Feasibility Assessment of the Production of Bioethanol from Lignocellulosic Biomass Pretreated with Acid Mine Drainage (AMD)

Nicholas W. Burman, Craig Sheridan, Kevin G. Harding*

Industrial and Mining Water Research Unit; Centre in Water Research and Development;

School of Chemical and Metallurgical Engineering

All of the University of the Witwatersrand, Johannesburg, Private Bag 3, Wits, 2050, South Africa

*Kevin.Harding@wits.ac.za

Declaration of Interest: none

A techno-economic evaluation of a lignocellulosic bioethanol facility that uses acid mine drainage for the pre-treatment of weeping love grass (*Eragrostis curvula*) was performed. Both separate hydrolysis and fermentation (SHF) and simultaneous saccharification and fermentation (SSF) reactor configurations were evaluated. Results were compared to an evaluation of the same process with biomass pre-treated with dilute H_2SO_4. Capital and operating costs were estimated and a simple economic evaluation was conducted. It was found that all scenarios made a loss except for biomass pre-treated with H_2SO_4 in the SHF reactor configuration, although the high capital cost resulted in a payback period of 80.7 years, which is unfeasible. SHF was found to produce more ethanol at a lower capital cost than SSF, indicating that it is more economically feasible. Incorporating the remediation of AMD into a simultaneous process could help improve process economics. It is thus recommended that a techno-economic evaluation be conducted on a process that produces bioethanol through SHF and simultaneously remediates AMD.

Keywords: Lignocellulosic Bioethanol; Economic Evaluation; Acid Mine Drainage (AMD); Pre-treatment; Separate Hydrolysis and Fermentation (SHF); Simultaneous Saccharification and Fermentation (SSF)

1 Introduction

The Intergovernmental Panel on Climate Change has concluded in its 5th Assessment Report that the burning of fossil fuels is “extremely likely” to be the cause of recent increase in atmospheric and oceanic temperatures [1]. Although starch-based bioethanol has been demonstrated to be a renewable alternative to petrol [2], it has various drawbacks including (amongst others) an increase in food prices, net energy losses, a reduction of available land for food production and land degradation [3].

Lignocellulosic biomass (agricultural waste, forestry residue and energy crops) has been identified as a source of biomass that can potentially be used to produce bioethanol without these drawbacks in an environmentally friendly manner [4]. Lignocellulosic biomass consists of three fractions, cellulose fibrils (linearly linked glucose molecules) surrounded by a matrix of hemicellulose and lignin [5]. In the production of bioethanol, cellulose is hydrolyzed to glucose by cellulase enzymes. Glucose is then fermented to produce bioethanol [6].

Unfortunately, the presence of the lignocellulosic matrix prevents cellulase enzymes from accessing cellulose fibrils, hindering enzymatic hydrolysis. To overcome this the ligno-hemicellulosic matrix needs to be disrupted in a pre-treatment process. Various pre-treatment processes have been investigated including physical, chemical, biological and physico-chemical. Dilute H_2SO_4 pre-treatment has been found to be the most commercially favorable process [5,7–10].

Another drawback to enzymatic hydrolysis is that the glucose produced inhibits cellulase activity. This is most evident in the separate hydrolysis and fermentation (SHF) reactor configuration, in which enzymatic hydrolysis and fermentation occur in separate reactors. To overcome this various reactor configurations, which aim to maintain a low glucose concentration, have been investigated. These include; simultaneous saccharification and fermentation (SSF), in which enzymatic hydrolysis and fermentation occur simultaneously in the same reactor; simultaneous saccharification and co-fermentation (SSCF) in which enzymatic hydrolysis of cellulose, fermentation of glucose and co-fermentation of hemicellulose produced in pre-treatment all occur in the same reactor; and consolidated bioprocessing (CBP) in which enzyme production, enzymatic hydrolysis, and fermentation all occur in the same reactor, with a host of different micro-organisms.

Recently there have been investigations into the use of acid mine drainage (AMD) for the pre-treatment of lignocellulosic biomass [11,12]. The H^+ ions present in the AMD catalyzes the hydrolyzes of hemicellulose, releasing sugars into the AMD, similar to dilute H_2SO_4 pre-treatment.

AMD is formed through a series of geochemical reactions when sulfate-rich minerals are exposed to oxygen and water, often through mining activity [13]. It is highly acidic (pH 1-3) with high sulfate (<20 g/L) and heavy metal (<5 g/L) concentration [14]. AMD has been found to harm aquatic and riparian ecosystems due to the toxic effects of increased concentration of acid, sulfate and heavy metals, on aquatic life. As the pH rises through natural processes dissolved heavy metals precipitate on the ecosystem floor [15].

Recently, there has been a study that determined the optimal pre-treatment times for biomass pre-treated with AMD, as well as the rate of enzymatic hydrolysis, fermentation, and SSF of this optimally pre-treated biomass [16].

It has also been shown that the sugars present on AMD after pre-treatment can be used by sulfate-reducing bacteria (SRB) in a process known as dissimilatory sulfate reduction [11,17]. This process partially remediates the water through a reduction of sulfate and heavy metal concentrations and an increase in pH. Although various work has been done on the simultaneous production of ethanol and remediation of AMD [10–12,17–19], there has yet to be a techno-economic evaluation of any aspect of this process.

There have been various techno-economic evaluations performed on the production of bioethanol from lignocellulosic biomass [20]. Although all of these studies were based on enzymatic hydrolysis and fermentation of lignocellulosic biomass, different processes and feedstocks have been investigated. Feedstocks evaluated included corn stover [21–25], switchgrass [20,26,27], hardwoods and softwoods [20,26,28,29] and paper sludge [30]. There have been various pre-treatments evaluated including, dilute acid pre-treatment [20,21,25,26,28], ammonia fiber explosion (AFEX) [23,24,27] and hot water [29]. Different reactor configurations for the enzymatic hydrolysis and fermentation process have been evaluated, including SHF [21], SSF [30], CBP [23,27] and SSCF [23].

Most of these techno-economic studies have been performed using a variety of process simulation, flow sheeting and engineering software, *e.g.* Aspen Plus®, MS Excel, and Capcost. Typically, flowsheets and stream tables are first developed, after which they are used to provide estimates of operating and capital costs which are used in a techno-economic evaluation of the process.

The study presented here investigated the production of bioethanol from *Eragrostis curvula* (Weeping lovegrass), pre-treated with AMD, and for comparison, pre-treated with H_2SO_4. Both SHF and SSF reactor configurations were investigated. The AMD remediation process is not investigated in this study.

