

A Techno-economic Analysis of Polyhydroxyalkanoate and Hydrogen Production from Syngas Fermentation of Gasified Biomass

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Abstract A techno-economic analysis was conducted to investigate the feasibility of a gasification-based hybrid biorefinery producing both hydrogen gas and polyhydroxyalkanoates (PHA), biodegradable polymer materials that can be an attractive substitute for conventional petrochemical plastics. The biorefinery considered used switchgrass as a feedstock and converted that raw material through thermochemical methods into syngas, a gaseous mixture composed mainly of hydrogen and carbon monoxide. The syngas was then fermented using *Rhodospirillum rubrum*, a purple non-sulfur bacterium, to produce PHA and to enrich hydrogen in the syngas. Total daily production of the biorefinery was assumed to be 12 Mg of PHA and 50 Mg of hydrogen gas. Grassroots capital for the biorefinery was estimated to be \$55 million, with annual operating costs at \$6.7 million. With a market value of \$2.00/kg assumed for the hydrogen, the cost of producing PHA was determined to be \$1.65/kg.

Keywords Syngas fermentation · Synthesis gas fermentation · Polyhydroxyalkanoate · PHA · Techno-economic analysis · Hydrogen · ASPEN Plus · *Rhodospirillum rubrum*

Introduction

The term biorefinery, a concept analogous to a conventional petrochemical refinery, has been widely used to describe the chemical refining of many different processes where the feedstock is organic material from recent biological origin, i.e., biomass or biorenewable resources [1, 2]. Biorefineries offer an alternative to fossil organic-material-based petrochemical refineries but require new and innovative processing methods than those traditionally used in the petroleum industry [1, 2]. One innovative processing method is the gasification of biomass followed by syngas fermentation. Gasification is a thermochemical conversion of biomass into a flammable vapor mixture and char. If gasification is oxygen-blown at temperatures above 900 °C, the non-condensable vapor mixture is mostly hydrogen (H₂), carbon monoxide (CO),

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and carbon dioxide (CO₂), which is known as syngas. If gasification is air-blown at temperatures between 700 °C and 900 °C, the mixture also includes substantial nitrogen originated from the air, which is known as producer gas [3]. 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. Gasification is overall an endothermic process and requires either an external heat source to maintain the reactions or partial combustion of the produced gas [4, 5]. 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.

After the gasification of biomass, contaminants must be removed before the syngas can be sent to the bioreactor for two major reasons. One, although the bacteria used as biocatalysts are capable of tolerating a wider range of contaminants compared to traditional metal-based catalysts, cleanup of the syngas may still be necessary to maintain maximal bacterial activity [6]. Two, char and tar accumulation in the syngas delivery lines can cause mechanical problems such as clogging, line breaking, and unstable gas flow rate [4]. The solid particulate matter, char and ash, is typically removed from the syngas stream before the tars at temperatures above 500 °C to prevent tars from condensing [5]. Particulate removal can be divided into two sections depending on the size of particles: cyclone filters and barrier filters [7]. Downstream from the gasifier, the first stage cleanup is usually high-efficiency cyclones, which are capable of removing particles of diameter greater than 5 µm. For the second stage cleanup, barrier filters such as ceramic candle filters and fabric bag filters can be used to further remove particles down to 0.5 µm in diameter [5, 7, 8]. After char removal, tar in the syngas stream can be cleaned up. Tar is a mixture of high-molecular-weight hydrocarbons and it can be removed by cooling and scrubbing with water or oil. However, this process is expensive and generates a new stream of contaminated water or oil which must be properly treated before disposal [3, 7]. For this analysis, tar was assumed to be reformed to additional syngas. To avoid complete oxidation of tar, steam was used as the sole oxidizer.

Syngas fermentation uses bacteria to mediate the biocatalytic conversion of a portion of the syngas, such as the CO and/or H₂, to a variety of chemicals. Chemicals produced from syngas fermentation can include hydrogen, methane, acetic acid, butyric acid, ethanol, butanol, and biopolymers [9]. Using bacteria as biocatalysts offers 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 H₂ in order to produce their desired chemicals. Finally, biological catalysts are less sensitive to the trace amount of contaminants in the syngas such as char, tar, ash, chlorine, and sulfur [10].

