O2
N2	CONV	NITROGEN	N2
CO	CONV	CARBON-MONOXIDE	CO
CO2	CONV	CARBON-DIOXIDE	CO2
CH4	CONV	METHANE	CH4
C2H4	CONV	ETHYLENE	C2H4
C2H2	CONV	ACETYLENE	C2H2
C2H6	CONV	ETHANE	C2H6
C3H8	CONV	PROPANE	C3H8
H2O	CONV	WATER	H2O
CHARASH	NC		
TAR	CONV	N-EICOSANE	C20H42
SWGRASS	NC		
P3HB	CONV		C4H6O2
DEXTROSE	CONV	DEXTROSE	C6H12O6
C	CONV	CARBON-GRAPHITE	C
SODIU-01	CONV	SODIUM-HYPOCHLORITE	NACLO

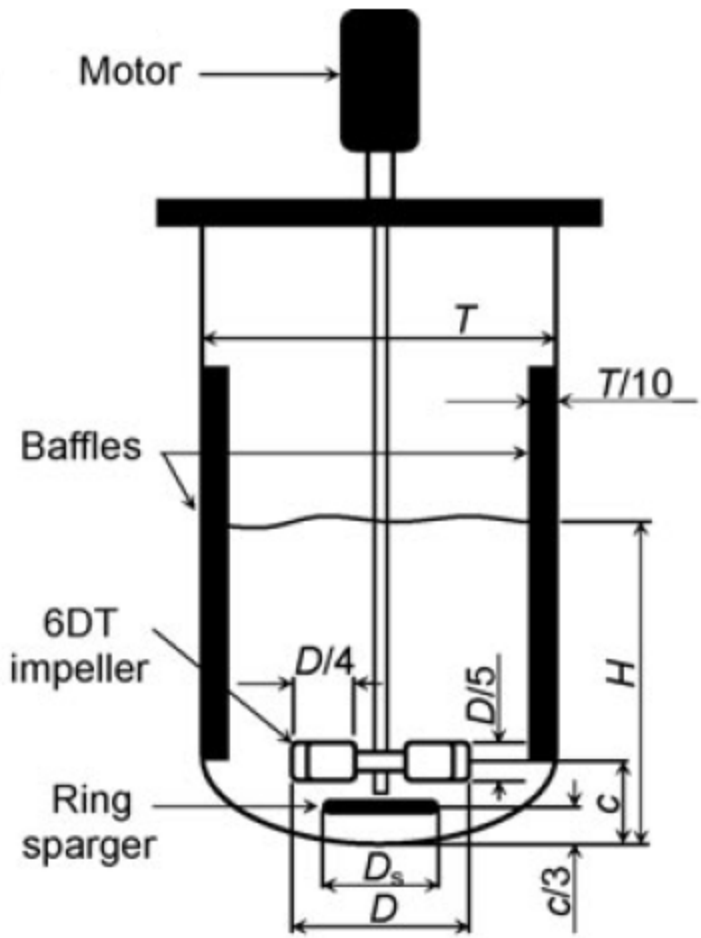

Figure 9. General stirred tank reactor geometry. Adapted from Kapic and Heindel (2006).

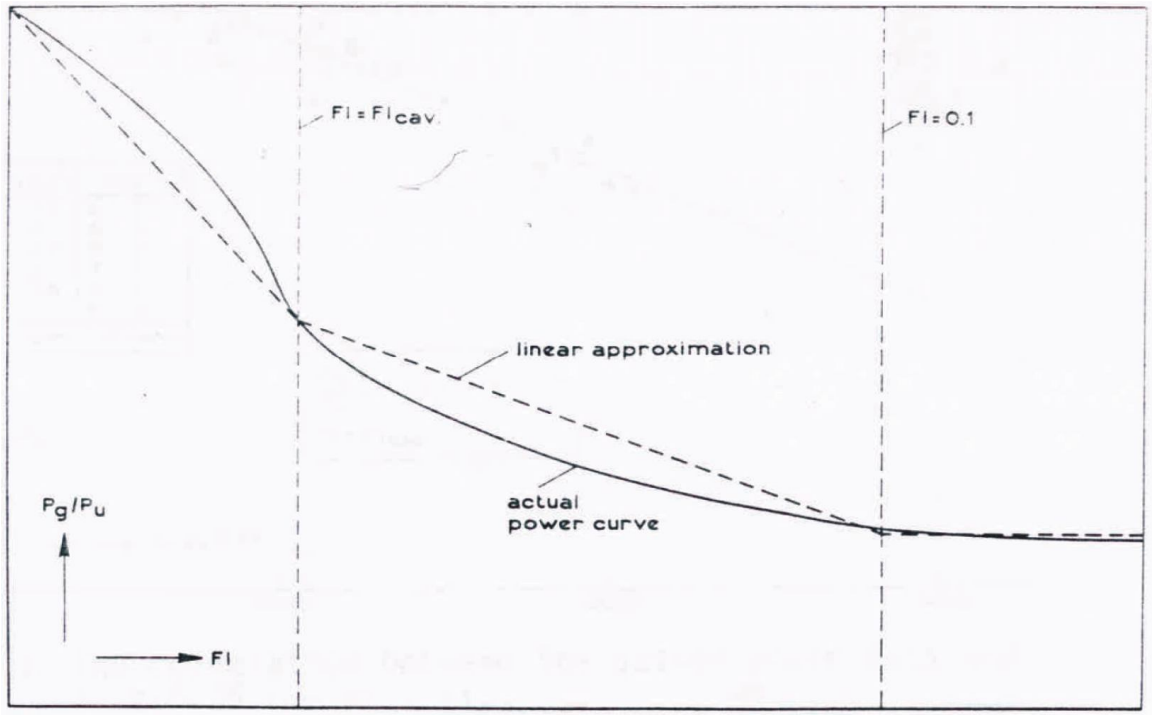

Figure 10. Gassed to ungassed impeller power ratio versus gas flow number. Adapted from Warmoekerken (1986). Note that on the graph, Flcav = (Fl)3-3 in the text.

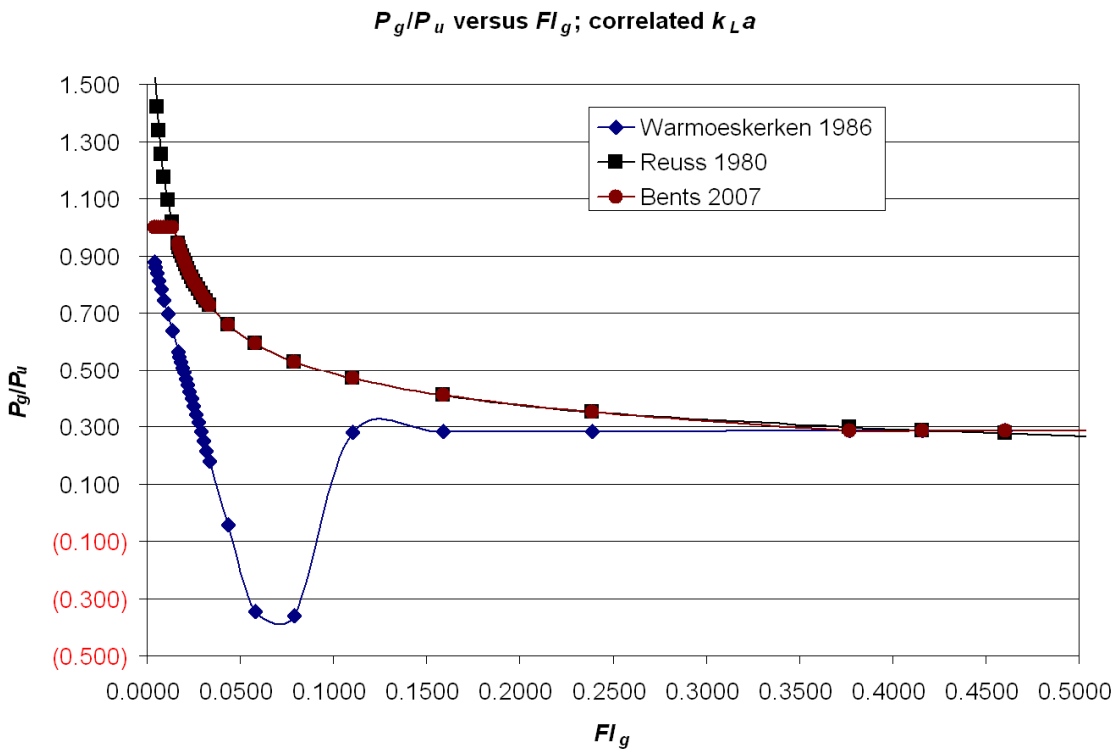

Figure 11. Correlations of gassed to ungassed impeller power versus gas flow number from Warmoeskerken (1986), Reuss (1980), and Bents (2007).

RESULTS & DISCUSSION

BIOREACTOR SIZE OPTIMIZATION

The bioreactor optimization was influenced mainly by three factors: carbon monoxide conversion, annual capital charges, and annual electrical costs. For all combinations of reactor diameter and speed, the total mass flow rate of syngas was always the same. Other factors, such as hours of annual operation, loan interest rate and life of loan were also kept constant. It can be seen from separate graphs of the three main factors listed above what the various effects were on the optimal operating point. A table summarizing the main results for both constant and correlated k_La cases is also available (Table 3).

CARBON MONOXIDE CONVERSION – CONSTANT & CORRELATED k_La

Conversion of carbon monoxide varied greatly between the bioreactor model using a constant k_La and the model using the correlated k_La. A volumetric mass transfer coefficient calculated using Kapic *et al.* caused CO conversion to asymptote to 1.0 at a steeper rate (Figure 12) as diameter increased than when using a constant k_La (Figure 13). This caused the optimal bioreactor diameter chosen to be smaller for the correlated k_La model than for the constant k_La model.

ANNUAL CAPITAL CHARGES & ELECTRICAL COSTS

A graph of bioreactor annual capital charges versus diameter (Figure 14) shows that capital charges increase with diameter. Since equipment costs are controlled by bioreactor diameter only, this graph does not change between using a constant volumetric mass transfer coefficient and using the correlated k_La.

Similarly, the annual electrical costs as a function of diameter did not change between the constant k_La and correlated k_La models for a given stirring speed (Figure 15).

CARBON MONOXIDE CONVERSION COST – CORRELATED k_La

Using the correlation from Kapic *et al.*, a volumetric mass transfer coefficient of 1.4 s^{-1} was calculated for the correlated k_La case. This value is outside the normal range

of 0.02 to 0.5 s^{-1} given in Paul *et al.*, which makes it difficult to accept as a realistic volumetric mass transfer coefficient. The CO conversion for this baseline reactor is 96%. A three-dimensional graph relating CO conversion cost ($/kg CO) to the bioreactor diameter for various stirring speeds is useful for finding the optimal CSTR diameter and stirring speed where cost is a minimum (Figure 16). Note that the dollar values shown on the graph are for the bioreactor capital and operating costs only. As opposed to the constant k_La model, the correlated k_La model shows a much smaller bioreactor of 6.6 m diameter being stirred at 2.5 rps to be optimum (Figure 17). Reactor volume at this optimal point is 230 m^3 and 1,100 kW of motor power needed for the stirring speed. The rapid climb in CO conversion to 1.0 explains the smaller optimal diameter needed for the correlated k_La model (Figure 12). Based on the unrealistic k_La value calculated from the correlation, the results from the constant k_La analysis were chosen to be presented in the text, while the correlated k_La results are given in the Appendices (Appendix B1-1 through B1-5).