The objectives of this study are to: develop process flow sheets for all scenarios; estimate the operating costs of the process; estimate the capital costs of the process, and; determine the economic feasibility through economic evaluation.

2 Methods

2.1 Process flowsheet development

2.1.1 Simulation Basis

The simulation was carried out using Aspen Plus® V8.4 (www.aspentech.com), with a basis of 90 ton/hr of milled (4mm) dry *Eragrostis curvula* (weeping lovegrass) grass with a composition of 37% cellulose, 29% xylan (hemicellulose), 19% acid-insoluble lignin, 6% acid-soluble lignin, 6% ash, and 3% protein [16].

Separate simulations were developed for both SHF and SSF, with pretreatment using AMD, and for comparison, H_2SO_4. There were thus four scenarios considered, *i.e.* AMD pre-treatment with SHF (A-SHF), H_2SO_4 pre-treatment with SHF (H-SHF), AMD pre-treatment with SSF(A-SSF), and H_2SO_4 pre-treatment with SSF (H-SSF).

The model made use of the NREL database for chemical compounds and structural components in lignocellulosic biomass that were used in the DW1102A Aspen Plus® simulation [21]. This study made use of the NRTL equations of state for modeling of vapor-liquid equilibrium.

2.1.2 Process description

The process consists of three sections: pre-treatment (Figure 1), hydrolysis and fermentation (either SHF (Figure 2) or SSF (Figure 3)) and product separation (Figure 4).

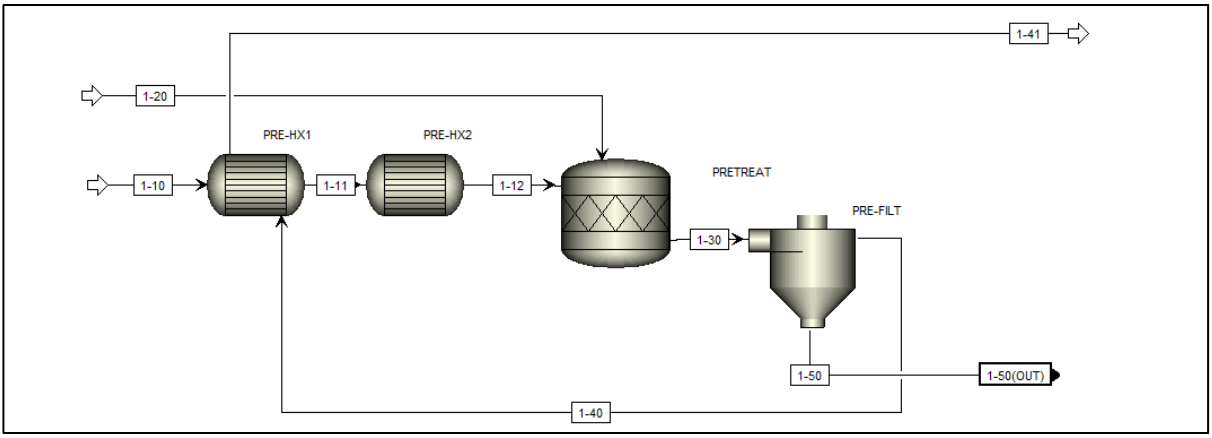

Figure 1: Layout of the pre-treatment section used in the Aspen Plus® simulation

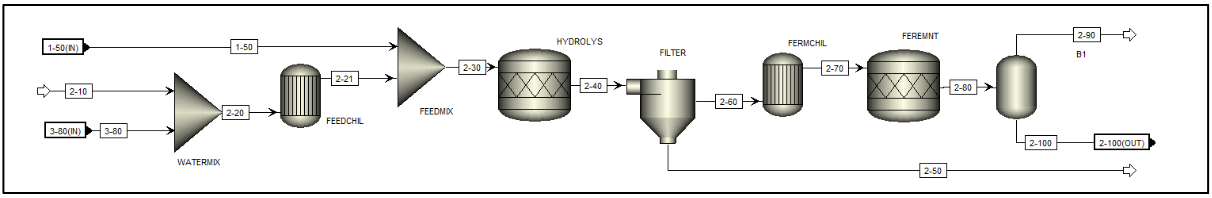

Figure 2: Layout of the SHF section used in the Aspen Plus® simulation

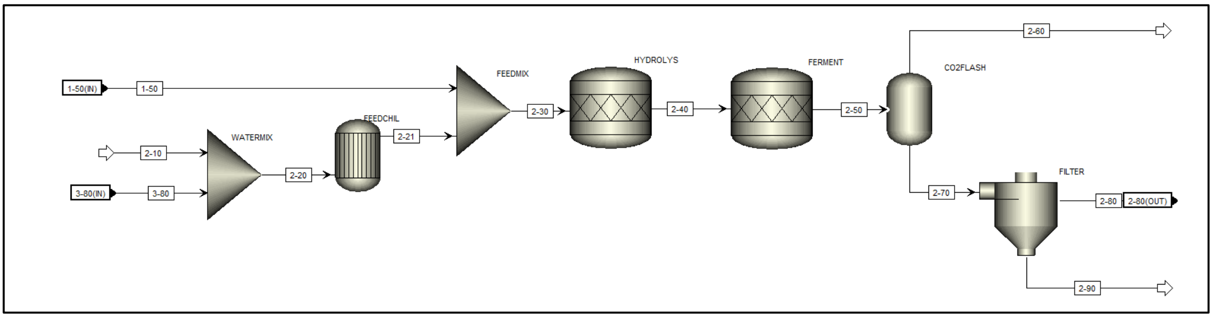

Figure 3: Layout of the SSF section used in the Aspen Plus® simulation

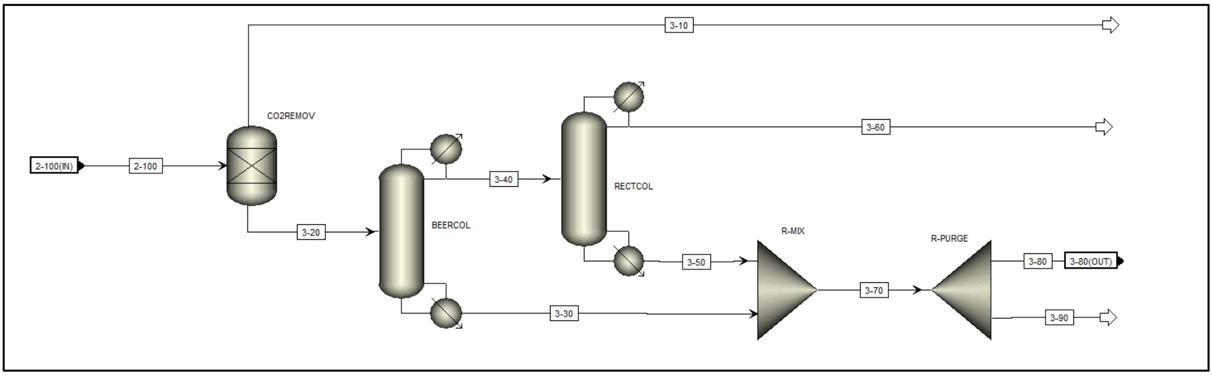

Figure 4: Layout of the product separation section used in the Aspen Plus® simulation