Rhodospirillum rubrum, a purple non-sulfur photosynthetic bacterium, is capable of syngas fermentation. *R. rubrum* has been used for the production of polyhydroxyalkanoates (PHA) as energy and carbon storage molecules in continuous stirred tank reactors (CSTR) fed with syngas. PHA can be extracted from bacterial cells and used as a biodegradable plastic with material properties similar to polypropylene [11]. In addition to PHA, *R. rubrum* can also produce H₂ [12]. Hydrogen is produced with a biocatalytic water–gas shift reaction mediated by carbon monoxide dehydrogenase (CODH) [4]:



To date, there has not been any study reported on the process analysis and techno-economic evaluation for PHA production by a gasification-based biorefinery. Techno-economic analysis of PHA production by the gasification-based biorefinery will allow for the estimation of PHA

production cost on a commercial scale and for the evaluation of the economic feasibility of PHA production. In this study, the biorefinery process was simulated based on the recently published information on the production and separation of PHA [4, 13–22].

Materials and Methods

Process Description

Techno-economic analysis for a gasification-based biorefinery producing 12 Mg/day of PHA was carried out using Aspen Plus software package (Aspen Technologies, Colorado Springs, CO, USA) unless otherwise stated. Four major steps were taken in the techno-economic analysis for this biorefinery. First, an optimization was performed on the bioreactors to determine their most cost-effective operating conditions. Next, the material and energy flows were determined by simulating the biorefinery (Fig. 1). 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 using spreadsheet software, Excel 2003 (Microsoft, Redmond, WA, USA).

Because the physical properties of switchgrass, char/ash, cellular biomass, and PHAs were not defined in the databanks of Aspen Plus software, empirical properties such as ultimate, proximate, and sulfur analyses were used to define them. Data for switchgrass and char/ash came from previous work by Lysenko [18]. PHA was modeled as the repeating unit ($C_4H_6O_2$) of PHA and the analysis did not account for polymerization energy. Microbial biomass was modeled as dextrose.

Bioreactor Optimization

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 to 25 m. Second, the bioreactor stirring speed was varied from 0 to 5 rps. Since carbon monoxide was the molecule consumed in the bacterial reactions, the parameter optimized was CO solubilization cost (\$/kg CO solubilized).

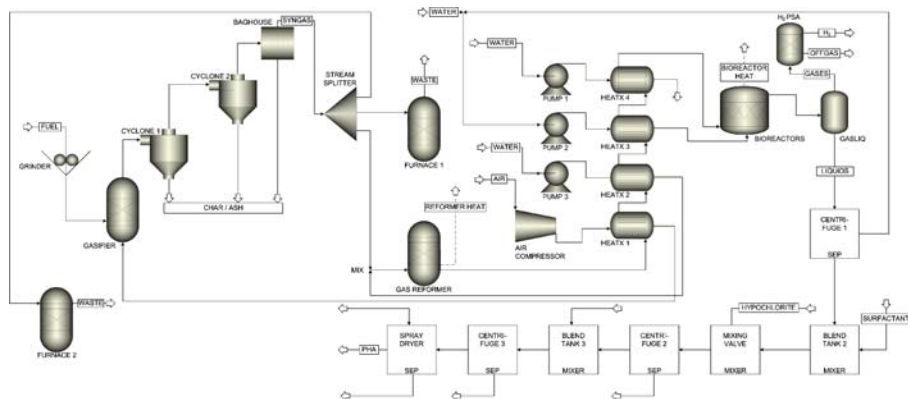


Fig. 1 Aspen Plus process flow diagram detailing the gasification-based hybrid biorefinery

The rate-limiting step in syngas fermentation by *R. rubrum* was the mass transfer of carbon monoxide from the syngas to the cell culture medium in the bioreactor [4]. Although mass transfer rate coefficients, $k_L a$, were expected to be a function of reactor diameter, stirring speed, etc. [16, 17], there was not sufficient data to model this functional dependence based on the range of values used in this study. Instead, a constant $k_L a$ of 0.05 s^{-1} was used based on work of Kapic et al. [16, 17]. For the bioreactor optimization model, it was assumed that the working fluid was water.

