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Research Article

Technoeconomics of Sugar Cane Bagasse Valorization to Lactic Acid Using Pinch Technology: Distillation vs Reactive Distillation

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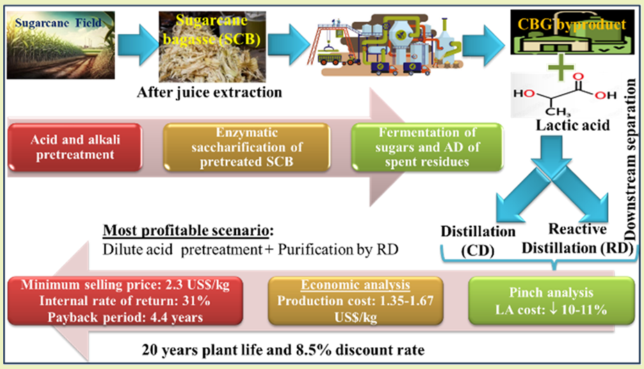
ABSTRACT: Sugar cane is one of the largest agricultural crops, and sugar cane bagasse (SCB), a major waste from sugar cane processing, is an abundant and inexpensive source of fermentable sugars for producing diverse platform chemicals. The present study evaluates the technoeconomic viability of L (+) lactic acid (LA) production from SCB with different stand-alone process scenarios modeled using the pinch method. It critically evaluates various cost-contributing factors when a sugar-rich hydrolysate is obtained via two different pretreatment methods: dilute acid and alkali. The cost−benefit of LA purification by conventional distillation (CD) is further compared to reactive distillation (RD). The pinch method cuts the LA manufacturing costs by 10−11%. Alkali pretreatment combined with RD involves a lower capital investment and utility consumption than the CD counterpart and slightly less LA manufacturing cost. However, LA production via dilute acid pretreatment and purification by RD emerges as the most profitable scenario due to capital investment, utility demand, and chemical consumption savings. This scenario offers the minimum LA selling price of 2.3 US$/kg for an 8.5% discount factor and a 5 year payback period. However, for a 20 year plant life and 2.5 US$/kg factory-gate LA selling price, the internal rate of return was 31% and the payback period was 4.4 years for an 8.5% discount factor.



KEYWORDS: *lactic acid, sugar cane bagasse, process modeling, pinch analysis, reactive distillation*

INTRODUCTION

Agricultural crop residues are perceived as one of the most promising bioresources as more than 60% of their structural component comprise polysaccharides, namely, cellulose and hemicellulose.[1] These polysaccharides are the central carbon blocks for producing an array of biofuels and biorenewables via biorefinery platforms. The crop residues are first pretreated and hydrolyzed to create renewable sugar platforms, which are further valorized to numerous chemical building blocks via the fermentative route. In India, after rice (33%) and wheat (21%), sugar cane (17%) is the third-largest crop contributing to maximum crop residue generation.[2] Fortunately, sugar cane processing is a well-established and mature technology in India, where sugar juice is extracted from sugar cane, leaving behind solid lignocellulosic residual fibrous biomass, known as sugar cane bagasse (SCB). SCB is thus a major byproduct of the sugar industry. However, unlike rice and wheat straw, the supply chain management of SCB is somewhat overridden due to high water content and unfavorable structural characteristics. In 2021−22, 439.43 million metric tons (MT) of sugar cane[3] was produced, of which 356.4 million MT was crushed in 506 sugar mills across India.[4] Presently, SCB is mostly used in sugar industries as a feedstock for the cogeneration of heat and electricity. As per the Ministry of New and Renewable Energy, this sector produced around 9434 MW of energy in 2023.[5] However, valorizing SCB to high-value chemical products has the potential to enhance the profitability of sugar mills. Besides its abundance, SCB is an inexpensive source of fermentable sugars, which makes it a promising biorefinery feedstock. Therefore, there is a favorable scenario to demonstrate the biomanufacturing of diversified products from SCB within the domain of circular biorefining in India. This approach is anticipated to significantly contribute toward decarbonizing the chemical sector, generating new jobs, increasing the farmer's income, and fostering the rural economy.[6] It can also be a vital step in reducing import dependence. However, some of the key drivers to make SCB-based biorefineries successful are the willingness of the industry to support innovations, choice and technology

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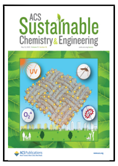

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readiness level of targeted products (main and side), process configurations, robust policy framework, and support from the government.

Lactic acid (LA) represents one such biobased platform chemical enlisted by the US Department of Energy, which is easily obtainable from biomass.[7,8] The popularity and significance of LA can easily be envisaged by its market size, which was 7.14 billion US$ in 2023.[9] The market demand for this versatile chemical is steadily growing due to the commercial exploitation of LA in diverse sectors ranging from biodegradable polymers to pharmaceuticals (pH regulator and biodegradable medical implants), food (acidulant and preservative), beverages, personal care, cosmetics (skin and hair care products), and textiles.[10] Owing to the presence of two different types of reactive functional groups, namely, carboxylic and hydroxyl groups, LA can easily undergo condensation, dehydration, dehydrogenation, and hydrogenation reactions, making it an important biorefinery platform chemical.[11] It can be catalytically transformed into an array of commodity chemicals, such as propylene glycol, acrylic acid, 2,3-pentanedione, pyruvic acid, ethyl acetate, and polylactic acid.[11,12] Nearly 1.5 million MT of LA was produced globally in 2022.[13] Even a developing country like India imported around 6391 MT of LA, its esters, and salts in 2023, with an import burden of about 10.91 million US$.[14] Therefore, it is high time for India to explore technological options to cater to the requirement of indispensable chemicals, such as LA, using numerous carbon-rich organic waste streams from the sugar industry, including SCB.