2.1.2.1 Pre-treatment

In the pre-treatment section, grass is fed into a semi-batch reactor (PRETREAT) where it undergoes pre-treatment by either AMD or H_2SO_4 which has been heated to 90°C (PRE-HX1 & PRE-HX2). Note: AMD and H_2SO_4 are not used in the same process but in different scenarios for comparison. In pre-treatment, xylan is hydrolyzed to xylose, breaking up the ligno-hemicellulosic structure, making cellulose more susceptible to enzymatic hydrolysis. This was represented in Aspen Plus® through the hydrolysis of xylan ($C_5H_8O_4$) to xylose ($C_5H_{10}O_5$). The pre-treated biomass is separated from the liquid (PREFILT) and sent to the hydrolysis and fermentation section. AMD or H_2SO_4 flow through the grass in the reactor continuously, while the grass is replenished at various intervals. Multiple pretreatment reactors are thus required to allow for the continuous operation of the process during loading/ removal of grass. The liquid product is first used to heat the incoming liquid stream before going to further treatment/ disposal (not considered in this study).

The flowrate of AMD/H_2SO_4 was estimated assuming that the ratio of biomass: AMD/H_2SO_4 consumed by the process was 0.2 as determined as optimal by a previous study [16]. The volume of pure H_2SO_4 that was required was then calculated assuming a 0.5% wt/wt H_2SO_4 concentration. A summary of the blocks used in the simulation and their specifications is given in Table 1.

2.1.2.2 SHF

In SHF, pre-treated biomass is fed into the batch hydrolysis the reactor (HYDROLYS) which is operated at 50°C. Make up water and water recycled from product separation section and cooled to 50°C, is fed into this reactor, along with cellulase enzymes, to achieve a solid loading of 20 wt% biomass. Cellulase enzymes catalyze the hydrolysis of cellulose to glucose. After hydrolysis is complete, the liquid fraction of the product stream is separated from the solid fraction (FILTER), cooled to 35°C (FERMCHIL) and fed into the fermenter (FERMENT). An inoculum of *Saccharomyces cerevisiae* is fed into the fermenter. *Saccharomyces cerevisiae* facilitates the conversion of glucose to ethanol and CO_2. Gas-phase CO_2 produced in fermentation will leave the top of the fermenter. Solid biomass is then separated from the liquid product stream (FILTER) which goes to the product separation section.

A summary of the blocks used in the simulation and their specifications is given in Table 1.

2.1.2.3 SSF

In SSF, pre-treated biomass is fed into the batch SSF reactor which is operated at 38°C. Make-up water and water recycled from the product separation section are blended and cooled to 38°C before passing into the SSF reactor, together with cellulase enzymes and *Saccharomyces cerevisiae*, to achieve a biomass solid loading of 20 wt%. In this reactor, there is the simultaneous hydrolysis of cellulose to glucose and fermentation of glucose to ethanol. Gas-phase CO_2 produced in fermentation will leave the top of the fermenter. Solid biomass is then separated from the liquid product stream (FILTER) which goes to the product separation section.

A summary of the blocks used in the simulation and their specifications is given in Table 1.

2.1.2.4 Product separation

The product separation section consists of two distillation columns. In the 1st distillation column (BEERCOL) the distillate stream contains 40% ethanol, with a 95% recovery of ethanol to the distillate. The second column (RECTCOL) produces a distillate of 90% ethanol with a recovery of 95% ethanol to the distillate. The bottoms stream from both columns is recycled/ purged as necessary.

A summary of the blocks used in the simulation and their specifications is given in Table 1.

2.1.3 Simulation specifications

All reactors were modeled using an RSTOICH block with conversions determined in previous experiments [16]. In SSF the hydrolysis and fermentation sections were modeled using separate blocks for hydrolysis (HDROLYSIS) and fermentation (FERMNET) although this process would occur in one reactor. This was done to increase model understanding and troubleshooting capabilities and is valid as the hydrolysis and fermentation reactions would have occurred in series anyway if they were in the same RSTOICH block. In both SHF and SSF a FLASH block (CO2FLASH) has been included after the FERMENT block to model the gas-liquid equilibrium of CO_2 and ethanol entering the product separation section.

Liquid streams entering/exiting reactors were heated/cooled to appropriate temperatures, by heat exchangers modeled by the HX block (2 stream heat exchanger) or HEATER block (heat exchanger with a utility) as required. The solid-liquid separation was modeled using SSPLIT block. Distillation columns were modeled with DSTWU block, which uses the Winn-Underwood-Gilliland shortcut method to model distillation columns based on the assumptions of constant relative volatilities and constant molar overflow.

The presence of CO_2 made the modeling of distillation with DSTWU blocks technically difficult, and hence it was assumed that there was no CO_2 present. This was accomplished by the incorporation of a SEP block (CO2REMOV) prior to distillation.

A summary of all block design specifications is presented in Table 1. A summary of the design specifications that were manipulated by Aspen Plus® is presented in Table 2.