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:

$$pQ_g = \dot{n} R \theta \quad (2)$$

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. The next important variable needed for the bioreactor model was the mean residence time (τ_R) of the syngas in the bioreactor [23]:

$$\tau_R = \frac{V_L}{Q_g} \quad (3)$$

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 was assumed that the bioreactor was a perfectly mixed CSTR with the gas to liquid mass transfer as the rate-limiting step of the process. Along with the volumetric mass transfer coefficient, the residence time was used to calculate the CO conversion (X_{CO}) by each bioreactor using Eq. 4 [23]:

$$X_{CO} = \frac{k_L a \tau_R}{1 + (k_L a \tau_R)} \quad (4)$$

Biomass Feedstock

The biomass feedstock entering the biorefinery was assumed to be switchgrass of length 0.6 to 1 m which was chopped to 0.03 m [18]. Power consumed by the dual-roll hammer mill grinder was 180 kW (Pesco Inc., Hokins, MN, USA). 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 [18]. To produce 12 Mg of PHA per day, the grinder was required to process 708 Mg of switchgrass or approximately 30 Mg/h based on the process flow sheet made in Aspen Plus. The grinder size used in the modeling reflected this.

Gasification

The gasifier chosen for this techno-economic analysis was a bubbling fluidized bed reactor (BFBR). The BFBR was sized with assistance from Frontline Bioenergy (Ames, IA, USA). For a BFBR using 708 Mg/day of biomass, a bed area of approximately 41 m^2 was required. Assuming a cylindrical reactor the diameter of the bed was then 7.25 m, the

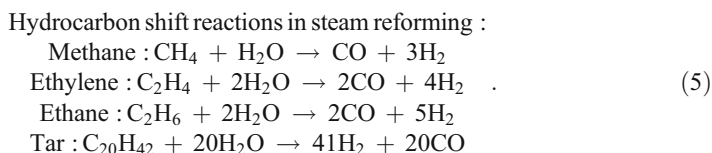
length of the reactor was assumed to be 10 m and the bed depth was 1 m. For costing purposes, the bed material was assumed to be 40 m³ of crushed limestone. In addition, the gasifier vessel was cost-estimated with a refractory brick lining of a 90% alumina firebrick backed by an insulating firebrick lining. Area of both linings was assumed to be 300 m². Operating temperature of the gasifier was 730 °C and the pressure was 2 bar. Gasifier mass balance and syngas composition were based on the experimental work of Lysenko [18].

Particulate Removal

For the purposes of hot gas cleanup, a particle size distribution of the char and ash exiting the gasifier was based on research done by Ritzert [21]. In the simulation, syngas exiting the gasifier was cleaned by two stages of cyclones followed by a fabric filter. The cyclones were modeled in Aspen Plus as high efficiency units using Leith–Licht correlations [24]. 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 m² 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 [20]. The total filter area was calculated to be 1,600 m² with a pressure drop of 250 N/m². The dust resistance coefficient used for this simulation was 60,000 Pa/[(kg/m²) (m/s)] based on a mean particle size of 55 µm in diameter [20]. Filter area for the bag house was estimated at 1,600 m² based on requirements given in the Aspen IPE software (Aspen Technologies) and volumetric flow rate of the syngas. Estimation of particulate removal efficiency was performed by the Aspen Plus software. The simulation results were below 10 mg/m³, which gave a char particle loading of 10 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.

Gas and Tar Reforming

For the Aspen Plus simulation, the tar was modeled as C₂₀H₄₂. High-temperature steam reforming was modeled as 100% conversion of all contaminants. The yield of H₂ and CO for light hydrocarbons and tar were based on the following stoichiometric reactions:



Three times the stoichiometric amount of steam was provided to the reformer [25], and the vessel operated at a temperature of 750 °C and a pressure of 1.5 bar [26]. Based on work reported in Spath et al. [22], 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 estimation purposes [15]. 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. The combustion of the syngas was modeled in a reactor block to give the effects of a furnace and provide the heat necessary for the gas reformer.