CARBON MONOXIDE CONVERSION COST – CONSTANT k_La

As mentioned earlier, the optimization performed on the bioreactors tended toward a smaller diameter bioreactor for the correlated k_La than the constant k_La model. Thus, for a constant k_La of 0.05 s^{-1} the optimum reactor size was a 14.8 m diameter being stirred at 0.6 rps (Figure 16). At this optimum size, carbon monoxide conversion is 94%, and a 14.8 m diameter reactor gives a 2,500 m^3 tank volume. It was determined that a reactor of this size required a motor of approximately 2,100 kW to power the agitator, which gives a carbon monoxide conversion cost of $0.21 per kilogram of absorbed CO.

MATERIAL AND ENERGY FLOWS – CONSTANT k_La

As mentioned earlier, this techno-economic analysis was performed for a biorefinery producing 50 Mg/day of hydrogen. This value was used to estimate all other material flows, as well as determine the sizes of the processing equipment. Based on the process flow sheet made in Aspen Plus, a biorefinery of this capacity requires 708 Mg/day of switchgrass feedstock to supply the raw material. The main product produced by the biorefinery, 95% pure PHA polymer, is made at a rate of 12 Mg/day. Other material and energy flows were also tabulated (Table 5).

Electricity consumed by the biorefinery was estimated to be 5,900 kW and determined mostly by using values given from the Aspen IPE software. Of this power, 2,500 kW are consumed by the blower providing air to the gasifier. The electricity consumed by the bioreactors came from the Excel spreadsheet model. For the grinder, the motor size of the grinder specified by Pesco Incorporated was used to determine its power consumption.

Heat required by the gas reformer was calculated by Aspen Plus, based on the equilibrium chemical reactions assumed to take place in the vessel. The total heat duty was determined to be 11 MW, meaning that the gas reformer requires a heat input to sustain its reactions. This heat duty requires 225 Mg/day of syngas.

As mentioned earlier, the spray dryer heat need was determined by using 50% more than the latent heat of vaporization for the water removed. Based on a water removal rate of 32 Mg/day and a latent heat of vaporization of 2,260 kJ/kg for water, this requires 1.3 MW of heat, or 25 Mg/day of syngas.

BIOREFINERY COSTS – CONSTANT k_La

A table summarizing the biorefinery base case results for both mass flows and costs is also available (Table 4).

CAPITAL

After exporting the simulation flow sheet from Aspen Plus into Aspen IPE all components were given necessary dimensions and material specifications to allow the software to calculate individual component equipment costs, as well as the costs for installation labor and materials (Table 6). For the direct costs, total (f.o.b.) equipment costs were calculated to be $23 million, while total materials for installation and total direct labor were $4.3 million and $1.6 million respectively. Bare module cost was calculated to be $36 million and total module $43 million. Grassroots capital was estimated to be $55 million. A breakdown of all equipment costs can be seen in the Appendix (Appendix A1-1).

OPERATING

Of the operating costs (Table 7) the biggest expense comes from the switchgrass feedstock at $12.8 million per year. This is a significant portion of total direct operating

costs, which are calculated to be $25 million/year. Of the indirect operating expenses, the overhead is most significant at $3.1 million/year. Total indirect operating expenses are $6.4 million/year. Combined direct and indirect operating costs total $31 million/year. From this value is subtracted the credit given by the sale of the biorefinery co-product of hydrogen gas. At a market value of $1.90/kg, sale of the hydrogen supplies an annual credit of $31 million. Annual capital charges were calculated from an assumed loan life of 20 years with an interest rate of 10%, giving a value of $7.4 million/year. Combining capital charges, operating costs, and co-product credits, one can find the annual operating cost for the biorefinery to be $8.3 million/year.

PHA PRODUCT COST

Daily PHA production is 12 Mg/day. This biorefinery was assumed to operate at a 90% plant capacity factor, meaning that out of 365 days each year it only operates approximately 329 of them. This means that annual PHA production is 4,000 Mg/year. Dividing annual operating cost by annual PHA production gives a PHA product cost of $2.05/kg.

COSTS – CORRELATED k_La

The baseline analysis for this paper was chosen to be a constant volumetric mass transfer coefficient of 0.05 s^{-1}. For comparison, however, an analysis was also performed based on a k_La that varied based on the superficial gas velocity, per the correlation from Kapic *et al*. As mentioned earlier, both the constant and correlated k_La bioreactor models showed approximately 95% CO conversion at their optimal operating point. This allowed the same Aspen Plus model to be used for calculating mass and energy balances in both cases. The only difference between the two was the size of the bioreactor and its optimal stirring speed, which for a correlated k_La was a 6.6 m diameter CSTR and a 2.5 rps impeller speed. This reduced capital and operating costs and thus significantly affected PHA product cost, which decreased from $2.05/kg to $0.51/kg. All other costs can be seen in the Appendices (Appendix B1-1 through B1-5). As mentioned earlier, this does not appear to be a realistic analysis because of the overly optimistic volumetric mass transfer coefficient of 1.4 s^{-1}.

COSTS – OTHER MODELS

In addition to the baseline (constant k_La) model and correlated k_La model, other analyses were created for natural gas rather than syngas as a heat source. While their results will not be detailed here, a full breakdown of all material flows, capital, operating, and products costs can be seen in the Appendices (Appendix A2-1 through A2-5 and B2-1 through B2-5).

SENSITIVITY ANALYSIS – CONSTANT k_La

SWITCHGRASS COST

For the baseline analysis, the switchgrass was assumed to cost $55/Mg ton delivered to the plant gate. As expected, the cost of producing PHA responded significantly to changes in the price of its feedstock. When the switchgrass cost was reduced to $25/Mg, the PHA cost was reduced to $0.12/kg. When the switchgrass cost increased by 100% to $110/Mg, the PHA cost increased by 171% from its baseline cost of $2.05 to $5.57/kg (Figure 18).

HYDROGEN MARKET VALUE

Similar to feedstock costs, the cost of PHA also responded significantly to changes in the market value of hydrogen. A baseline value of $1.90/kg of hydrogen produced was assumed, and when this value was reduced to $0.38/kg the PHA cost increased to $8.14/kg. This is an increase of 296%. When hydrogen production was increased in value to $2.38/kg, the PHA cost decreased to $0.15/kg, a decrease of 93% (Figure 19).

OPERATING LABOR COST

Compared to switchgrass cost and hydrogen market value, the cost of operating labor had a relatively small effect on the cost of PHA production. The baseline value of $25/man·hour was decreased to $20/man·hour, and PHA cost decreased by 8.4% to $1.88/kg. When operating labor was increased to $30/man·hour, PHA cost increased to $2.23/kg, a linear increase of 8.4% (Figure 20).

ELECTRICITY COST

Of the four variables examined in the sensitivity analyses, a change in the cost of electricity had the smallest overall effect on PHA cost. When the baseline cost of $0.0425/kWh was increased by 100% to $0.085/kWh, the PHA cost increased by 27% to $2.60/kg. When electricity costs increased by 200% to $0.1275/kWh, PHA product cost increased to $3.15/kg, a change of 53% (Figure 21). No decreases in electricity cost were examined.

Table 3. A summary of the main results for the bioreactor optimzation study. Both constant and correlated kLa values are shown.

	Constant $k_L a$	Correlated $k_L a$
Volumetric Mass Transfer Coefficient ($k_L a$, s^{-1})	0.05	1.36
Optimal Reactor Diameter (m)	14.8	6.6
Optimal Stirring Speed (rps)	0.6	2.5
Agitator Stirring Power (kW)	2,060	1,145
Total CO Conversion (%)	0.9391	0.9617
Annual Capital Cost ($/yr)	$1,477,536	$182,896
Annual Stirring Cost ($/yr)	$690,779	$384,026
CO Conversion Cost ($/kg CO converted)	$0.2097	$0.1853

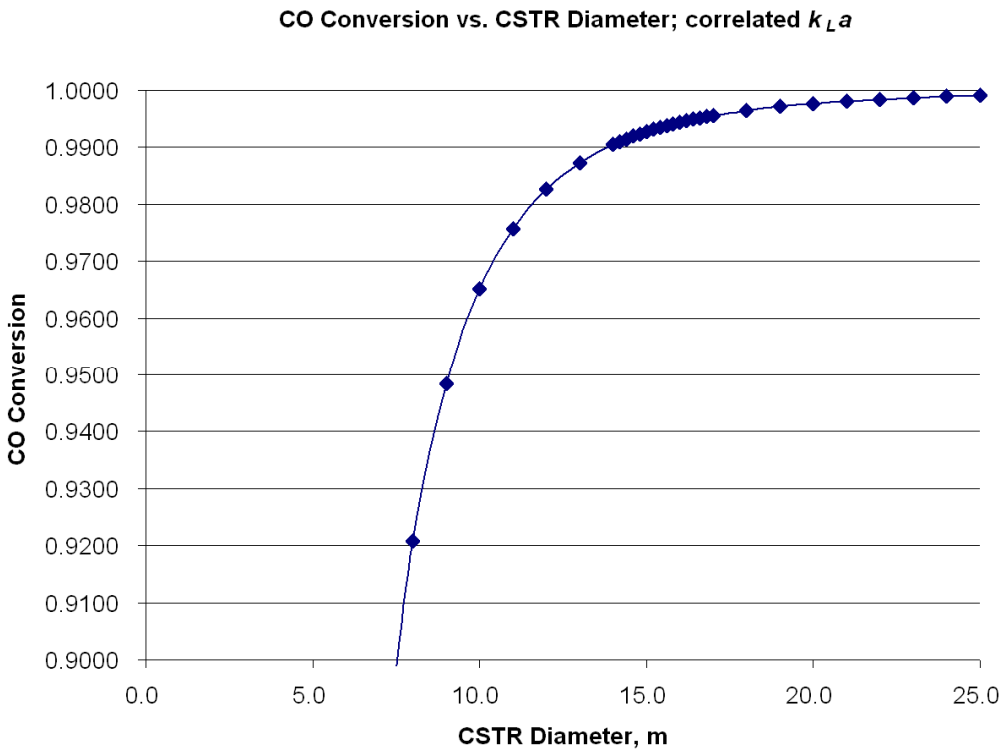

Figure 12. Carbon monoxide conversion versus CSTR diameter varying from 1 to 25 meters in diameter assuming a correlated kLa. Calculated at 1.0 rps impeller speed.

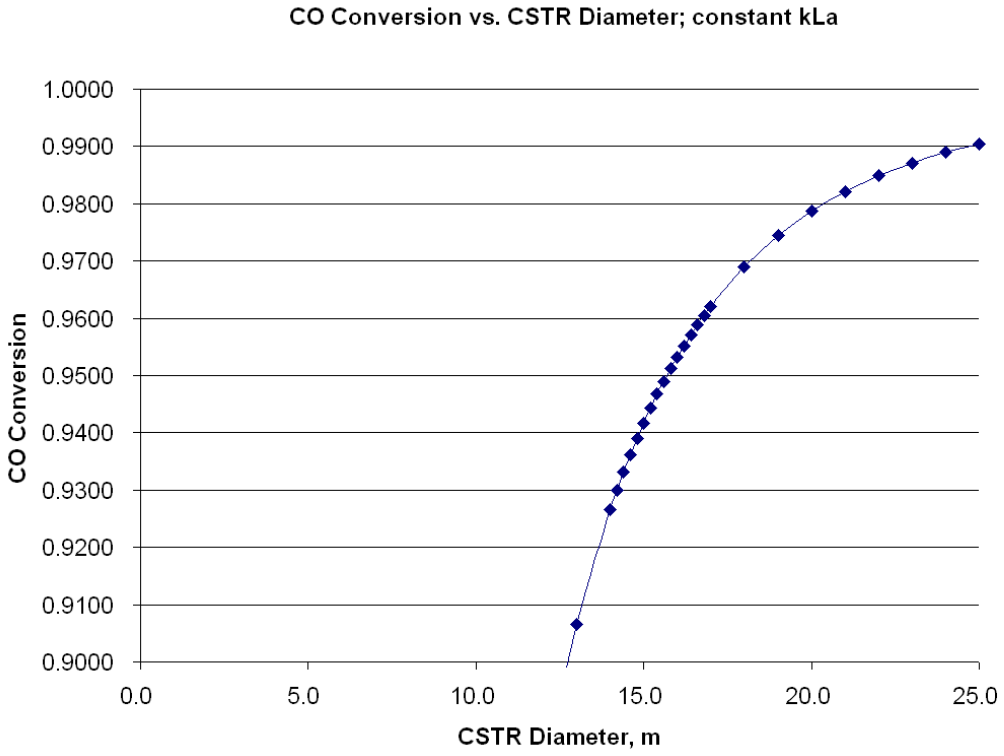

Figure 13. Carbon monoxide conversion versus CSTR diameter varying from 1 to 25 meters in diameter assuming a constant kLa. Calculated at 1.0 rps impeller speed.