Table 1: Summary of block specifications used in Aspen Plus® simulations

	Block Name	Block Type	Specification
Pre-treatment	FEEDCHILL	HEATER	$T_{hot, out}$ = 50°C
	PRE- HX1	HX	$T_{hot, out}$ = 30°C
	PRE- HX2	HEATER	$T_{cold, out}$ = 90°C
	PRETREAT	RSTOICH	RX1: Xylan → Xylose =0.5
	PREFILT	SSPLIT	1-50 = 100% solids 1-41 = 90 % liquid

SHF	HYDROLYSIS	RSTOICH	Time = 168 Hrs RX1: Cellulose → Glucose
	FILTER	SSPLIT	2-50 = 100% solid 2-60= 95% liquids
	FERMCHILL	HEATER	$T_{cold, out}$ = 35°C
	FERMENT	RSTOICH	RX1: Glucose → 2CO2 + 2 EtOH X=0.90
	B1	FLASH	T=35°C
SSF	FEEDCHILL	HEATER	$T_{hot, out}$ = 38
	HYDROLYSIS	RSTOICH	time = 168 Hrs RX1: Cellulose → Glucose
	FERMENT	RSTOICH	RX1: Glucose → 2CO2 + 2 EtOH X=0.90
	CO2FLASH	FLASH	$T_{cold, out}$ = 38°C
	FILTER	SSPLIT	2-90 = 100% solid 2-80= 95% liquids
SEP	CO2REMOV	SEP	3-10 = 100% CO2
	BEERCOL	DSTWU	RRATIO = 1.1 times minimum
	RECTCOL	DSTWU	RRATIO = 1.1 times minimum

Table 2: Summary of design specifications used in Aspen Plus® simulation

Design Specification	**Specification**	**Adjusted variable**
DS1	Reaction time = 168 hrs	Glucose conversion in HYDROLYS block
DS2	40% ethanol in BEERCOL distillate	Recovery of water to RECTCOL distillate
DS3	90% ethanol in RECTCOL distillate	Recovery of water RECTCOL to distillate
DS4	Flow rate of water in reactor feed = 20000 kg/hr	Flow rate of make-up water to FEEDMIX

In hydrolysis, the conversion of cellulose to glucose, and conversion of glucose to ethanol, was modeled using kinetics determined in a previous study [16] (Table 3). The conversion of cellulose to glucose was varied using a design specification on the total reaction time.

Table 3: Summary of empirical equations

Reaction	**Equation**	
SHF Hydrolysis	$G = (m_{1,M}W + C_{1,M})ln(t) + (m_{1,C}W + C_{1,C})$	
SHF Fermentation	$G = G_0 - r_g \times t_f$	$for\ t_f \in 0{:}6\ hr$
	$G = G_0 - r_{lg} \times 6 - r_s \times (t_f - 6)$	$for\ t_f \in 6{:}12\ hr$
SSF	$E = (m_{2,M}W + C_{2,M})ln(t) + (m_{2,C}ln(W) + C_{2,C})$	

Where G is the glucose concentration (g/L), W is the solid loading fraction of biomass (wt%) t_h, t_f, t_{ssf} are the hydrolysis, fermentation and SSF time respectively (hrs), G_0 is the initial glucose concentration at the start of fermentation (g/L), r_g and r_s are the rates of fermentation in different phases of fermentation (g/L/hr), E is the ethanol concentration in SSF (g/L), and $m_{i,j}$ and $c_{i,j}$ are empirically determined constants [16] .

Pre-treatment time required for AMD pre-treatment (3 days) and H_2SO_4 pre-treatment (1 day) was based on previous studies [16].

2.2 Operating Costs

Estimation of operating costs was performed using the Aspen Plus® inbuilt utility and operating cost tools. This was done by defining three utilities and then assigning them to certain operating blocks. The three utilities that were defined are low-pressure steam, cooling water and refrigerated water (Table 4). Low-pressure steam, cooling water, and refrigerated water were chosen as they are suitable for the heating of incoming AMD/H_2SO_4, the condensation of distillate streams, and the cooling of hydrolysate from the hydrolysis reactor (50°C) before it enters the fermenter (35°C), respectively.

The cost of the utilities was estimated based on the method of Ulrich and Vasudevan (2006), assuming that steam was produced in a natural gas boiler and the electricity used in the production of cooling and refrigeration water was produced in a coal-based power plant. The cost of fuel was assumed to be 3.57 USD/GJ for natural gas and 0.95 USD/GJ for coal[32].

Table 4: Summary of the utilities used in the Aspen Plus® process simulation

	Low-pressure steam	**Cooling water**	**Refrigerated water**
Cost (USD/GJ)	6.15	1.06	5.08
Tin	125	30	20
Tout	124	45	30
Enthalpy change kJ/kg	2191	62.59	41.74
Used at	All reboilers	All condensers, FEEDCHILL (SHF)	FERMCHILL (SHF) FEEDCHILL (SSF)
Pressure (atm)	2.29	1	1
Vapor fraction inlet/ outlet	1/0	0/0	0/0

The DSTWU block does not allow for the allocation of utilities. The utility requirements were thus calculated manually and added to utilities calculated in Aspen Plus®.

The cost of the grass was taken to 35 USD/ton, as this represents the lowest feedstock cost found in literature. This was based investigation into the market value of the feedstock.

Due to the lack of physical property data enzyme were not included in the Aspen Plus® simulation, however, the cost of enzyme was taken into account. It was assumed enzyme was dosed at 0.20 mg/g pre-treated biomass based on previous studies [33]. It was assumed that the cost of enzyme was (1.25 USD/kg enzyme). This is once again the cheapest enzyme cost found in literature [34]. The cost of H_2SO_4 was taken to be 80 USD/ton [35].

The market value of the product was taken to be 815.00 USD/ton [2]

2.3 Capital Costs

The size of all heat exchangers, columns and pumps were taken from the Aspen Plus® simulation. Fortran script was written in calculator blocks to evaluate the volumes of all reactors (PRETREAT, HYDROLYSIS, FERMENT) based on the process flow rates and kinetics of reactions determined previously [16] (Table 3). All equations used for the determination of reactor volumes are presented in the supplementary data.

An estimation of the capital costs for individual process units was performed using the Capcost2017 Program (www.richardturton.faculty.wvu.edu). A summary of the equipment accounted for and its estimated cost is presented in the supplementary data. The cost of the (hydrolysis, fermentation, and pre-treatment reactors) was estimated using prices from the NREL 2011 [21] design report adjusted to 2017 prices using the Chemical Engineering Price Cost Index (CEPCI). Due to the PRETREAT reactor having similar solid loading, batch time and temperatures to the HYDROLYSIS reactor, it was assumed that the price per volume of these reactors would be the same. The total installed capital cost was estimated from the total equipment cost using the Lang factor method with a Lang factor of 4.74 [36].

2.4 Economic Evaluation

A simple economic evaluation in which the non-discounted payback period was determined for the process based on the estimated capital costs and annual profit. This evaluation only considered the operating costs mentioned in the operating costs section but did not consider other operating costs such as salaries or tax.

3 Results and Discussion

3.1 Process flow sheet

A full stream table of all streams can be found in the supplementary data.

The feedstock requirements for scenarios with the same pre-treatment are the same (Table 5). This is due to all scenarios have the same basis (90 tons/hr grass) as well as having the same mass balance around the pre-treatment process section, resulting in the same quantity of biomass entering the hydrolysis and fermentation section and hence the same enzyme usage. Scenarios that use H_2SO_4 pre-treatment also require H_2SO_4.