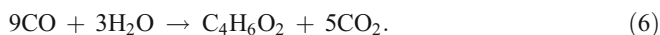
Heat Exchanger Network

In this simulation, four stages of heat exchangers 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. In the Aspen Plus software, the heat exchangers were modeled independent of detailed heat exchanger geometry. Only the desired cold stream outlet temperatures were specified from which the simulation software estimated heat exchanger areas. It was assumed that the overall heat transfer coefficient of first heat exchanger was 60 W/m² K for the first heat exchanger and 230 W/m² K for the remaining heat exchangers [20]. To find the cost of the exchangers, the data were 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.

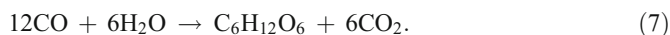
Bioreactors

The reactors were assumed to be enclosed, fully jacketed, and agitated tank reactors with a shell of 304 stainless steel [27] and a jacket of low carbon steel [28]. Design pressure and temperature were 3.45 bar and 125 °C, respectively. The actual operating temperature and pressure 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 makeup water entering the bioreactor at 20 °C and also to maintain the bioreactor at the necessary 25 °C.

In addition to modeling gas–liquid exchange in the bioreactors, the chemical reactions taking place inside them had to be simulated as well. The reactions were based on the metabolism of *R. rubrum*. Of the carbon monoxide anaerobically oxidized by the bacteria, 80% of it was assumed to be consumed in the biologically mediated water gas shift reaction shown in Eq. 1 [4]. The remaining 20% of the metabolized carbon monoxide was assumed to be incorporated into bacterial cell biomass, of which 40% was PHA [4]. For this analysis, the PHA was assumed to be poly-3-hydroxybutyrate (P3HB), with the repeating unit of C₄H₆O₂. The reaction to produce the repeating unit of P3HB is given by:



All non-PHA biomass was assumed to be dextrose (C₆H₁₂O₆), with a production reaction of:



In the PHA and dextrose reactions, only the energy needed to form the monomers was accounted for. Based on work by Do et al. [4], 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.

Hydrogen PSA

Separation and purification of H₂ (Fig. 1) was modeled as a pressure swing adsorption (PSA) unit [13]. 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) were taken directly from a previous analysis performed by Lysenko [18].

PHA Separation

Separating PHA from the bacterial cell is typically one of the most costly parts of production [28]. For this analysis, the methods of Choi and Lee [14] were adapted for a continuous process. Surfactant is first used to break down the cell wall, and then a solution of sodium hypochlorite further solubilizes the cell material. Centrifugation and washing steps are then used to separate the PHA granules from the remaining cell biomass and water solution. The *R. rubrum* simulated in this analysis had an optimal cell density of 0.19% total solids. This requires significant dehydration before the bacteria can be treated with the surfactant and hypochlorite solutions.

To dry the 95% pure PHA granules, a continuous spray drying system was used. 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].

Project Cost Estimation

After results for the mass and energy flows in the biorefinery were achieved, an analysis of the biorefinery economics was performed. Free-on-board (f.o.b.) equipment costs (C_P), labor costs to install the components (C_L), and the costs of the associated material used for the installation (C_M) were estimated for each of the major equipment components of the biorefinery.

The most of these costs were derived from Aspen IPE with one major exception. 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 [18]. All costs were adjusted to be in US dollars, year 2005 basis.

Co-Product Value

For accounting purposes, H_2 produced by the biorefinery was considered to be a co-product with a market value of \$2.00/kg based on the US Department of Energy's target price for hydrogen fuel [29]. The main product was assumed to be PHA, and the techno-economic analysis estimated the cost of this using all other inputs.

Material and Energy 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 [14] and adjusting for inflation so that the value would be in US dollars, year 2005 basis. The sodium hypochlorite solution cost, \$0.12/kg, was also from a previous study by Choi and Lee [14]. The surfactant solution was similarly determined to be \$1.85/kg in US dollars, year 2005 basis.

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 [30]. The cost of wastewater treatment was assumed to be \$0.0006/kg [31]. Both values were adjusted for inflation.

Labor Inputs

Operator labor input was assumed to be \$25/man-hour based on Lysenko's work [18]. The number of operators needed to run the biorefinery was based on equipment requirements presented in other studies [1, 31, 32]. For the baseline biorefinery, the number of operators was calculated to be 7.4 per shift.