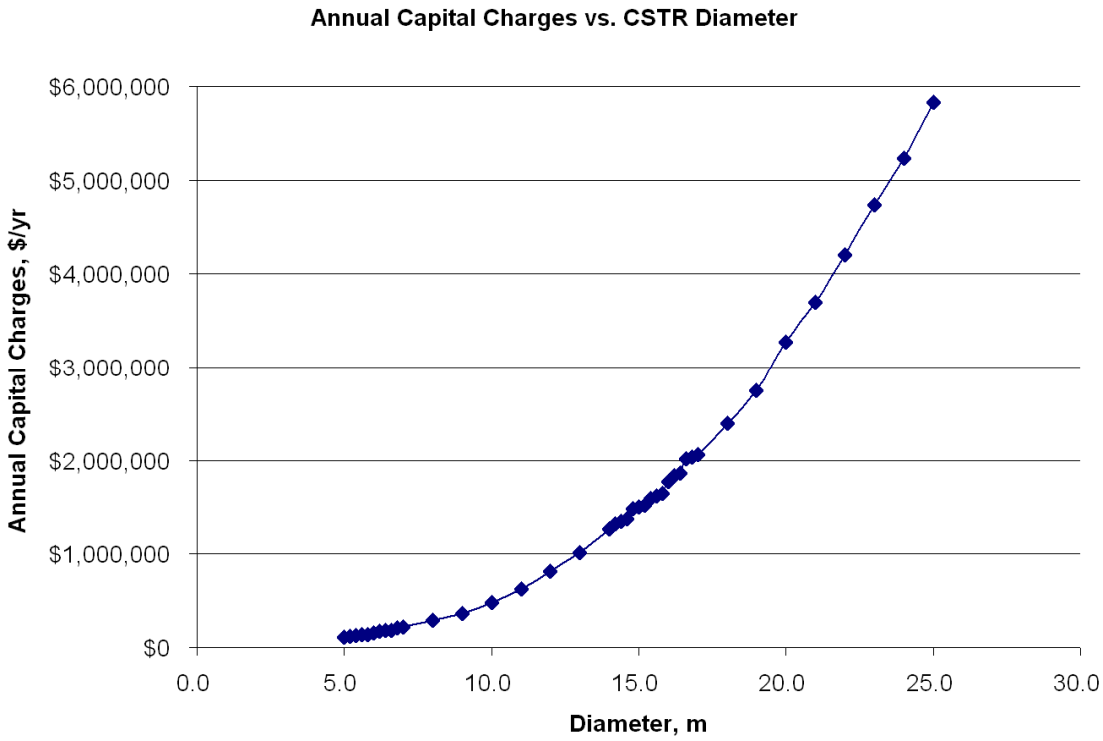

Figure 14. Annual capital charges versus CSTR diameter varying from 1 to 25 meters

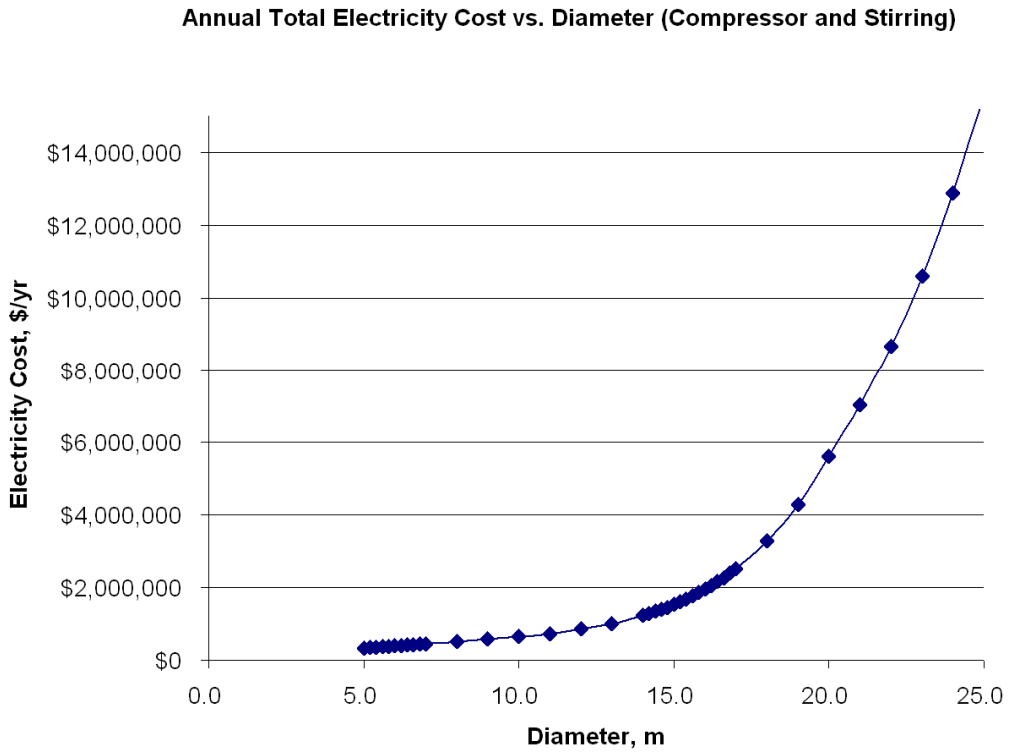

Figure 15. Annual bioreactor stirring costs versus CSTR diameter varying from 1 to 25 meters. A stirring speed of 0.6 rps is shown.

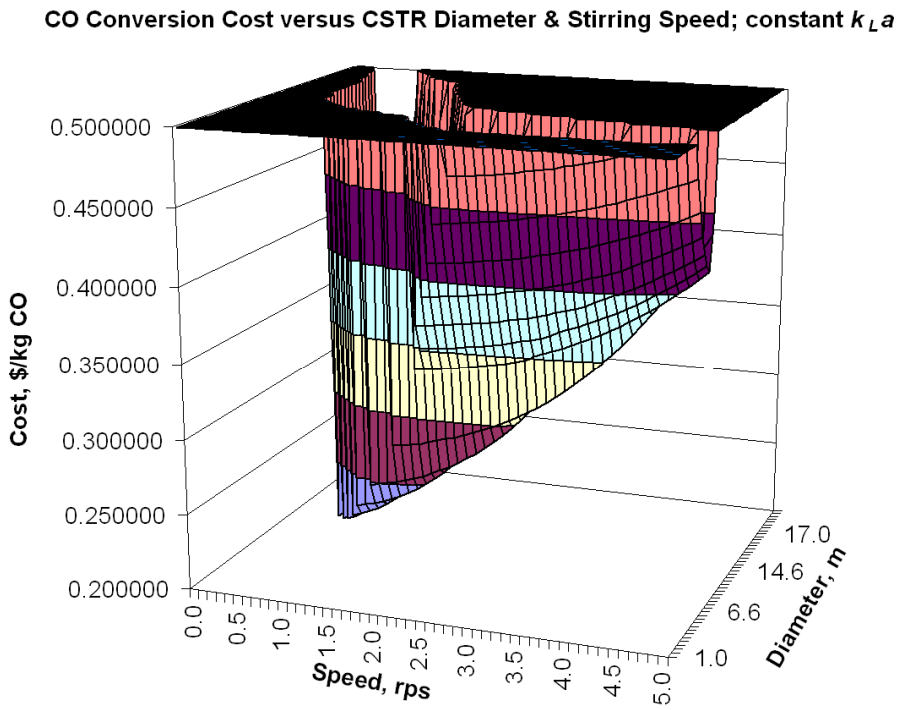

Figure 16. Carbon monoxide conversion cost versus CSTR diameter from 1 to 25 meters and impeller speed from 0.0 to 5.0 rps. Calculated using a constant kLa.

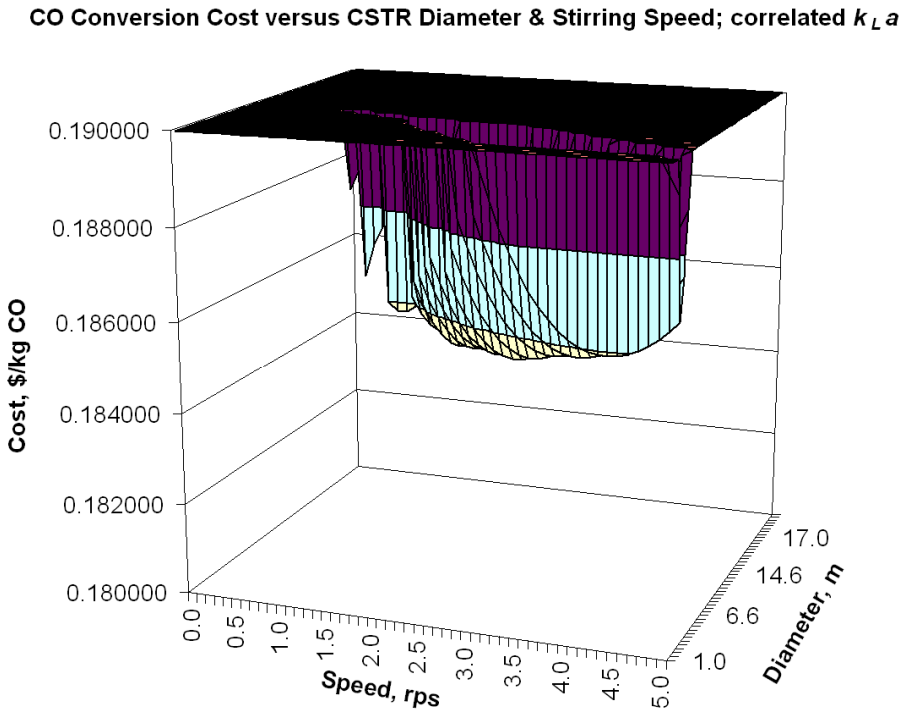

Figure 17. Carbon monoxide conversion cost versus CSTR diameter from 1 to 25 meters and impeller speed from 0.0 to 5.0 rps. Calculated using a correlated kLa.

Table 4. A summary of the main results for the bioreactor economic study. Base case (constant kLa) values are shown.