Table 5: Summary of the raw material costs

Raw material	unit value	H_2SO_4 Pre-treatment		AMD pre-treatment	
	USD/kg	ton/yr	MUSD/yr	ton/yr	MUSD/yr
Grass	0.035	750 000	25.5	750 000	25.5
Enzyme	1.25	5 500	6.93	5500	6.93
H_2SO_4	0.08	18 000	1.50	0	0
Total			33.9		32.4

The amount of ethanol produced in different scenarios varied substantially ranging from 38 000 to 60 000 ton/year (Table 6). Scenarios with H_2SO_4 pre-treatment produced more ethanol than the scenarios with AMD pre-treatment. The scenarios with SHF reactor configuration produced more ethanol than the scenarios with SSF reactor configuration. The higher final ethanol volumes (in SHF compared to SSF and H_2SO_4 compared to AMD) are due to higher concentrations of ethanol achieved in fermentation. This reflects the experimental results on which the reaction models used in this study are based (Table 3) [16].

Table 6: Summary of ethanol yield, volume produced and revenue from sales for different scenarios.

Scenario*	Ethanol Yield L/dry ton	Ethanol Volume ton/Year	Revenue MUSD/yr
A-SHF	58.4	44 000	35.7
H-SHF	80.7	60 000	49.3
A-SSF	50.3	38 000	30.7
H-SSF	53.7	40 000	32.8

* A = AMD; H = H_2SO_4

The ethanol yield ranged from 58.4 – 80.7 L/dry ton. This is low in comparison to other techno-economic evaluations that report yields of up to 341 L/dry ton [37]. One explanation of the comparatively low yield is that other studies are fermenting both C5 and C6 sugars [21], whereas in this study the C5 sugars are required as a carbon source for the SRB. Another explanation is that the yields in this study are based on experiments that were conducted without access to tailored cellulase mixtures, advanced bioreactors or genetically modified fermentative organisms [16].

The heating and cooling duty vary with each scenario from 2 340 to 2 830 TJ/yr (Table 7). Total duties required are higher for H_2SO_4 pre-treatment than AMD pre-treatment and higher for SHF reactor configuration than SSF reactor configuration. The variation in the heating/cooling duties can mainly be attributed to the different reflux/reboiler requirements in each scenario.

Table 7: Summary of utility duties and utility costs for different scenarios.

Scenario*	Utility Duty TJ/yr	Utility Cost MUSD/yr
A-SHF	2 690	11.4

H-SHF	2 830	11.9
A-SSF	2 340	9.06
H-SSF	2 360	9.13

* A = AMD; H = H2SO4

3.2 Operating costs and revenue

As can be seen in Table 5 the feedstock costs are the same for scenarios with the same pre-treatments (*i.e.* A-SHF & A-SSF; H-SHF & H-SSF). Scenarios with AMD pre-treatment do not require H_2SO_4 and hence have a lower raw material cost. Although there are many other feedstocks, only grass, cellulase enzyme, and H_2SO_4 were accounted for as these are considered to be the most significant costs.

The variation in ethanol revenue (30.7 MUSD/yr – 49.3 MUSD/yr) follows the same trends as the variation in ethanol produced (Table 6).

The trends in the utility costs follow the trend in utility duty (Table 7), with H-SHF (11.9 MUSD/yr) being the highest, followed by A-SHF (11.4 MUSD/yr) followed by H-SSF (9.13 MUSD/yr) and lastly A-SSF (9.06 MUSD/yr).

For all scenarios except for H-SHF, the operating costs are higher than the revenue and hence not profitable (Figure 5). This is mainly due to low ethanol yield and hence revenue. Although scenario H-SHF makes a profit, it is small (3.5 MUSD/yr). Considering that this evaluation assumes the cheapest raw material costs, favorable ethanol price, and ignores various other operating costs (salaries, tax, *etc.*), it is extremely unlikely that this scenario is feasible. The low revenue achieved in each scenario is due to the product yields achieved in hydrolysis and fermentation.

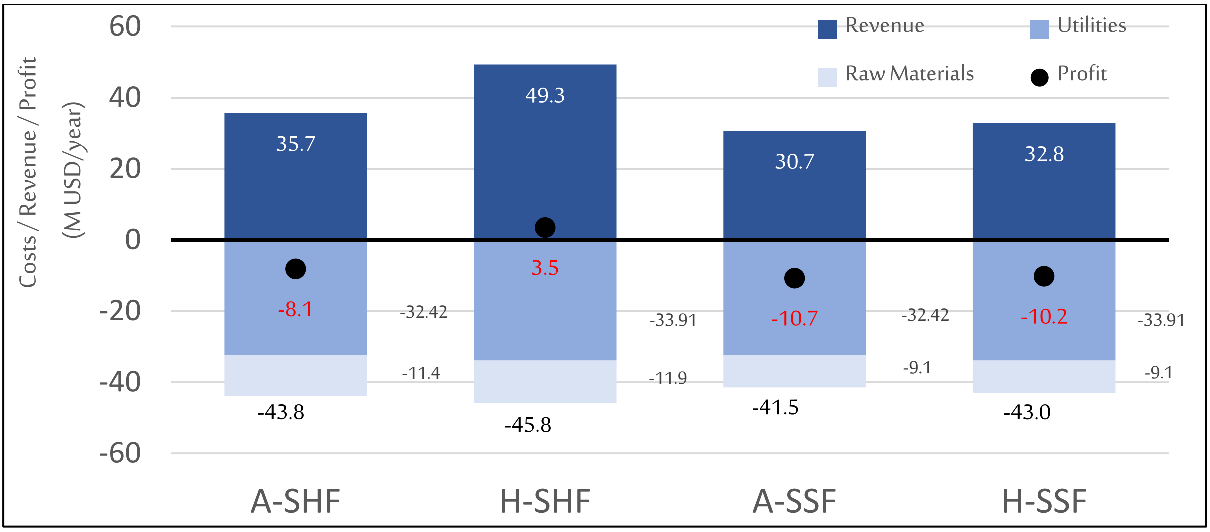

Figure 5: Summary of operating costs, revenue, and profit for different scenarios (A = AMD; H = H_2SO_4)

3.3 Capital Costs

A summary of the estimated capital costs for different scenarios is presented in Figure 6.