Project Costs

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. Estimation of indirect costs for this analysis such as the taxes, insurance, and engineering expenses was done by assuming them to be a percentage of the direct project expenses (Table 3).

Operating Costs

The plant capacity factor (f_0) defines the percentage of each year that the plant operates and allows calculation of the annual hours of production. For this analysis, a plant capacity factor of 90% was used, which gave 7,889.4 h of annual operation assuming 365.25 days each year. Direct operating costs included raw material, energy, labor, laboratory, and patent, and royalties costs [1]. Indirect costs included expenses such as insurance, taxes, and administrative costs.

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

$$C_{OC} = C_{CC} + C_{CP} + C_{DE} + C_{IE}. \quad (8)$$

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

$$C_{PHA} = \frac{C_{OC}}{A_{PHA}}. \quad (9)$$

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:

$$C_{CO} = \frac{(C_{OC})_{\text{bioreactor}}}{A_{CO}} \quad (10)$$

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

Sensitivity Analysis

To evaluate the response of PHA cost to change in various process variables, a sensitivity analysis was 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 determined. Specifically, the switchgrass cost, H_2 market value, operating labor cost, and electricity cost were varied to check PHA cost sensitivity.

Results

Bioreactor Size Optimization

The minimum operating cost to solubilize CO in the syngas bioreactor was \$0.21 per kilogram of dissolved CO. The optimal condition occurs for a reactor of 14.8-m diameter stirred at a rate of 0.6 rps (Fig. 2A). This corresponds to a reactor volume of 2,500 m³, an electric power consumption of 2,100 kW to stir the tank, and a CO conversion of 94%. The bioreactor optimization was influenced mainly by three factors: CO solubilization, 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. Both capital charges and electricity costs increase with diameter. The CO solubilization efficiency approaches a maximum at the optimal diameter (Fig. 2B). A table summarizing the main results is available (Table 1).

Fig. 2 Bioreactor design optimization using a constant $k_L a$ value of 0.05 s^{-1} . **A** CO solubilization cost as a function of impeller speed and continuous stirred tank reactor (CSTR) diameter (ϕ Diameter). **B** Annual cost of electricity (filled circle), capital charge (empty circle), and CO solubilization efficiency (square, CSE) as a function of CSTR diameter. The optimal CSTR diameter was 14.8 m

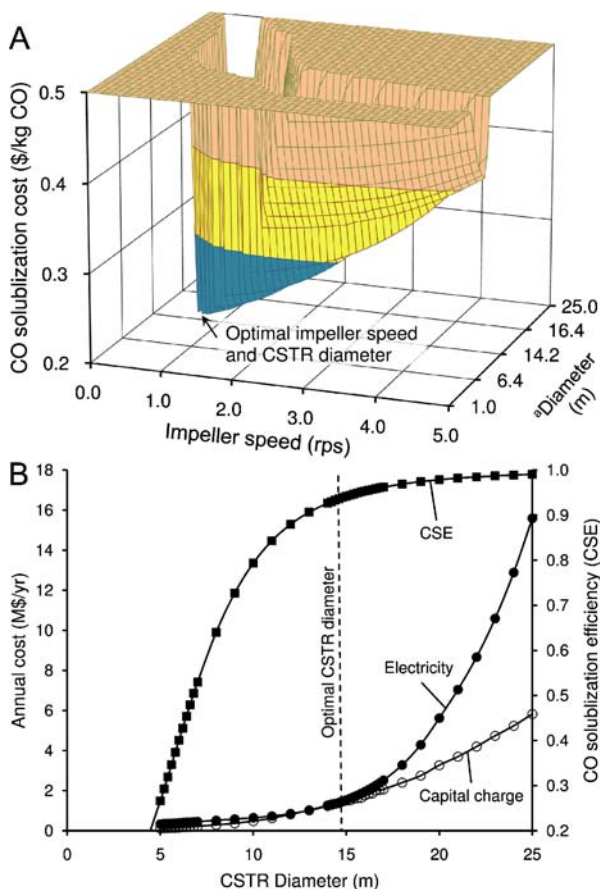


Table 1 Bioreactor design optimization results summary for a constant $k_L a$.