Biorefinery Base Case Results Summary	
Hydrogen Produced (Mg/yr)	16,153
PHA Produced (Mg/yr)	4,034
Switchgrass Consumed (Mg/yr)	232,737
Water Consumed (Mg/yr)	1,022,636
Grassroots Capital ($)	$55,457,679
By-products credit (H_2 sale, $/yr)	($30,690,215)
Annual Capital Charges ($/yr)	$7,360,863
Annual Operating Cost ($/yr)	$8,289,484
PHA Product Cost ($/kg)	$2.05

Table 5. Biorefinery material and energy flows using a constant kLa and 95% CO conversion

PHA/H2 Plant Material & Energy Flows	
from: PHA_Plant_Combined_rev030.apw	
Inputs	
Switchgrass, kg/day	708,000
Surfactant, kg/day	1,608
Hypochlorite solution, kg/day	31,074
Water:	
Gas Reformer	179,353
Bioreactor make-up	678,174
Final syngas cooling	2,000,000
PHA Washing	253,388
Total Water, kg/day	3,110,915
Gas Reformer Energy, kW	11,366
Electricity, kW	5,934
Outputs Daily	
Syngas, post-filter, kg/day	1,691,268
Syngas LHV, pre-reformer, kJ/kg	4,368
95% pure (10% moisture) PHA, kg/day	12,273
Hydrogen, kg/day	49,138
Spray dryer water vapor, kg/day	31,909
Wastewater:	
Waste cooling water	2,000,000
Centrifuge 2	666,478
Centrifuge 3	257,475
Total Wastewater, kg/day	2,923,953
Char & Ash:	
Cyclone stage 1	32,686
Cyclone stage 2	1,576
Candle filter	610
Total Char & Ash, kg/day	34,872
Bioreactor Heat, kW	53
Outputs Annual	
95% Pure PHA, Mg/yr	4,034
Hydrogen, Mg H_2/yr	16,153

Table 6. Biorefinery capital costs for a constant kLa and 95% CO conversion

Capital Cost			
Direct Costs			
Equipment (f.o.b.)	C_P from Icarus		$23,224,640
Materials for installation	C_M from Icarus		$4,283,585
Direct labor	C_L from Icarus		$1,564,649
Total Direct Costs	$C_D = C_P + C_M + C_L$		$29,072,874
Indirect Costs			
Freight, Insurance, taxes	$C_{FIT} = 0.08 \times C_P$		$1,857,971
Construction overhead	$C_O = 0.7 \times C_L$		$1,095,254
Engineering expenses	$C_E = 0.15 \times (C_P + C_M)$		$4,126,234
Total Indirect Costs	$C_{ID} = C_{FIT} + C_O + C_E$		$7,079,459
Bare module cost	$C_{BM} = C_D + C_{ID}$		$36,152,333
Contingency & fee	$C_{CF} = 0.18 \times C_{BM}$		$6,507,420
Total Module Cost	$C_{TM} = C_{BM} + C_{CF}$		$42,659,753
Auxiliary facilities	$C_{AF} = 0.30 \times C_{TM}$		$12,797,926
Grassroots capital	$\mathbf{C_{GR} = C_{TM} + C_{AF}}$		**$55,457,679**

Table 7. Biorefinery operating costs for constant kLa and 95% CO conversion

Operating Cost	
	2005 dollars
Direct Expenses ($/yr)	
Raw materials	
Switchgrass	$12,800,552
Water	$1,190,083
Surfactant	$922,452
Hypochlorite Solution	$1,188,750
Operating labor	$1,534,488
Supervisory labor	$230,173
Utilities	
Electricity (major components)	$1,989,646
Wastewater treatment	$574,184
Maintenance & repairs	$3,327,461
Operating supplies	$499,119
Laboratory charges	$230,173
Patents and royalties	$734,612
Direct Subtotal	**$25,221,693**
Indirect & General Expenses ($/yr)	
Overhead	$3,055,273
Local taxes	$831,865
Insurance	$388,204
General expenses	$2,121,800
Indirect subtotal	**$6,397,143**

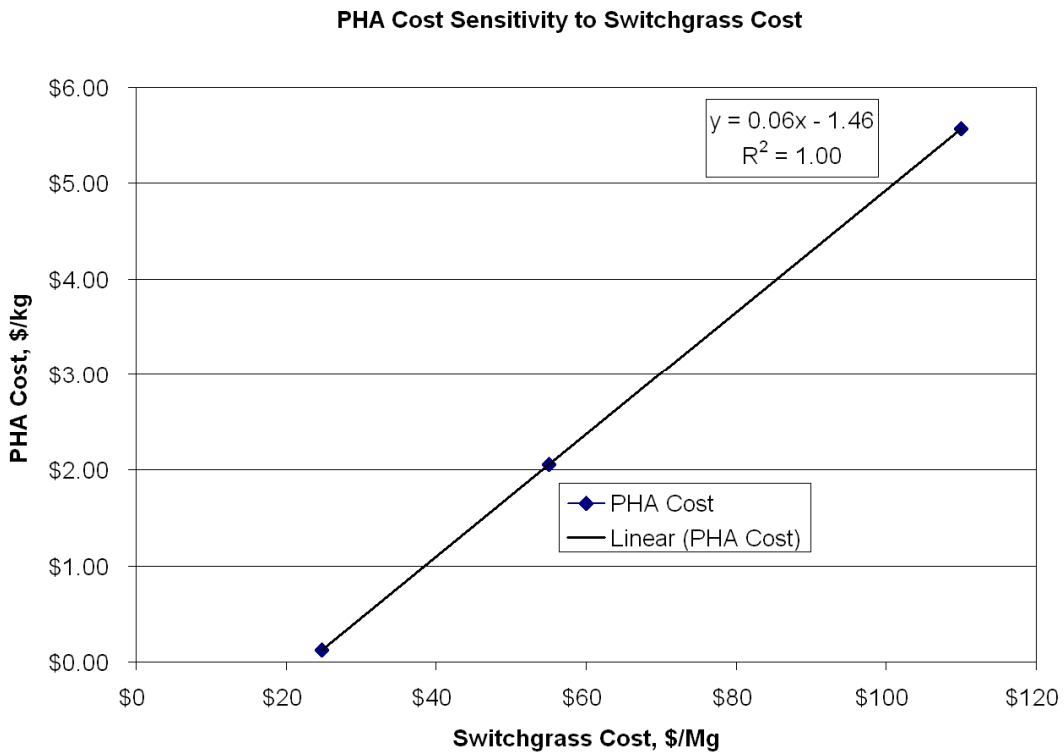

Figure 18. PHA cost sensitivity to switchgrass cost for a bioreactor with constant kLa and 95% CO conversion.

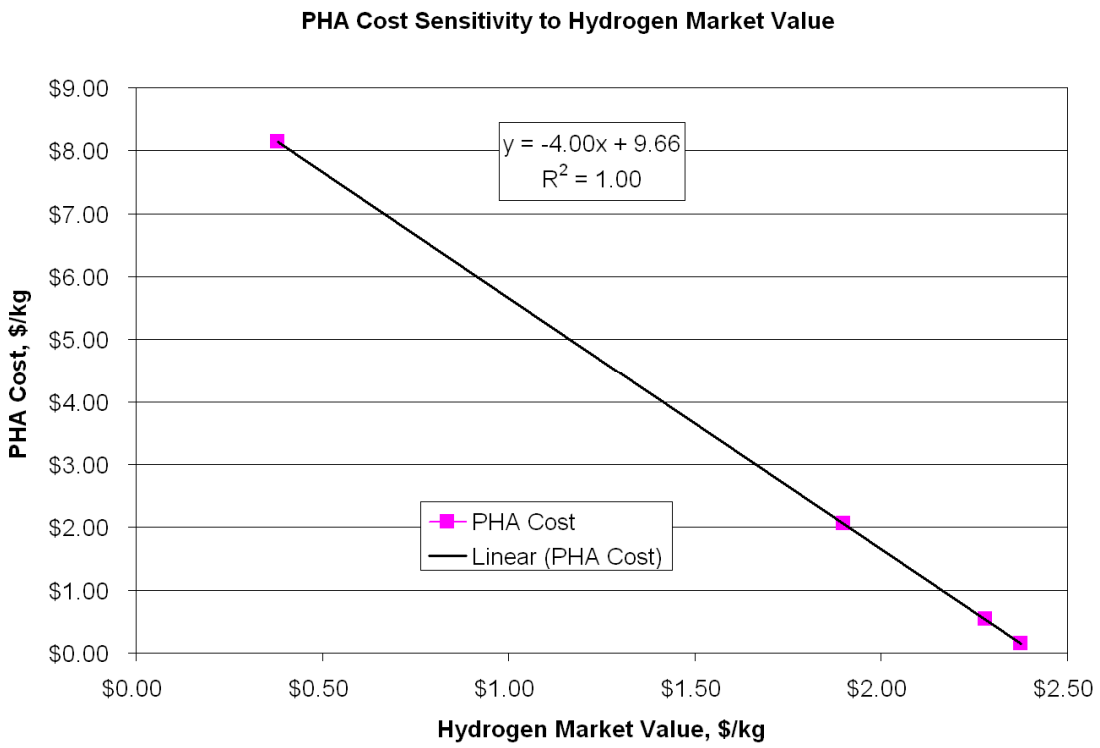

Figure 19. PHA cost sensitivity to hydrogen market value for a bioreactor with constant kLa and 95% CO conversion.

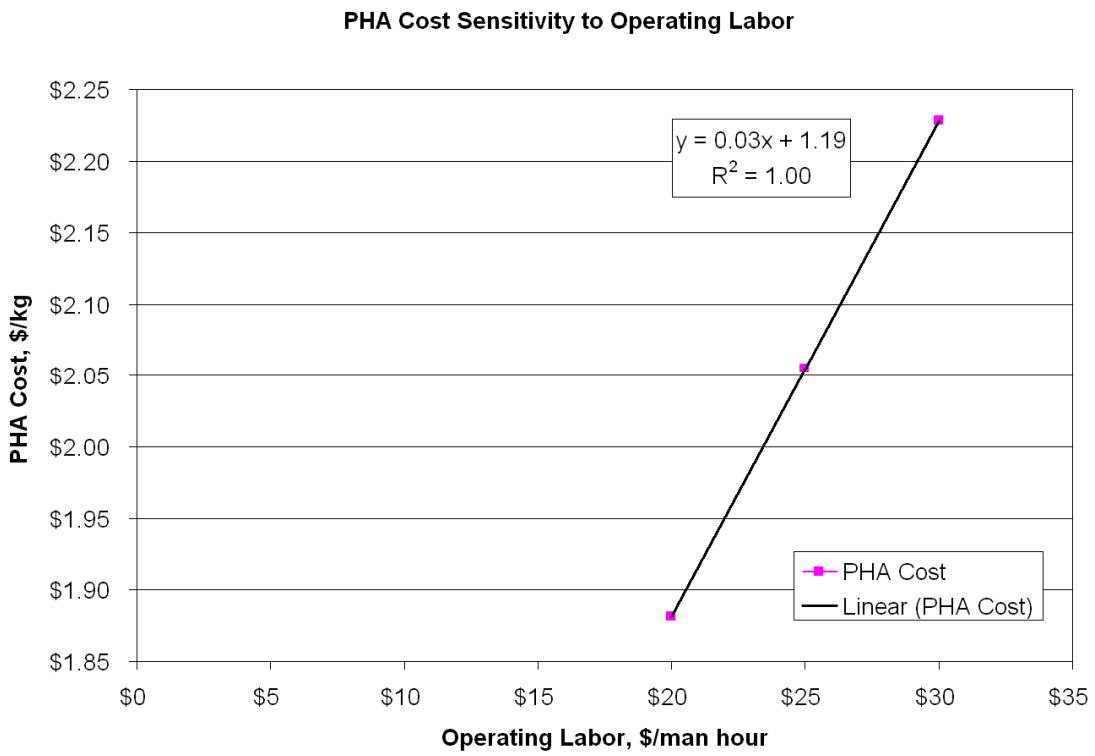

Figure 20. PHA cost sensitivity to operating labor for a bioreactor with constant kLa and 95% CO conversion.