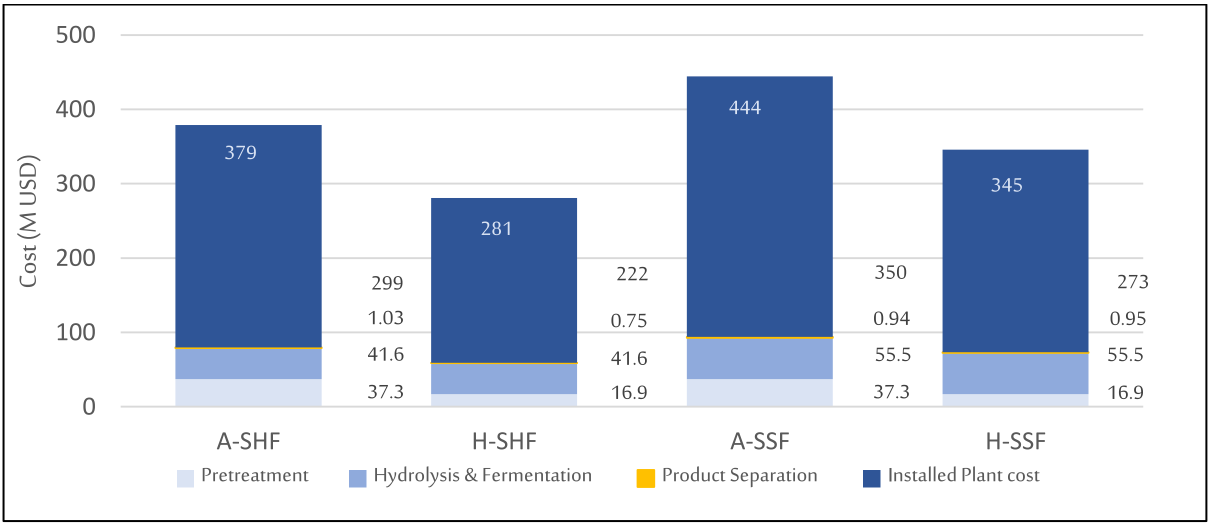

Figure 6: Summary of the capital costs for each processes section, and installed plant cost (accounting for purchase and installation all major and ancillary equipment) for the different scenarios (A = AMD; H = H_2SO_4)

As can be seen in Figure 6 (Table 8) the capital cost for the product separation section is substantially less than the capital cost for pre-treatment and hydrolysis and fermentation sections. The large capital cost of the pre-treatment and hydrolysis and fermentation sections is due to the large reactor volumes required for both pre-treatment and hydrolysis. The capital cost for pre-treatment is approximately the same for scenarios with the same type of pre-treatment *i.e.* AMD or H_2SO_4. The capital cost for hydrolysis and fermentation is approximately the same for scenarios with the same hydrolysis and fermentation configuration *i.e.* SSF or SHF.

The capital cost for scenarios with H_2SO_4 pre-treatment was found to be lower than scenarios with AMD pre-treatment. This can be attributed to a lower capital cost of the pre-treatment area, for scenarios with H_2SO_4 pretreatment, compared with scenarios with AMD pre-treatment. Scenarios with H_2SO_4 pre-treatment have a shorter pre-treatment time (1 day) than scenarios with AMD pretreatment (3.5 days), to achieve the desired level of pre-treatment. The shorter pre-treatment time results in smaller pre-treatment reactor volumes, which are less expensive.

The capital cost for scenarios with SHF was found to be lower than scenarios with SSF. This is due to the hydrolysis reactor having a simpler design, and hence less expensive, than the SHF reactor. Although the SHF scenarios require an additional fermentation reactor, the cost of this is small in comparison to the hydrolysis and SHF reactors due to a significantly shorter batch time, and hence volume.

The installed plant cost (including capital cost, transportation, and installation of the entire process) was estimated using the Lang Factor method. This method assumes that the total installed plant cost can be estimated by multiplying the capital cost of the major process units by a Lang factor. This is inclusive of the capital cost of all major and ancillary equipment (piping, electrical, control, *etc.*); transportation and installation of major and ancillary equipment; required civil works; and engineering services. A Lang factor of 4.74 was assumed for this study [36]. The total installed plat cost ranges from 281 MUSD to 444MUSD.

A previous techno-economic evaluation [21] determined a total installed plant cost of 232 MUSD, which is the same order of magnitude. The study by Humbird *et al*. (2011) [21] included various process sections such as enzyme production and wastewater remediation that were not included in this evaluation. The total installed plant cost determined in this evaluation is thus significantly higher, even if compared to an inflation-adjusted value. This high installed plant cost can be attributed to the large reactor volumes required for both pre-treatment and hydrolysis, resulting in a large capital cost for these sections.

3.4 Economic Evaluation

Table 8: Summary of operating costs, capital cost and payback period

Scenario Name*	Capital Cost MUSD	Operating Cost MUSD/yr	Revenue MUSD/yr	Profit MUSD/yr	Payback Period yr
A-SHF	378.8	43.83	35.69	-8.14	-
H-SHF	281.0	45.82	49.30	3.48	80.7
A-SSF	444.1	41.47	30.72	-10.75	-
H-SSF	345.3	43.04	32.83	-10.21	-

* A = AMD; H = H_2SO_4

The payback period was only calculated for scenario H-SHF, as this was the only scenario that makes a profit (Table 8).

The payback period for Scenario H-SHF is extremely long (80.7 years), indicating that this process is not economically feasible. Considering that this evaluation assumed favorable economic conditions and did not take into account various operating costs (tax, salaries) this scenario would be of even less feasibility. The major issue making this process unfeasible is the low yield of ethanol from feedstock. This results in a low revenue as well as a high capital cost as the enzymatic hydrolysis time has been extended to try to achieve higher product yield.

To reduce the capital cost and hence payback period all scenarios were analyzed using a hydrolysis/ SSF reaction time of 84 hours as opposed to 168 hours. This resulted in a slightly lower volume of ethanol produced, and a significantly lower capital cost for the hydrolysis and fermentation section. Although this reduces the capital cost for all scenarios, the decreased ethanol production, and hence revenue, resulted in all scenarios, including H-SHF making a loss.

Although this evaluation indicates that all scenarios are currently unfeasible, some insightful observations can be made. The SHF reactor configuration is significantly cheaper and produces more ethanol than the SSF configurations. This is true for both pre-treatment with AMD and pre-treatment with H_2SO_4. The SHF reactor configuration also allows for the production of various products through different biochemical transformations of the glucose intermediary. The production of small quantities of high-value chemicals, in addition to large quantities of biofuels, can contribute towards the economic feasibility of a process [12]. It is thus recommended that all future studies into the production of bioethanol using AMD pre-treated biomass should focus on the SHF reactor configuration.