Volumetric mass transfer coefficient ($k_L a$, s^{-1})	0.05
Optimal reactor diameter (m)	14.8
Optimal stirring speed (rpm)	0.6
Agitator stirring power (kW)	2060
Total CO solubility efficiency (%)	94
Annual capital cost (\$/year)	1,477,536
Annual stirring cost (\$/year)	690,779
CO solubilization cost (\$/kg CO)	0.21

Material and Energy Flows

This techno-economic analysis was performed for a biorefinery producing 12 Mg/day of PHA. 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 was 95% pure PHA polymer. Other material and energy flows were also tabulated (Table 2). Electricity consumed by the biorefinery was estimated to be 5,900 kW and determined by using values given from the Aspen IPE software. Of this power, 2,500 kW was consumed by the blower providing air to the gasifier.

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

Table 2 Material and energy flows of the gasification-based hybrid biorefinery.

Inputs (kg/day)		Outputs (kg/day)	
Material			
Switchgrass	708,000	Syngas, post-filter	1,691,268
Surfactant	1,608	95% pure PHA	12,273
Hypochlorite solution	31,074	Hydrogen	49,138
Water		Spray dryer water vapor	31,909
Gas reformer	179,353	Wastewater	
Bioreactor make-up	678,174	Waste cooling water	2,000,000
Final syngas cooling	2,000,000	Centrifuge 2	666,478
PHA washing	253,388	Centrifuge 3	257,475
Total water	3,110,915	Total wastewater	2,923,953
		Char and ash	
		Cyclone stage 1	32,686
		Cyclone stage 2	1,576
		Candle filter	610
		Total char and ash	34,872
Energy			
Gas reformer energy (kW)	11,366	Bioreactor heat (kW)	53
Electricity (kW)	5,934	Syngas, LHV (kJ/kg)	4,368

Table 3 Project cost estimation for the gasification-based hybrid biorefinery.**GRASSROOTS CAPITAL ESTIMATION SUMMARY (US dollars, year 2005 basis)**

Direct project costs (C_D)	$C_D = C_P + C_M + C_L$	\$29,072,874
Equipment (f.o.b.) (C_P)	C_P from Icarus	\$23,224,640
Materials for installation (C_M)	C_M from Icarus	\$4,283,585
Direct labor (C_L)	C_L from Icarus	\$1,564,649
Indirect project costs (C_{ID})	$C_{ID} = C_{FIT} + C_O + C_E$	\$7,079,459
Freight, insurance, and taxes (C_{FIT})	$C_{FIT} = 0.08C_P$	\$1,857,971
Construction overhead (C_O)	$C_O = 0.70 C_L$	\$1,095,254
Engineering costs (C_E)	$C_E = 0.15(C_P + C_M)$	\$4,126,234
Other costs (C_{OT})	$C_{OT} = C_{CF} + C_{AF}$	\$19,305,346
Contingency and fee cost (C_{CF})	$C_{CF} = 0.18 (C_D + C_{ID})$	\$6,507,420
Auxiliary facilities cost (C_{AF})	$C_{AF} = 0.30 (C_{CF} + C_D + C_{ID})$	\$12,797,926
Grassroots capital cost (C_{GR})	$C_{GR} = C_D + C_{ID} + C_{OT}$	\$55,457,679

ANNUAL OPERATING COST (US dollars, year 2005 basis)