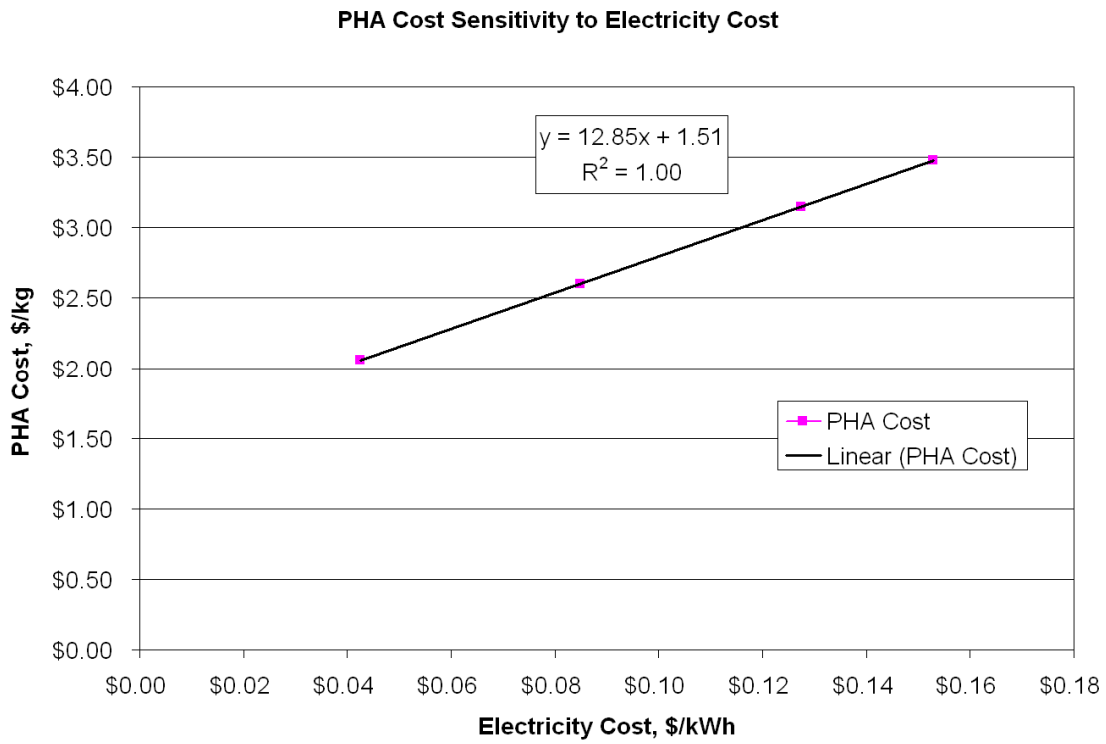

Figure 21. PHA cost sensitivity to electricity cost for a bioreactor with constant kLa and 95% CO conversion.

CONCLUSIONS

Results of this techno-economic analysis demonstrate that the production of PHA from the fermentation of syngas using *R. rubrum* is economically viable and technically feasible. The cost of producing the PHA via syngas fermentation is less expensive than producing PHA by sugar fermentation [29], which ranged from $4 to $6/kg. The operating cost of the biorefinery is heavily subsidized by the production and sale of the hydrogen gas, which has been counted as a co-product. However, this evaluation is fair because the market value ($1.90/kg) given to the hydrogen is actually less than $2/GGE (gallon gasoline equivalent). The DOE Hydrogen Posture Plan published in December 2006 [43] gave a hydrogen cost goal of $2 to $3/GGE. A hydrogen cost within that range would make this biorefinery even more attractive economically.

OPPORTUNITIES FOR FURTHER RESEARCH

There are opportunities for further investigation in this biorefinery that were not explored fully in this techno-economic analysis, and they were mentioned earlier. Some of the more important opportunities will be listed here. For the gasification portion of the biorefinery, a comparison of a bubbling fluidized bed reactor to an entrained flow reactor would be useful. Each reactor has advantages and disadvantages both technically and economically, and integrating a comparison of the two types of gasifiers within the context of a syngas fermenting biorefinery would help to better understand overall capital costs.

The cleaning of the syngas stream could also be explored further. As mentioned earlier, the cost for the bag house was estimated with the standard fabric bags, since the Aspen IPE software did not offer alternative materials. A more accurate cost for this piece of equipment would be useful, since a fabric with greater temperature resistance is likely to cost more than the standard fabric. Also, the gas reformer could be analyzed with less than 100% conversion of the long chain hydrocarbons to more accurately reflect actual conditions.

The bioreactors analyzed here were only of a single type, the CSTR. Other reactor types are available for gas-liquid dispersions, and they could also be explored to determine their optimum economical operation. Air-lift and bubble column reactors require lower operating costs because they do not use an agitator like CSTRs and show

higher conversions [50]. The trickle bed reactors studied by Klasson *et al*. also showed high CO conversion [33].

Another area of the biorefinery that could be investigated further is the PHA separation process. A large amount of water is used in this area, and in the analysis here the sodium hypochlorite waste was assumed to leave the process and be treated separately. A cost was then assigned to the treatment of this waste stream. A fuller accounting of the biorefinery, however, would include this treatment and its associated equipment and costs. In addition, the chemical usage could be analyzed on a different basis. For this analysis, the chemicals were based on the amount of PHA produced, and scaled up from the *E. coli* in the Choi and Lee process [29]. However, the *R. rubrum* bacteria have a different percentage of PHA in their cells than the *E. coli*, and this analysis could be modified to estimate chemical amounts on the cell biomass rather than the PHA produced.

Another opportunity in the area of gas cleanup is to explore uses for the char and ash streams leaving the cyclones and bag house. In the simulation explored in this analysis, these streams exited the biorefinery with no recycling or heat recovery. At 35 Mg/day, this stream has potential for other uses. The first obvious use is the removal of ash from the stream and recycling of the char to the gasifier for further syngas production. Another opportunity could lie in utilizing the material outside the biorefinery. First, the char and ash could be cooled while some process heat is recovered. Then, the mixture could be added to the topsoil in a field. The ash would provide some lost nutrients to the soil, and the char would sequester carbon, which has economic value. On 07 March 2007 a metric ton of carbon dioxide traded at 1.1 Euros [51]. Based on an exchange rate of 0.76 Euros per US dollar, this is a value of $1.45/Mg of CO2, or $5.31/Mg of carbon. Assuming the char produced by this biorefinery is 100% carbon, this provides a potential revenue stream of $61,000/year.

SUMMARY

This techno-economic analysis investigated the feasibility of a hybrid biorefinery producing both hydrogen gas and PHA, a biorenewable polymer. The biorefinery considered used switchgrass as a feedstock and converted that raw material through thermochemical methods into syngas, a combination mainly of hydrogen gas and carbon monoxide. The syngas was then fermented using *Rhodospirillum rubrum* bacteria to produce more hydrogen gas and PHA. The hydrogen was separated from the other gases

using a pressure swing adsorption system and the PHA was removed using a combination of surfactant and sodium hypochlorite to break down the cell material. The remaining material was then centrifuged to remove the PHA. Total daily production of the biorefinery was 50 Mg of hydrogen gas and 12 Mg of PHA.

Grassroots capital for the biorefinery was estimated to be $55 million, with annual operating costs at $8.3 million. With a market value of $1.90/kg assumed for the hydrogen, the cost of producing PHA was determined to be $2.05/kg.

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APPENDIX A. CONSTANT $k_L a$; ADDITIONAL RESULTS

APPENDIX A1-1. CONSTANT k_La; SYNGAS HEAT SOURCE; BIOREFINERY INDIVIDUAL COMPONENT COSTS

Costed using Icarus 2004.0.6 on PHA_Plant_Combined_rev028; software cost base is 1Q2004

					1994 CE PCI	368.1									
					2004 CE PCI	444.2									
					2005 CE PCI	468.2	Base dollars	2005 dollars	Base dollars	Base dollars	2005 dollars		Base dollars	2005 dollars	
Component	Qty	Size	Unit	Electricity, kW	Operators/unit/shift	Operators/shift	C_P		$C_P + C_M$	C_M		MMF = C_M/C_P	C_L		LMF = $C_L/(C_P+C_M)$
AIRCOMP	1	35,370.92	m^3/h	2,500.000	0.15	0.15	$287,300	$303,455	$341,927	$54,027	$56,946	0.1877	$40,412	$42,595	0.1182
BIOREACT	1	2,546	m^3	2,060.185	0.5	0.5	$11,307,300	$11,918,230	$12,228,378	$921,078	$970,844	0.0815	$350,749	$369,700	0.0287
BLNDTNK2	1	75.0	m^3	106.001	0.5	0.5	$315,500	$332,546	$439,335	$123,835	$130,526	0.3925	$56,928	$60,004	0.1296
BLNDTNK3	1	4.7	m^3	15.000	0.5	0.5	$69,300	$73,677	$133,115	$63,215	$66,630	0.9044	$29,844	$31,456	0.2242
BAGHOUSE	1	1,600	m^2		0.2	0.2	$367,300	$386,829	$406,853	$39,853	$42,006	0.1086	$33,580	$35,394	0.0825
CENTRIF1	4	920	mm	680.000	0.13	0.52	$2,097,500	$2,210,933	$2,364,982	$267,382	$281,829	0.1275	$98,680	$104,012	0.0417
		3,350	mm	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
CENTRIF2	1	920	mm	170.000	0.13	0.13	$524,400	$552,733	$591,246	$66,846	$70,458	0.1275	$24,670	$26,003	0.0417
		3,350	mm	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
CENTRIF3	1	920	mm	170.000	0.13	0.13	$524,400	$552,733	$591,246	$66,846	$70,458	0.1275	$24,670	$26,003	0.0417
		3,350	mm	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
CYCLONE1 Steel	5	1,500	mm	N/A	0	0	$139,500	$147,037	$255,068	$115,568	$121,812	0.8284	$47,657	$50,232	0.1868
CYCLONE1 Gunned Lining	5	15	m^2	N/A	0	0	$51,500	$54,283	$51,500	$0	$0	0.0000	$0	$0	0.0000
CYCLONE2 Steel	5	1,500	mm	N/A	0	0	$139,500	$147,037	$255,069	$115,569	$121,813	0.8285	$47,662	$50,237	0.1869
CYCLONE2 Gunned Lining	5	15	m^2	N/A	0	0	$51,500	$54,283	$51,500	$0	$0	0.0000	$0	$0	0.0000
FURNACE1	1	11.36	MW		0.5	0.5	$566,400	$597,002	$707,226	$140,826	$148,435	0.2486	$75,191	$79,254	0.1063
FURNACE2	1	1.32	MW		0.5	0.5	$208,500	$219,765	$276,817	$68,317	$72,008	0.3277	$42,677	$44,983	0.1542
GASIFIER Vessel	1	7.25	m	N/A	0.5	0.5	$295,400	$311,360	$779,142	$483,742	$509,878	1.6376	$148,042	$156,041	0.1900
		10	m	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
GASIFIER Refractory Brick	1	300	m^2	N/A	0	0	$232,900	$245,484	$232,900	$0	$0	0.0000	$0	$0	0.0000
GASIFIER Firebrick	1	300	m^2	N/A	0	0	$66,500	$70,198	$66,600	$0	$0	0.0000	$0	$0	0.0000
GASIFIER Limestone Packing	1	40	m^3	N/A	0	0	$16,700	$17,602	$16,700	$0	$0	0.0000	$8,074	$8,510	0.4835
GASLIQ-flash vessel	1	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
GASREFRM Vessel	1	7.25	m	N/A	0.5	0.5	$295,400	$311,360	$779,142	$483,742	$509,878	1.6376	$148,042	$156,041	0.1900
		10	m	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
GASREFRM Refractory Brick	1	300	m^2	N/A	0	0	$232,900	$245,484	$232,900	$0	$0	0.0000	$0	$0	0.0000
GASREFRM Firebrick	1	300	m^2	N/A	0	0	$66,500	$70,198	$66,600	$0	$0	0.0000	$0	$0	0.0000
GASREFRM Limestone Packing	1	40	m^3	N/A	0	0	$1,114,113	$1,417,081	$1,114,113	$0	$0	0.0000	$8,074	$8,510	0.0072
GRINDER	1	30	Mg/h	180.000	0.75	0.75	$900,300	$948,627	$902,678	$2,678	$2,823	0.0030	$5,498	$5,795	0.0061
H2PSA	1	50	Mg/d		1	1	$44,300	$46,377	$52,800	$8,800	$9,275	0.2000	$4,300	$4,532	0.0814
HEATX1	1	2,241.17	m^2	N/A	0.1	0.1	$889,300	$937,349	$1,372,493	$483,193	$509,300	0.5433	$84,165	$88,712	0.0613
HEATX2	1	823.65	m^2	N/A	0.1	0.1	$270,500	$285,220	$516,805	$246,205	$259,507	0.9098	$50,196	$52,908	0.0971
HEATX3	1	68.48	m^2	N/A	0.1	0.1	$20,500	$21,713	$59,439	$38,839	$40,937	1.8854	$22,431	$23,643	0.3774
HEATX4	1	1,999.97	m^2	N/A	0.1	0.1	$309,400	$326,117	$448,801	$139,401	$146,933	0.4506	$59,481	$62,695	0.1325
MIX1	1	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
MIX2	1	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
MIX3	1	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
PUMP1	1	2.29	L/s	0.750	0	0	$3,100	$3,267	$12,728	$9,628	$10,148	3.1058	$9,169	$9,664	0.7204
PUMP2	1	188.46	L/s	30.000	0	0	$13,300	$14,546	$57,078	$43,278	$45,616	3.1361	$18,319	$19,309	0.3209
PUMP3	1	13.51	L/s	22.000	0	0	$15,400	$16,232	$31,117	$15,717	$16,566	1.0206	$10,360	$10,920	0.3329
SPLIT1	1	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
SPRAYDRY	1	1,400	kg/h		1	1	$366,100	$385,880	$431,523	$65,423	$68,958	0.1787	$35,574	$37,496	0.0824
			Totals:	5,933.936	7.39	7.78	$21,803,313	$23,224,640	$25,867,821	$4,064,008	$4,283,585	N/A	$1,484,445	$1,564,649	N/A