Incorporating the process of bioethanol production into a process that simultaneously remediates AMD could also improve its feasibility. After pre-treatment AMD contains xylose released during pre-treatment, which could be utilized as a carbon source for sulfate-reducing bacteria to remediate the AMD. The integration of the two processes would be financially beneficial to both as the cost of pre-treatment of the biomass could be shared with both processes. As the remediation of AMD already has a cost associated with it, any savings on this could be attributed as a profit stream for the integrated process. It is thus recommended that a techno-economic evaluation of this envisioned integrated bio-ethanol production/AMD remediation process be conducted.

As the product yield was found to be low, it is recommended that further experimental work be carried to determine the optimal conditions of enzymatic hydrolysis in the SHF configuration. Tailored enzyme mixtures should be investigated in conjunction with hydrolysis operating conditions such as temperature, pH and mixing.

4 Conclusion

This techno-economic evaluation found scenarios A-SHF, A-SSF and H-SHF to be unprofitable, while scenario H-SHF was only marginally profitable (3.5 MUSD/year). Although the H-SHF scenario was profitable, the payback period calculated was too long to be feasible (80.5 years). Although all scenarios are unfeasible SHF was shown to be more favorable than SSF.

Due to a lack of previous quantitative research, this study was limited to data from only one previous study, which was both feedstock (Weeping lovegrass) and product (ethanol) specific and resulted in a low product yield (58.4 – 80.7 L/dry ton) [16]. The low product yield decreased the feasibility of the process, especially considering that ethanol is a low value biochemical.

Optimization of enzymatic hydrolysis, through improved enzymes and operating conditions, could substantially increase product yield and improve the economic feasibility of the process. The economic feasibility could also be substantially improved if it were to be coupled with an AMD remediation process. AMD remediation has a cost associated with its so any savings could be considered as a source of income.

Although this process is not currently feasible, further research and process development are encouraged. This process has the potential to produce environmentally friendly alternatives to fossil fuel products, while simultaneously remediating AMD. This could be highly beneficial for a developing country such as South Africa, as it will help protect the environment and increase both energy and water security without impacting food production.

5 Acknowledgments

This work is based on research supported in part by the National Research Foundation of South Africa (Grant Numbers: 111864). The support of the University of the Witwatersrand, Johannesburg is also acknowledged.

6 References

[1] IPCC, Climate Change 2014: Contribution of Working Groups I, II and III to the Fifth Assessment Report of the Intergovernmental Panel on Climate Change, in: Core Writing Team, R.K. Pachauri, L.A. Meyer (Eds.), IPCC, Geneva, Switzerland, 2014: p. 151.

[2] E4TECH, RE-CORD, WUR, From the Sugar Platform to biofuels and biochemicals, 2015. doi:contract No. ENER/C2/423-2012/SI2.673791.

[3] J. Lange, Lignocellulose conversion : an introduction to chemistry , Biofuels, Bioprod. Biorefining. 1 (2007) 39–48. doi:10.1002/bbb.

[4] E. Searcy, P.C. Flynn, Processing of Straw / Corn Stover : Comparison of Life Cycle Emissions, Int. J. Green Energy. 5 (2008) 423–437. doi:10.1080/15435070802498010.

[5] N. Mosier, C. Wyman, B. Dale, R. Elander, Y.Y. Lee, M. Holtzapple, M. Ladisch, Features of promising technologies for pretreatment of lignocellulosic biomass, Bioresour. Technol. 96 (2005) 673–686. doi:10.1016/j.biortech.2004.06.025.

[6] Z. Yu, H. Zhang, Ethanol fermentation of acid-hydrolyzed cellulosic pyrolysate with Saccharomyces cerevisiae, Bioresour. Technol. 90 (2003) 95–100. doi:10.1016/S0960-8524(03)00093-2.

[7] P. Alvira, E. Tomas-Pejo, M. Ballesteros, M.J. Negro, Pretreatment technologies for an efficient bioethanol production process based on enzymatic hydrolysis: A review, Bioresour. Technol. 101 (2010) 4851–4861. doi:10.1016/j.biortech.2009.11.093.

[8] D.P. Maurya, A. Singla, S. Negi, An overview of key pretreatment processes for biological conversion of lignocellulosic biomass to bioethanol, 3 Biotech. 5 (2015) 597–609. doi:10.1007/s13205-015-0279-4.

[9] M.J. Taherzadeh, K. Karimi, Pretreatment of lignocellulosic wastes to improve ethanol and biogas production: A review, Int. J. Mol. Sci. 9 (2008) 1621–1651. doi:10.3390/ijms9091621.

[10] N.W. Burman, C. Sheridan, L. van Dyk, K.G. Harding, Modelling of low temperature dilute sulfuric acid pre-treatment of South African grass, Bioresour. Technol. Reports. 4 (2018) 21–28. doi:10.1016/j.biteb.2018.08.014.

[11] E. Magowo, K. Rumbold, C. Sheridan, The Utilization of Cellulosic Biomass in treating AMD and the Subsequent Generation of Fermentable Sugars, in: 10th Int. Conf. Acid Rock Drain. IMWA Anu. Conf., 2015: pp. 1–12.

[12] N.W. Burman, K.G. Harding, C.M. Sheridan, L. Van Dyk, Evaluation of a combined lignocellulosic / waste water bio-refinery for the simultaneous production of valuable biochemical products and the remediation of acid mine drainage, Biofuels, Bioprod. Biorefining. 12 (2018) 649–664. doi:10.1002/bbb.1880.

[13] D.B. Johnson, K.B. Hallberg, Acid mine drainage remediation options: A review, Sci. Total Environ. 338 (2005) 3–14. doi:10.1016/j.scitotenv.2004.09.002.

[14] D.B. Johnson, K.B. Hallberg, Biogeochemistry of the compost bioreactor components of a composite acid mine drainage passive remediation system, Sci. Total Environ. 338 (2005) 81–93. doi:10.1016/j.scitotenv.2004.09.008.

[15] G.S. Simate, S. Ndlovu, Acid mine drainage: Challenges and opportunities, J. Environ. Chem. Eng. 2 (2014) 1785–1803. doi:10.1016/j.jece.2014.07.021.

[16] N.W. Burman, K.G. Harding, C.M. Sheridan, Lignocellulosic bioethanol production from grasses pre-treated with acid mine drainage: Modeling and comparison of SHF and SSF Author links open overlay panel, Bioresour. Technol. Reports. 7 (2019). doi:10.1016/j.biteb.2019.100299.