Annual capital charges (C_{CC})	$C_{CC} = (C_{TC}i(1+i)^n/[(1+i)^n - 1])$	\$7,360,863
Working capital cost (C_{WC})	$C_{WC} = 0.13C_{GR}$	\$7,209,498
Total capital cost (C_{TC})	$C_{TC} = C_{GR} + C_{WC}$	\$62,667,178
Direct operating costs (C_{DE})	$C_{DE} = C_R + C_{OL} + C_{SL} + C_{MR} + C_{OS} + C_{LE} + C_{PR}$	\$25,221,693
Raw material costs (C_R)		
Switchgrass		\$12,800,552
Water		\$1,190,083
Surfactant		\$922,452
Hypochlorite solution		\$1,188,750
Operating labor		\$1,534,488
Supervisory labor (C_{SL})	$C_{SL} = 0.15C_{OL}$	\$230,173
Utilities		
Electricity (major components)		\$1,989,646
Wastewater treatment		\$574,184
Maintenance and repairs (C_{MR})	$C_{MR} = 0.06C_{FC}$	\$3,327,461
Operating supplies (C_{OS})	$C_{OS} = 0.15C_{MR}$	\$499,119
Laboratory charges (C_{LE})	$C_{LE} = 0.15C_{OL}$	\$230,173
Patents and royalties cost (C_{PR})	$C_{PR} = 0.30 (C_R + C_{OL} + C_{SL} + C_{MR} + C_{OS} + C_{LE})$	\$734,612
Indirect operating costs (C_{IE})	$C_{IE} = C_{LT} + C_{IN} + C_{AE} + C_{DM} + C_{OH}$	\$6,397,143
Overhead cost (C_{OH})	$C_{OH} = 0.60 (C_{OL} + C_{SL} + C_{MR})$	\$3,055,273
Local taxes (C_{LT})	$C_{LT} = 0.015C_{FC}$	\$831,865
Insurance (C_{IN})	$C_{IN} = 0.007C_{FC}$	\$388,204
General costs		
Administration costs (C_{AE})	$C_{AE} = 0.15C_{OL}$	\$230,173
Distributing and marketing cost (C_{DM})	$C_{DM} = 0.075C_{DE}$	\$1,891,627
Annual by-product credit (C_{CP})		(\$32,305,490)
Annual biorefinery operating cost (C_{OC})	$C_{OC} = C_{CC} + C_{CP} + C_{DE} + C_{IE}$	\$6,674,210

determined to be 11 MW_t, meaning that the gas reformer requires a heat input to sustain its reactions. This heat duty requires 225 Mg/day of syngas.

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_t of heat, or 25 Mg/day of syngas.

Biorefinery Costs

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 3). 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 cost was \$43 million. Grassroots capital was estimated to be \$55 million.

The largest operating cost for the biorefinery was the switchgrass feed stock at \$12.8 million per year (Table 3). This was a significant portion of total direct operating costs, which were calculated to be \$25 million per year. Of the indirect operating expenses, the overhead was most significant at \$3.1 million per year. 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. Combined operating costs were \$39 million, but a credit for H₂ co-product reduced net operating costs to \$6.7 million.

Daily PHA production was 12 Mg/day. This biorefinery was assumed to operate at a 90% plant capacity factor. Therefore, annual PHA production was 4,000 Mg/year, resulting in product cost of \$1.65/kg. Table 4 summarizes the results for both mass flows and costs associated with the biorefinery.

Sensitivity Analysis

For the baseline analysis, the switchgrass was assumed to cost \$55/Mg delivered to the plant gate. The cost of producing PHA responded significantly to changes in the price of its feedstock. When the switchgrass cost was reduced to \$22/Mg, the PHA cost was reduced to −\$0.05/kg. When the switchgrass cost increased by 60% to \$88/Mg, the PHA cost increased by 115% beyond the baseline cost to \$3.56/kg (Fig. 3A, B).

Table 4 Summary of the main results of the gasification-based hybrid biorefinery study.

Hydrogen produced (Mg/year)	16,153
PHA produced (Mg/year)	4,043
Switchgrass consumed (Mg/year)	232,737
Water consumed (Mg/year)	1,022,636
Grassroots capital (\$)	\$55,457,679
By-products credit, H ₂ sale (\$/year)	(\$32,305,490)
Annual capital charges (\$/year)	\$7,360,863
Annual operating cost (\$/year)	\$6,674,210
PHA production cost (\$/kg)	\$1.65

Similar to feedstock costs, the cost of PHA also responded significantly to changes in the market value of H_2 . A baseline value of \$2.0/kg of H_2 produced was assumed. When this value was reduced to \$0.8/kg, the PHA cost was increased by 191% to \$6.46/kg. When H_2 production was increased in value to \$3.2/kg, the PHA cost decreased to −\$3.15/kg (Fig. 3A, C).