APPENDIX A2-1. CONSTANT k_La; NATURAL GAS HEAT SOURCE; BIOREFINERY INDIVIDUAL COMPONENT COSTS

Costed using Icarus 2004.0.6 on PHA_Plant_Combined_rev028; software cost base is 1Q2004

					1994 CE PCI	368.1									
					2004 CE PCI	444.2									
					2005 CE PCI	468.2	Base dollars	2005 dollars	Base dollars	Base dollars	2005 dollars		Base dollars	2005 dollars	
Component	Qty	Size	Unit	Electricity, kW	Operators/unit/shift	Operators/shift	C_P		$C_P + C_M$	C_M		MMF = C_M/C_P	C_L		LMF = $C_L/(C_P+C_M)$
AIRCOMP	1	35,370.92	m^3/h	2,500.000	0.15	0.15	$287,900	$303,455	$341,927	$54,027	$56,946	0.1877	$40,412	$42,595	0.1182
BIOREACT	1	2,546	m^3	2,060.185	0.5	0.5	$11,307,300	$11,918,230	$12,228,378	$921,078	$970,844	0.0815	$350,749	$369,700	0.0287
BLNDTNK2	1	75.0	m^3	106.001	0.5	0.5	$315,500	$332,546	$439,335	$123,835	$130,526	0.3925	$56,928	$60,004	0.1296
BLNDTNK3	1	4.7	m^3	15.000	0.5	0.5	$69,900	$73,677	$133,115	$63,215	$66,630	0.9044	$29,844	$31,456	0.2242
BAGHOUSE	1	1,600	m^2		0.2	0.2	$367,000	$386,829	$406,853	$39,853	$42,006	0.1086	$33,580	$35,394	0.0825
CENTRIF1	4	920	mm	680.000	0.13	0.52	$2,097,600	$2,210,933	$2,364,982	$267,382	$281,829	0.1275	$98,680	$104,012	0.0417
		3,350	mm	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
CENTRIF2	1	920	mm	170.000	0.13	0.13	$524,400	$552,733	$591,246	$66,846	$70,458	0.1275	$24,670	$26,003	0.0417
		3,350	mm	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
CENTRIF3	1	920	mm	170.000	0.13	0.13	$524,400	$552,733	$591,246	$66,846	$70,458	0.1275	$24,670	$26,003	0.0417
		3,350	mm	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
CYCLONE1 Steel	5	1,500	mm	N/A	0	0	$139,500	$147,037	$255,068	$115,568	$121,812	0.8284	$47,657	$50,232	0.1868
CYCLONE1 Gunned Lining	5	15	m^2	N/A	0	0	$51,500	$54,283	$51,500	$0	$0	0.0000	$0	$0	0.0000
CYCLONE2 Steel	5	1,500	mm	N/A	0	0	$139,500	$147,037	$255,069	$115,569	$121,813	0.8285	$47,662	$50,237	0.1869
CYCLONE2 Gunned Lining	5	15	m^2	N/A	0	0	$51,500	$54,283	$51,500	$0	$0	0.0000	$0	$0	0.0000
FURNACE1	1	11.36	MW		0.5	0.5	$566,400	$597,002	$707,226	$140,826	$148,435	0.2486	$75,191	$79,254	0.1063
FURNACE2	1	1.32	MW		0.5	0.5	$208,500	$219,765	$276,817	$68,317	$72,008	0.3277	$42,677	$44,983	0.1542
GASIFIER Vessel	1	7.25	m	N/A	0.5	0.5	$295,400	$311,360	$779,142	$483,742	$509,878	1.6376	$148,042	$156,041	0.1900
		10	m	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
GASIFIER Refractory Brick	1	300	m^2	N/A	0	0	$232,900	$245,484	$232,900	$0	$0	0.0000	$0	$0	0.0000
GASIFIER Firebrick	1	300	m^2	N/A	0	0	$66,600	$70,198	$66,600	$0	$0	0.0000	$0	$0	0.0000
GASIFIER Limestone Packing	1	40	m^3	N/A	0	0	$16,700	$17,602	$16,700	$0	$0	0.0000	$8,074	$8,510	0.4835
GASLIQ-flash vessel	1	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
GASREFRM Vessel	1	7.25	m	N/A	0.5	0.5	$295,400	$311,360	$779,142	$483,742	$509,878	1.6376	$148,042	$156,041	0.1900
		10	m	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
GASREFRM Refractory Brick	1	300	m^2	N/A	0	0	$232,900	$245,484	$232,900	$0	$0	0.0000	$0	$0	0.0000
GASREFRM Firebrick	1	300	m^2	N/A	0	0	$66,600	$70,198	$66,600	$0	$0	0.0000	$0	$0	0.0000
GASREFRM Limestone Packing	1	40	m^3	N/A	0	0	$1,114,113	$1,417,081	$1,114,113	$0	$0	0.0000	$8,074	$8,510	0.0072
GRINDER	1	30	Mg/h	180.000	0.75	0.75	$900,000	$948,627	$902,678	$2,678	$2,823	0.0030	$5,498	$5,795	0.0061
H2PSA	1	50	Mg/d		1	1	$44,000	$46,377	$52,800	$8,800	$9,275	0.2000	$4,300	$4,532	0.0814
HEATX1	1	1,740.05	m^2	N/A	0.1	0.1	$684,700	$721,694	$1,037,687	$352,987	$372,059	0.5155	$66,914	$70,529	0.0645
HEATX2	1	729.60	m^2	N/A	0.1	0.1	$249,700	$263,191	$495,558	$245,858	$259,142	0.9846	$49,947	$52,646	0.1008
HEATX3	1	14.49	m^2	N/A	0.1	0.1	$14,200	$14,967	$39,578	$25,378	$26,749	1.7872	$18,140	$19,120	0.4583
HEATX4	1	1,514.18	m^2	N/A	0.1	0.1	$232,900	$245,484	$339,352	$106,452	$112,204	0.4571	$47,993	$50,586	0.1414
MIX1	1	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
MIX2	1	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
MIX3	1	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
PUMP1	1	2.29	L/s	0.750	0	0	$3,100	$3,267	$12,728	$9,628	$10,148	3.1058	$9,169	$9,664	0.7204
PUMP2	1	188.46	L/s	30.000	0	0	$13,800	$14,546	$57,078	$43,278	$45,616	3.1361	$18,319	$19,309	0.3209
PUMP3	1	13.51	L/s	22.000	0	0	$15,400	$16,232	$31,117	$15,717	$16,566	1.0206	$10,360	$10,920	0.3329
SPLIT1	1	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
SPRAYDRY	1	1,400	kg/h		1	1	$366,100	$385,880	$431,523	$65,423	$68,958	0.1787	$35,574	$37,496	0.0824
			Totals:	5,933.936	7.39	7.78	$21,495,413	$22,899,577	$25,382,458	$3,887,045	$4,097,061	N/A	$1,451,166	$1,529,572	N/A

APPENDIX A2-2. CONSTANT k_La; NATURAL GAS HEAT SOURCE; BIOREFINERY MATERIAL & ENERGY FLOWS

PHA/H2 Plant Material & Energy Flows	
from: PHA_Plant_Combined_rev029.apw	
Inputs	
Switchgrass, kg/day	604,000
Surfactant, kg/day	1,609
Hypochlorite solution, kg/day	31,100
Water:	
Gas Reformer	179,500
Bioreactor make-up	678,081
Final syngas cooling	2,000,000
PHA Washing	253,620
Total Water, kg/day	3,111,201
Gas Reformer Energy, kW	11,186
Electricity, kW	5,934
Outputs Daily	
Syngas, post-filter, kg/day	1,442,833
Syngas LHV, pre-reformer, kJ/kg	4,368
95% pure (10% moisture) PHA, kg/day	12,283
Hydrogen, kg/day	49,178
Spray dryer water vapor, kg/day	31,936
Wastewater:	
Waste cooling water	2,000,000
Centrifuge 2	667,053
Centrifuge 3	257,710
Total Wastewater, kg/day	2,924,763
Char & Ash:	
Cyclone stage 1	27,939
Cyclone stage 2	1,313
Candle filter	498
Total Char & Ash, kg/day	29,749
Bioreactor Heat, kW	54
Outputs Annual	
95% Pure PHA, Mg/yr	4,038
Hydrogen, Mg H_2/yr	16,166

APPENDIX A2-3. CONSTANT k_La; NATURAL GAS HEAT SOURCE; BIOREFINERY CAPITAL COSTS

Capital Cost				
Direct Costs				
Equipment (f.o.b.)	C_P from Icarus		$22,899,577	
Materials for installation	C_M from Icarus		$4,097,061	
Direct labor	C_L from Icarus		$1,529,572	
Total Direct Costs	$C_D = C_P + C_M + C_L$		$28,526,210	
Indirect Costs				
Freight, Insurance, taxes	$C_{FIT} = 0.08 \times C_P$		$1,831,966	
Construction overhead	$C_O = 0.7 \times C_L$		$1,070,700	
Engineering expenses	$C_E = 0.15 \times (C_P + C_M)$		$4,049,496	
Total Indirect Costs	$C_{ID} = C_{FIT} + C_O + C_E$		$6,952,162	
Bare module cost	$C_{BM} = C_D + C_{ID}$		$35,478,372	
Contingency & fee	$C_{CF} = 0.18 \times C_{BM}$		$6,386,107	
Total Module Cost	$C_{TM} = C_{BM} + C_{CF}$		$41,864,479	
Auxiliary facilities	$C_{AF} = 0.30 \times C_{TM}$		$12,559,344	
Grassroots capital	$\mathbf{C_{GR} = C_{TM} + C_{AF}}$		**$54,423,823**	