[17] B. Ramla, C. Sheridan, The potential utilisation of indigenous South African grasses for acid mine drainage remediation, Water SA. 41 (2015) 247–252. doi:10.4314/wsa.v41i2.10.

[18] N.W. Burman, L. van Dyk, F. Postma, C. Sheridan, G.S. Simate, K.G. HArding, Flow Sheet and Sensitivity Analyses for the Bio-Remediation of Acid Mine Drainage Using Sulfate Reducing Bacteria and South African Grasses, in: 2nd Int. Conf. Energy, Evironment Clim. Chang., Pointe Aux Piments, Mauritius, 2017.

[19] D.K. Westensee, K. Rumbold, K.G. Harding, C.M. Sheridan, L.D. van Dyk, G.S. Simate, F. Postma, The availability of second generation feedstocks for the treatment of acid mine drainage and to improve South Africa's bio-based economy, Sci. Total Environ. 637–638 (2018) 132–136. doi:10.1016/j.scitotenv.2018.04.410.

[20] E. Gnansounou, A. Dauriat, Bioresource Technology Techno-economic analysis of lignocellulosic ethanol : A review, Bioresour. Technol. 101 (2010) 4980–4991. doi:10.1016/j.biortech.2010.02.009.

[21] D. Humbird, R. Davis, L. Tao, C. Kinchin, D. Hsu, A. Aden, P. Schoen, J. Lukas, B. Olthof, M. Worley, D. Sexton, D. Dudgeon, Process Design and Economics for Biochemical Conversion of Lignocellulosic Biomass to Ethanol, Golden, Co., 2011. http://www.nrel.gov/docs/fy11osti/47764.pdf.

[22] F.K. Kazi, J.A. Fortman, R.P. Anex, D.D. Hsu, A. Aden, A. Dutta, G. Kothandaraman, Techno-economic comparison of process technologies for biochemical ethanol production from corn stover q, Fuel. 89 (2010) S20–S28. doi:10.1016/j.fuel.2010.01.001.

[23] E. Sendich, M. Laser, S. Kim, H. Alizadeh, L. Laureano-perez, B. Dale, L. Lynd, Recent process improvements for the ammonia fiber expansion (AFEX) process and resulting reductions in minimum ethanol selling price, Bioresour. Technol. 99 (2008) 8429–8435. doi:10.1016/j.biortech.2008.02.059.

[24] B. Bals, C. Wedding, V. Balan, E. Sendich, B. Dale, Evaluating the impact of ammonia fiber expansion (AFEX) pretreatment conditions on the cost of ethanol production, Bioresour. Technol. 102 (2011) 1277–1283. doi:10.1016/j.biortech.2010.08.058.

[25] D. Klein-marcuschamer, P. Oleskowicz-popiel, B.A. Simmons, H.W. Blanch, Technoeconomic analysis of biofuels : A wiki-based platform for lignocellulosic biorefineries, Biomass and Bioenergy. 34 (2010) 1914–1921. doi:10.1016/j.biombioe.2010.07.033.

[26] H. Huang, S. Ramaswamy, W. Al-dajani, U. Tschirner, R.A. Cairncross, Effect of biomass species and plant size on cellulosic ethanol : A comparative process and economic analysis, Biomass and Bioenergy. 33 (2009) 234–246. doi:10.1016/j.biombioe.2008.05.007.

[27] M. Laser, E. Larson, B.E. Dale, M. Wang, N. Greene, L.R. Lynd, Comparative analysis of efficiency , environmental impact , and process economics for mature biomass refi ning scenarios, Biofuels, Bioprod. Biorefining. 3 (2009) 247–270. doi:10.1002/bbb.

[28] C. Piccolo, F. Bezzo, A techno-economic comparison between two technologies for bioethanol production from lignocellulose, Biomass and Bioenergy. 33 (2009) 478–491. doi:10.1016/j.biombioe.2008.08.008.

[29] National Accademy of Sciences, National Academy of Engineering, National Research Council, The national academies press, 1st ed., The National Academies Press, Wachington, D.C., 2009. doi:10.17226/12620.

[30] C.L.L. Robus, L.D. Gottumukkala, E. van Rensburg, J.G. Görgens, Feasible process development and techno-economic evaluation of paper sludge to bioethanol conversion : South African paper mills scenario, 92 (2016) 333–345. doi:10.1016/j.renene.2016.02.017.

[31] G.D. Ulrich, P.T. Vasudevan, How to Estimate Utility Costs for a number of utilities, Chem. Eng. (2006) 66–69.

[32] Department of Energy, 2018 Energy Price Report, Pretoria, 2018. http://www.energy.gov.za/files/media/explained/Energy-Price-Report-2018.pdf.

[33] S. Ellilä, L. Fonseca, C. Uchima, J. Cota, G.H. Goldman, M. Saloheimo, V. Sacon, M. Siika-Aho, Development of a low-cost cellulase production process using Trichoderma reesei for Brazilian biorefineries, Biotechnol. Biofuels. 10 (2017) 1–17. doi:10.1186/s13068-017-0717-0.

[34] G. Liu, J. Zhang, J. Bao, Cost evaluation of cellulase enzyme for industrial-scale cellulosic ethanol production based on rigorous Aspen Plus modeling Cost evaluation

of cellulase enzyme for industrial-scale cellulosic ethanol production based on rigorous Aspen Plus modeling, Bioprocess Biosyst. Eng. 39 (2016) 133–140. doi:10.1007/s00449-015-1497-1.

[35] Argus Media, Argus Sulfuric Acid, London, 2018. https://www.argusmedia.com/-/media/Files/sample-reports/argus-sulphuric-acid.ashx?la=en&hash=28D8CDEF485998FED5806750D90A916D3F3DED19.

[36] R. Turton, R.C. Bailie, W.B. Whiting, J.A. Shaeiwitz, Analysis, Synthesis, and Design of Chemical Processes, 1st ed., Pretince Hall, Upper Saddle River, 1998.

[37] A. Aden, M. Ruth, K. Ibsen, J. Jechura, K. Neeves, J. Sheehan, B. Wallace, L. Montague, A. Slayton, J. Lukas, Lignocellulosic Biomass to Ethanol Process Design and Economics Utilizing Co-Current Dilute Acid Prehydrolysis and Enzymatic Hydrolysis for Corn Stover Lignocellulosic Biomass to Ethanol Process Design and Economics Utilizing Co-Current Dilute Acid Prehyd, Golden , Co, 2002.