Compared to switchgrass cost and H_2 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 4.2% to \$1.58/kg. When

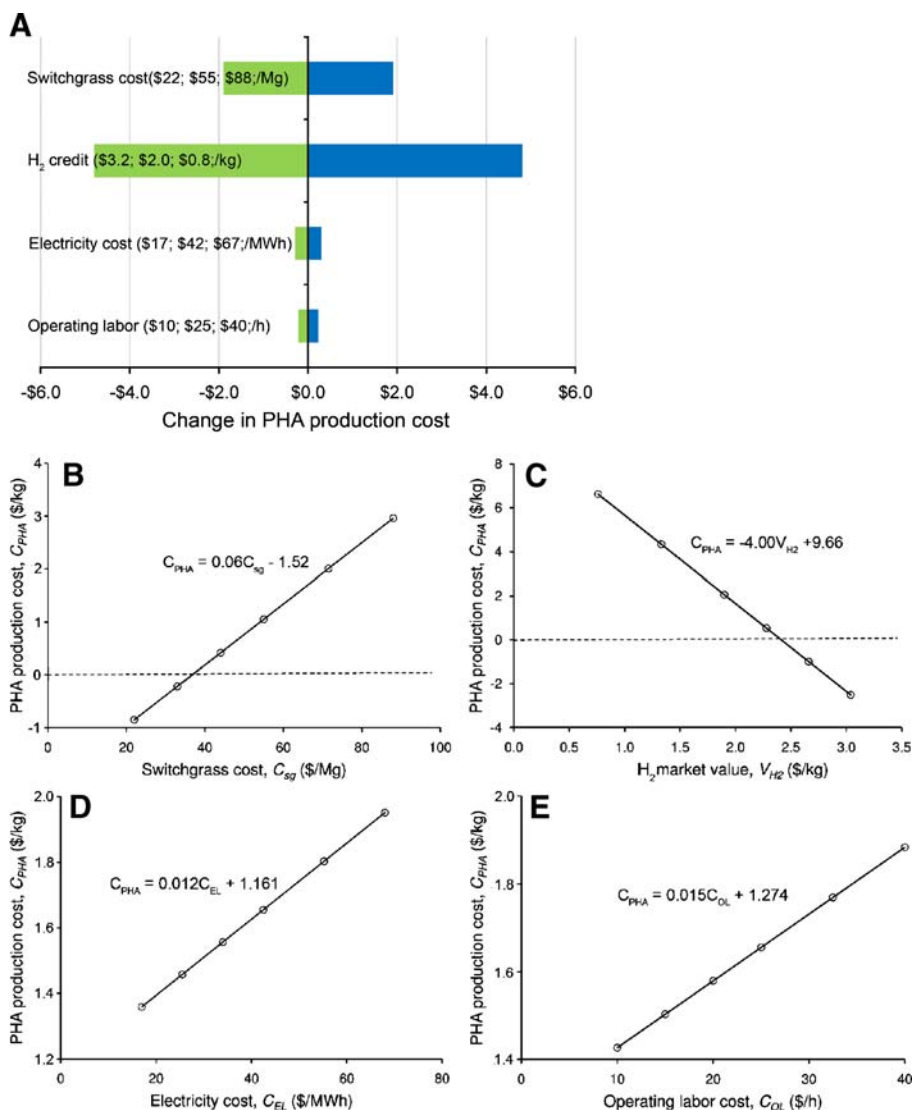


Fig. 3 Polyhydroxyalkanoate production cost (C_{PHA}) sensitivity analysis. Summary (A), PHA production cost changes in response to switchgrass cost (B), hydrogen market value (C), electricity cost (D), and operating labor cost (E)

operating labor was increased to \$30/man-hour, PHA cost increased to \$1.77/kg, a linear increase of 7.3% (Fig. 3A, D).

The cost of electricity also had minimal effect on the cost of PHA production. When the baseline cost of \$42.5/MWh was increased by 60% to \$68/MWh, the PHA cost increased by 18% to \$1.95/kg. When the electricity cost was decreased to \$25.50/MWh, PHA production cost was decreased to \$1.36/kg, a change of 12% (Fig. 3A, E).

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, which ranged from \$4 to \$6 per kilogram [14]. 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 would be fair because the market value, \$2.0/kg, given to H₂ reflects the most optimistic view of the DOE Hydrogen Posture Plan published in December 2006 which gave a H₂ cost goal of \$2 to \$3 per kilogram [29]. Hydrogen co-product value greater than \$2/kg would make this biorefinery even more attractive economically.

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