APPENDIX A2-4. CONSTANT k_La; NATURAL GAS HEAT SOURCE; BIOREFINERY OPERATING COSTS

Operating Cost	
	2005 dollars
Direct Expenses ($/yr)	
Raw materials	
Switchgrass	$10,920,245
Water	$1,190,193
Surfactant	$923,208
Hypochlorite Solution	$1,189,726
Operating labor	$1,534,488
Supervisory labor	$230,173
Utilities	
Electricity (major components)	$1,989,646
Gas reform heat	$2,472,121
Spray dryer heat	$276,933
Wastewater treatment	$574,343
Maintenance & repairs	$3,265,429
Operating supplies	$489,814
Laboratory charges	$230,173
Patents and royalties	$758,595
Direct Subtotal	**$26,045,087**
Indirect & General Expenses ($/yr)	
Overhead	$3,018,055
Local taxes	$816,357
Insurance	$380,967
General expenses	$2,183,555
Indirect subtotal	**$6,398,933**

APPENDIX A2-5. CONSTANT k_La; NATURAL GAS HEAT SOURCE; BIOREFINERY PRODUCT COSTS

Product Cost	
	2005 dollars
By-product credits (sale of H_2)	($30,715,462)
Annual capital charges ($/yr)	$7,223,640
Annual operating cost ($/yr)	$8,952,199
Product cost ($/kg PHA)	$2.2172

APPENDIX B. CORRELATED $k_L a$; ADDITIONAL RESULTS

APPENDIX B1-1. CORRELATED k_La; SYNGAS GAS HEAT SOURCE; BIOREFINERY INDIVIDUAL COMPONENT COSTS

Costed using Icarus 2004.0.6 on PHA_Plant_Combined_rev028; software cost base is 1Q2004

					1994 CE PCI	368.1									
					2004 CE PCI	444.2									
					2005 CE PCI	468.2	Base dollars	2005 dollars	Base dollars	Base dollars	2005 dollars		Base dollars	2005 dollars	
Component	Qty	Size	Unit	Electricity, kW	Operators/unit/shift	Operators/shift	C_P		$C_P + C_M$	C_M		MMF = C_M/C_P	C_L		LMF = $C_L/(C_P+C_M)$
AIRCOMP	1	35,370.92	m^3/h	2,500.000	0.15	0.15	$287,900	$303,455	$341,927	$54,027	$56,946	0.1877	$40,412	$42,595	0.1182
BIOREACT	1	226	m^3	1,145.323	0.5	0.5	$1,248,300	$1,315,745	$1,458,584	$210,284	$221,646	0.1685	$98,542	$103,866	0.0676
BLNDTNK2	1	75.0	m^3	106.001	0.5	0.5	$315,500	$332,546	$439,335	$123,835	$130,526	0.3925	$56,928	$60,004	0.1296
BLNDTNK3	1	4.7	m^3	15.000	0.5	0.5	$69,900	$73,677	$133,115	$63,215	$66,630	0.9044	$29,844	$31,456	0.2242
BAGHOUSE	1	1,600	m^2		0.2	0.2	$367,000	$386,829	$406,853	$39,853	$42,006	0.1086	$33,580	$35,394	0.0825
CENTRIF1	4	920	mm	680.000	0.13	0.52	$2,097,600	$2,210,933	$2,364,982	$267,382	$281,829	0.1275	$98,680	$104,012	0.0417
		3,350	mm	N/A	N/A	N/A	\/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
CENTRIF2	1	920	mm	170.000	0.13	0.13	$524,400	$552,733	$591,246	$66,846	$70,458	0.1275	$24,670	$26,003	0.0417
		3,350	mm	N/A	N/A	N/A	\/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
CENTRIF3	1	920	mm	170.000	0.13	0.13	$524,400	$552,733	$591,246	$66,846	$70,458	0.1275	$24,670	$26,003	0.0417
		3,350	mm	N/A	N/A	N/A	\/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
CYCLONE1 Steel	5	1,500	mm	N/A	0	0	$139,500	$147,037	$255,068	$115,568	$121,812	0.8284	$47,657	$50,232	0.1868
CYCLONE1 Gunned Lining	5	15	m^2	N/A	0	0	$51,500	$54,283	$51,500	$0	$0	0.0000	$0	$0	0.0000
CYCLONE2 Steel	5	1,500	mm	N/A	0	0	$139,500	$147,037	$255,069	$115,569	$121,813	0.8285	$47,662	$50,237	0.1869
CYCLONE2 Gunned Lining	5	15	m^2	N/A	0	0	$51,500	$54,283	$51,500	$0	$0	0.0000	$0	$0	0.0000
FURNACE1	1	11.36	MW		0.5	0.5	$566,400	$597,002	$707,226	$140,826	$148,435	0.2486	$75,191	$79,254	0.1063
FURNACE2	1	1.32	MW		0.5	0.5	$208,500	$219,765	$276,817	$68,317	$72,008	0.3277	$42,677	$44,983	0.1542
GASIFIER Vessel	1	7.25	m	N/A	0.5	0.5	$295,400	$311,360	$779,142	$483,742	$509,878	1.6376	$148,042	$156,041	0.1900
		10	m	N/A	N/A	N/A	\/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
GASIFIER Refractory Brick	1	300	m^2	N/A	0	0	$232,900	$245,484	$232,900	$0	$0	0.0000	$0	$0	0.0000
GASIFIER Firebrick	1	300	m^2	N/A	0	0	$66,600	$70,198	$66,600	$0	$0	0.0000	$0	$0	0.0000
GASIFIER Limestone Packing	1	40	m^3	N/A	0	0	$16,700	$17,602	$16,700	$0	$0	0.0000	$8,074	$8,510	0.4835
GASLIQ-flash vessel	1	N/A	N/A	N/A	N/A	N/A	\/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
GASREFRM Vessel	1	7.25	m	N/A	0.5	0.5	$295,400	$311,360	$779,142	$483,742	$509,878	1.6376	$148,042	$156,041	0.1900
		10	m	N/A	N/A	N/A	\/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
GASREFRM Refractory Brick	1	300	m^2	N/A	0	0	$232,900	$245,484	$232,900	$0	$0	0.0000	$0	$0	0.0000
GASREFRM Firebrick	1	300	m^2	N/A	0	0	$66,600	$70,198	$66,600	$0	$0	0.0000	$0	$0	0.0000
GASREFRM Limestone Packing	1	40	m^3	N/A	0	0	$1,114,113	$1,417,081	$1,114,113	$0	$0	0.0000	$8,074	$8,510	0.0072
GRINDER	1	30	Mg/h	180.000	0.75	0.75	$900,000	$948,627	$902,678	$2,678	$2,823	0.0030	$5,498	$5,795	0.0061
H2PSA	1	50	Mg/d		1	1	$44,000	$46,377	$52,800	$8,800	$9,275	0.2000	$4,300	$4,532	0.0814
HEATX1	1	2,241.17	m^2	N/A	0.1	0.1	$889,300	$937,349	$1,372,493	$483,193	$509,300	0.5433	$84,165	$88,712	0.0613
HEATX2	1	823.65	m^2	N/A	0.1	0.1	$270,600	$285,220	$516,805	$246,205	$259,507	0.9098	$50,196	$52,908	0.0971
HEATX3	1	68.48	m^2	N/A	0.1	0.1	$20,600	$21,713	$59,439	$38,839	$40,937	1.8854	$22,431	$23,643	0.3774
HEATX4	1	1,999.97	m^2	N/A	0.1	0.1	$309,400	$326,117	$448,801	$139,401	$146,933	0.4506	$59,481	$62,695	0.1325
MIX1	1	N/A	N/A	N/A	N/A	N/A	\/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
MIX2	1	N/A	N/A	N/A	N/A	N/A	\/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
MIX3	1	N/A	N/A	N/A	N/A	N/A	\/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
PUMP1	1	2.29	L/s	0.750	0	0	$3,100	$3,267	$12,728	$9,628	$10,148	3.1058	$9,169	$9,664	0.7204
PUMP2	1	188.46	L/s	30.000	0	0	$13,800	$14,546	$57,078	$43,278	$45,616	3.1361	$18,319	$19,309	0.3209
PUMP3	1	13.51	L/s	22.000	0	0	$15,400	$16,232	$31,117	$15,717	$16,566	1.0206	$10,360	$10,920	0.3329
SPLIT1	1	N/A	N/A	N/A	N/A	N/A	\/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
SPRAYDRY	1	1,400	kg/h		1	1	$366,100	$385,880	$431,523	$65,423	$68,958	0.1787	$35,574	$37,496	0.0824
			Totals:	5,019.074	7.39	7.78	$11,744,813	$12,622,155	$15,098,027	$3,353,214	$3,534,387	N/A	$1,232,238	$1,298,815	N/A

APPENDIX B1-2. CORRELATED k_La; SYNGAS GAS HEAT SOURCE; BIOREFINERY MATERIAL & ENERGY FLOWS

PHA/H2 Plant Material & Energy Flows	
from: PHA_Plant_Combined_rev030.apw	
Inputs	
Switchgrass, kg/day	708,000
Surfactant, kg/day	1,608
Hypochlorite solution, kg/day	31,074
Water:	
Gas Reformer	179,353
Bioreactor make-up	678,174
Final syngas cooling	2,000,000
PHA Washing	253,388
Total Water, kg/day	3,110,915
Gas Reformer Energy, kW	11,366
Electricity, kW	5,019
Outputs Daily	
Syngas, post-filter, kg/day	1,691,268
Syngas LHV, pre-reformer, kJ/kg	4,368
95% pure (10% moisture) PHA, kg/day	12,273
Hydrogen, kg/day	49,138
Spray dryer water vapor, kg/day	31,909
Wastewater:	
Waste cooling water	2,000,000
Centrifuge 2	666,478
Centrifuge 3	257,475
Total Wastewater, kg/day	2,923,953
Char & Ash:	
Cyclone stage 1	32,686
Cyclone stage 2	1,576
Candle filter	610
Total Char & Ash, kg/day	34,872
Bioreactor Heat, kW	53
Outputs Annual	
95% Pure PHA, Mg/yr	4,034
Hydrogen, Mg H_2/yr	16,153

APPENDIX B1-3. CORRELATED k_La; SYNGAS GAS HEAT SOURCE; BIOREFINERY CAPITAL COSTS

Capital Cost				
Direct Costs				
Equipment (f.o.b.)	C_P from Icarus		$12,622,155	
Materials for installation	C_M from Icarus		$3,534,387	
Direct labor	C_L from Icarus		$1,298,815	
Total Direct Costs	$C_D = C_P + C_M + C_L$		$17,455,357	
Indirect Costs				
Freight, Insurance, taxes	$C_{FIT} = 0.08 \times C_P$		$1,009,772	
Construction overhead	$C_O = 0.7 \times C_L$		$909,171	
Engineering expenses	$C_E = 0.15 \times (C_P + C_M)$		$2,423,481	
Total Indirect Costs	$C_{ID} = C_{FIT} + C_O + C_E$		$4,342,424	
Bare module cost	$C_{BM} = C_D + C_{ID}$		$21,797,782	
Contingency & fee	$C_{CF} = 0.18 \times C_{BM}$		$3,923,601	
Total Module Cost	$C_{TM} = C_{BM} + C_{CF}$		$25,721,383	
Auxiliary facilities	$C_{AF} = 0.30 \times C_{TM}$		$7,716,415	
Grassroots capital	$\mathbf{C_{GR} = C_{TM} + C_{AF}}$		**$33,437,797**	

APPENDIX B1-4. CORRELATED k_La; SYNGAS GAS HEAT SOURCE; BIOREFINERY OPERATING COSTS

Operating Cost	
	2005 dollars
Direct Expenses ($/yr)	
Raw materials	
Switchgrass	$12,800,552
Water	$1,190,083
Surfactant	$922,452
Hypochlorite Solution	$1,188,750
Operating labor	$1,534,488
Supervisory labor	$230,173
Utilities	
Electricity (major components)	$1,682,893
Wastewater treatment	$574,184
Maintenance & repairs	$2,006,268
Operating supplies	$300,940
Laboratory charges	$230,173
Patents and royalties	$679,829
Direct Subtotal	**$23,340,785**
Indirect & General Expenses ($/yr)	
Overhead	$2,262,558
Local taxes	$501,567
Insurance	$234,065
General expenses	$1,980,732
Indirect subtotal	**$4,978,921**

APPENDIX B1-5. CORRELATED k_La; SYNGAS GAS HEAT SOURCE; BIOREFINERY PRODUCT COSTS

Product Cost	
	2005 dollars
By-product credits (sale of H_2)	($30,690,215)
Annual capital charges ($/yr)	$4,438,178
Annual operating cost ($/yr)	$2,067,669
Product cost ($/kg PHA)	$0.5125

APPENDIX B2-1. CORRELATED k_La; NATURAL GAS HEAT SOURCE; BIOREFINERY INDIVIDUAL COMPONENT COSTS

Costed using Icarus 2004.0.6 on PHA_Plant_Combined_rev028; software cost base is 1Q2004

					1994 CE PCI	368.1									
					2004 CE PCI	444.2									
					2005 CE PCI	468.2	Base dollars	2005 dollars	Base dollars	Base dollars	2005 dollars		Base dollars	2005 dollars	
Component	Qty	Size	Unit	Electricity, kW	Operators/unit/shift	Operators/shift	C_P		$C_P + C_M$	C_M		MMF = C_M/C_P	C_L		LMF = $C_L/(C_P+C_M)$
AIRCOMP	1	35,370.92	m^3/h	2,500.000	0.15	0.15	$287,900	$303,455	$341,927	$54,027	$56,946	0.1877	$40,412	$42,595	0.1182
BIOREACT	1	226	m^3	1,145.323	0.5	0.5	$1,248,300	$1,315,745	$1,458,584	$210,284	$221,646	0.1685	$98,542	$103,866	0.0676
BLNDTNK2	1	75.0	m^3	106.001	0.5	0.5	$315,600	$332,546	$439,335	$123,835	$130,526	0.3925	$56,928	$60,004	0.1296
BLNDTNK3	1	4.7	m^3	15.000	0.5	0.5	$69,900	$73,677	$133,115	$63,215	$66,630	0.9044	$29,844	$31,456	0.2242
BAGHOUSE	1	1,600	m^2		0.2	0.2	$367,000	$386,829	$406,853	$39,853	$42,006	0.1086	$33,580	$35,394	0.0825
CENTRIF1	4	920	mm	680.000	0.13	0.52	$2,097,600	$2,210,933	$2,364,982	$267,382	$281,829	0.1275	$98,680	$104,012	0.0417
		3,350	mm	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
CENTRIF2	1	920	mm	170.000	0.13	0.13	$524,400	$552,733	$591,246	$66,846	$70,458	0.1275	$24,670	$26,003	0.0417
		3,350	mm	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
CENTRIF3	1	920	mm	170.000	0.13	0.13	$524,400	$552,733	$591,246	$66,846	$70,458	0.1275	$24,670	$26,003	0.0417
		3,350	mm	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
CYCLONE1 Steel	5	1,500	mm	N/A	0	0	$139,500	$147,037	$255,068	$115,568	$121,812	0.8284	$47,657	$50,232	0.1868
CYCLONE1 Gunned Lining	5	15	m^2	N/A	0	0	$51,500	$54,283	$51,500	$0	$0	0.0000	$0	$0	0.0000
CYCLONE2 Steel	5	1,500	mm	N/A	0	0	$139,500	$147,037	$255,069	$115,569	$121,813	0.8285	$47,662	$50,237	0.1869
CYCLONE2 Gunned Lining	5	15	m^2	N/A	0	0	$51,500	$54,283	$51,500	$0	$0	0.0000	$0	$0	0.0000
FURNACE1	1	11.36	MW		0.5	0.5	$566,400	$597,002	$707,226	$140,826	$148,435	0.2486	$75,191	$79,254	0.1063
FURNACE2	1	1.32	MW		0.5	0.5	$208,600	$219,765	$276,817	$68,317	$72,008	0.3277	$42,677	$44,983	0.1542
GASIFIER Vessel	1	7.25	m	N/A	0.5	0.5	$295,400	$311,360	$779,142	$483,742	$509,878	1.6376	$148,042	$156,041	0.1900
		10	m	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
GASIFIER Refractory Brick	1	300	m^2	N/A	0	0	$232,900	$245,484	$232,900	$0	$0	0.0000	$0	$0	0.0000
GASIFIER Firebrick	1	300	m^2	N/A	0	0	$66,600	$70,198	$66,600	$0	$0	0.0000	$0	$0	0.0000
GASIFIER Limestone Packing	1	40	m^3	N/A	0	0	$16,700	$17,602	$16,700	$0	$0	0.0000	$8,074	$8,510	0.4835
GASLIQ-flash vessel	1	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
GASREFRM Vessel	1	7.25	m	N/A	0.5	0.5	$295,400	$311,360	$779,142	$483,742	$509,878	1.6376	$148,042	$156,041	0.1900
		10	m	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
GASREFRM Refractory Brick	1	300	m^2	N/A	0	0	$232,900	$245,484	$232,900	$0	$0	0.0000	$0	$0	0.0000
GASREFRM Firebrick	1	300	m^2	N/A	0	0	$66,600	$70,198	$66,600	$0	$0	0.0000	$0	$0	0.0000
GASREFRM Limestone Packing	1	40	m^3	N/A	0	0	$1,114,113	$1,417,081	$1,114,113	$0	$0	0.0000	$8,074	$8,510	0.0072
GRINDER	1	30	Mg/h	180.000	0.75	0.75	$900,000	$948,627	$902,678	$2,678	$2,823	0.0030	$5,498	$5,795	0.0061
H2PSA	1	50	Mg/d		1	1	$44,000	$46,377	$52,800	$8,800	$9,275	0.2000	$4,300	$4,532	0.0814
HEATX1	1	1,740.05	m^2	N/A	0.1	0.1	$684,700	$721,694	$1,037,687	$352,987	$372,059	0.5155	$66,914	$70,529	0.0645
HEATX2	1	729.60	m^2	N/A	0.1	0.1	$249,700	$263,191	$495,558	$245,858	$259,142	0.9846	$49,947	$52,646	0.1008
HEATX3	1	14.49	m^2	N/A	0.1	0.1	$14,200	$14,967	$39,578	$25,378	$26,749	1.7872	$18,140	$19,120	0.4583
HEATX4	1	1,514.18	m^2	N/A	0.1	0.1	$232,900	$245,484	$339,352	$106,452	$112,204	0.4571	$47,993	$50,586	0.1414
MIX1	1	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
MIX2	1	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
MIX3	1	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
PUMP1	1	2.29	L/s	0.750	0	0	$3,100	$3,267	$12,728	$9,628	$10,148	3.1058	$9,169	$9,664	0.7204
PUMP2	1	188.46	L/s	30.000	0	0	$13,600	$14,546	$57,078	$43,278	$45,616	3.1361	$18,319	$19,309	0.3209
PUMP3	1	13.51	L/s	22.000	0	0	$15,400	$16,232	$31,117	$15,717	$16,566	1.0206	$10,360	$10,920	0.3329
SPLIT1	1	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
SPRAYDRY	1	1,400	kg/h		1	1	$366,100	$385,880	$431,523	$65,423	$68,958	0.1787	$35,574	$37,496	0.0824
			Totals:	5,019.074	7.39	7.78	$11,436,413	$12,297,092	$14,612,664	$3,176,251	$3,347,863	N/A	$1,198,959	$1,263,738	N/A

APPENDIX B2-2. CORRELATED k_La; NATURAL GAS HEAT SOURCE; BIOREFINERY MATERIAL & ENERGY FLOWS

PHA/H2 Plant Material & Energy Flows	
from: PHA_Plant_Combined_rev029.apw	
Inputs	
Switchgrass, kg/day	604,000
Surfactant, kg/day	1,609
Hypochlorite solution, kg/day	31,100
Water:	
Gas Reformer	179,500
Bioreactor make-up	678,081
Final syngas cooling	2,000,000
PHA Washing	253,620
Total Water, kg/day	3,111,201
Gas Reformer Energy, kW	11,186
Electricity, kW	5,019
Outputs Daily	
Syngas, post-filter, kg/day	1,442,833
Syngas LHV, pre-reformer, kJ/kg	4,368
95% pure (10% moisture) PHA, kg/day	12,283
Hydrogen, kg/day	49,178
Spray dryer water vapor, kg/day	31,936
Wastewater:	
Waste cooling water	2,000,000
Centrifuge 2	667,053
Centrifuge 3	257,710
Total Wastewater, kg/day	2,924,763
Char & Ash:	
Cyclone stage 1	27,939
Cyclone stage 2	1,313
Candle filter	498
Total Char & Ash, kg/day	29,749
Bioreactor Heat, kW	54
Outputs Annual	
95% Pure PHA, Mg/yr	4,038
Hydrogen, Mg H_2/yr	16,166

APPENDIX B2-3. CORRELATED k_La; NATURAL GAS HEAT SOURCE; BIOREFINERY CAPITAL COSTS

Capital Cost				
Direct Costs				
Equipment (f.o.b.)	C_P from Icarus		$12,297,092	
Materials for installation	C_M from Icarus		$3,347,863	
Direct labor	C_L from Icarus		$1,263,738	
Total Direct Costs	$C_D = C_P + C_M + C_L$		$16,908,693	
Indirect Costs				
Freight, Insurance, taxes	$C_{FIT} = 0.08 \times C_P$		$983,767	
Construction overhead	$C_O = 0.7 \times C_L$		$884,617	
Engineering expenses	$C_E = 0.15 \times (C_P + C_M)$		$2,346,743	
Total Indirect Costs	$C_{ID} = C_{FIT} + C_O + C_E$		$4,215,127	
Bare module cost	$C_{BM} = C_D + C_{ID}$		$21,123,821	
Contingency & fee	$C_{CF} = 0.18 \times C_{BM}$		$3,802,288	
Total Module Cost	$C_{TM} = C_{BM} + C_{CF}$		$24,926,109	
Auxiliary facilities	$C_{AF} = 0.30 \times C_{TM}$		$7,477,833	
Grassroots capital	$\mathbf{C_{GR} = C_{TM} + C_{AF}}$		**$32,403,941**	

APPENDIX B2-4. CORRELATED k_La; NATURAL GAS HEAT SOURCE; BIOREFINERY OPERATING COSTS

Operating Cost	
	2005 dollars
Direct Expenses ($/yr)	
Raw materials	
Switchgrass	$10,920,245
Water	$1,190,193
Surfactant	$923,208
Hypochlorite Solution	$1,189,726
Operating labor	$1,534,488
Supervisory labor	$230,173
Utilities	
Electricity (major components)	$1,682,893
Gas reform heat	$2,472,121
Spray dryer heat	$276,933
Wastewater treatment	$574,343
Maintenance & repairs	$1,944,236
Operating supplies	$291,635
Laboratory charges	$230,173
Patents and royalties	$703,811
Direct Subtotal	**$24,164,179**
Indirect & General Expenses ($/yr)	
Overhead	$2,225,339
Local taxes	$486,059
Insurance	$226,828
General expenses	$2,042,487
Indirect subtotal	**$4,980,712**

APPENDIX B2-5. CORRELATED k_La; NATURAL GAS HEAT SOURCE; BIOREFINERY PRODUCT COSTS

Product Cost	
	2005 dollars
By-product credits (sale of H_2)	($30,715,462)
Annual capital charges ($/yr)	$4,300,955
Annual operating cost ($/yr)	$2,730,384
Product cost ($/kg PHA)	$0.6762