At present, about 70−90% of LA is produced commercially by the fermentative route, but it relies heavilyon edible carbohydrate feedstocks, such as sugar, starch, and sugar beet syrup. However, the abundant, nonedible, and cheap agricultural crop residues, including SCB, are attractive alternative source of fermentable sugars for LA production. This strategy is essential to promoting sustainability and circularity without compromising the food supply for the ever-growing world population. Though research outcomes toward valorizing lignocellulosic biomass to LA are promising, it is imperative to judge the economic performance of these processes for their successful commercialization. Motivated by the thriving need, a few technoeconomic analyses have been performed using various starting materials, such as SCB, leaves,[15] corn stove,[16] lignocellulosic feedstock,[17] food wastes,[18] and bread waste.[19] State-of-the-art further reveals that the technoeconomic feasibility of LA production from SCB has been explored in the past, either as a main product or as a coproduct.[15,20−23] However, most previous studies aimed at developing biorefineries annexed to sugar mills where SCB and/or molasses were diverted for LA production, along with coproducts. Besides, limited technoeconomic analyses undermine the scope of multiple possible process configurations for individual processing steps to arrive at the most profitable scenario. Therefore, the present work explores the potential of SCB for sustainable LA production in a stand-alone biorefinery facility close to the sugar mill, accounting for raw materials and energy costs, using current state-of-the-art experimental data for each stage of the process.

The feasibility analysis hinges on the detailed process modeling for the precise estimation of total capital investment (TCI) and material-energy consumption. The processes are designed using the appropriate thermodynamic property methods and rigorous unit operation models available in Aspen Plus software for reliable estimates of the process economics. Besides, unlike most of the earlier studies, pinch analysis is employed for process integration in each of the scenarios. Pinch analysis is an essential tool for designing the heat exchanger network by matching a hot stream with appropriate cold streams for maximum utilization of the process heat energy, thereby minimizing external utility consumption.

The present study specifically assesses the technocommercial feasibility of various scenarios of L (+) LA production using SCB as the starting raw material. The study also considers the biogas as a byproduct, which is obtained by the anaerobic digestion (AD) of the solid residues left out after enzymatic saccharification of pretreated SCB and liquid fractions after LA extraction. Specifically, the cost−benefit analysis in the current investigation is limited to three different process scenarios: (i) alkali pretreatment with LA separation by conventional distillation (CD), (ii) alkali pretreatment with LA separation by reactive distillation (RD), and (iii) acid pretreatment with LA separation by RD.

METHODOLOGY

SCB Composition and Plant Capacity. Baral et al. reported the dry composition of SCB as 40.49 ± 1.95 wt % cellulose, 27.55 ± 0.31 wt % hemicellulose, 21.91 ± 0.52 wt % acid-insoluble lignin, 2.03 ± 0.07 wt % acid-soluble lignin, and 3.84 ± 0.32 wt % ash.[24] The extractive content in dry SCB was considered as 4.18 wt % for composition balance closure, which was denoted using gluconic acid as a typical soluble organic acid. The water content of SCB was taken as 35 wt %. The process was designed based on the above SCB composition. The cellulose was represented by a linear combination of 10,000 β-D-glucose monomer units connected at 1,4 positions. The hemicellulose was assumed to be composed of 80% xylan and 20 wt % glucomannan, which were considered polysaccharides of 200 xylose and mannose monomer units, respectively. The lignin was taken as solid with an elemental composition of 71.6 wt % carbon, 11.4 wt % hydrogen, and 17 wt % oxygen.[25] The cellulose, hemicellulose, lignin, extractive, and gypsum ($CaSO_4{\cdot}2H_2O$) are nondatabank components in Aspen Plus. Thermodynamic properties, such as heat of formation, vapor pressure, heat of vaporization, solid/liquid molar volume, and heat capacity, of these components were included in Aspen Plus from the NREL databank.[25] In India, Maharashtra state alone processed 132 million MT of sugar cane in 2021−22.[6] Some of the large sugar mills in India process up to 12,000 MT of sugar cane per day, generating around 3000 MT of wet SCB. On the other hand, NREL and Idaho National Laboratory (INL) demonstrated that the transportation costs overpowered the economy-of-scale benefits above 2000 MT (dry)/day plant capacity for lignocellulosic biorefinery.[26] Based on the above facts, the present biorefinery was designed for a daily wet SCB refining capacity of 2000 MT, equivalent to about 573−605 MT of LA per day. The following scenarios were considered in the present work:

1. This scenario represents LA production via cofermentation of glucose and xylose, which are derived using alkali pretreatment of SCB, followed by enzymatic hydrolysis of the solid carbohydrate fraction. The downstream LA purification in this scenario is based on the well-established commercial method. It employs sequential

Scheme 1. Reaction Stoichiometry for LA Fermentation and Cell Biomass Growth

Substrate	Reaction	ΔH^{0}_{298K}, kJ/mol	
LA fermentation			
Glucose/Mannose	$C_6H_{12}O_6 \rightleftharpoons 2C_3H_6O_3$	-225.3/-98.1	(i)
Xylose	$3C_5H_{10}O_5 \rightleftharpoons 5C_3H_6O_3$	-131.5	(ii)
Cell biomass growth			
Glucose/Mannose	$C_6H_{12}O_6 \rightleftharpoons 4.938CH_{1.64}O_{0.39} + 1.062CO_2 + 1.951H_2O$	-348.9/-255.2	(iii)
Xylose	$C_5H_{10}O_5 \rightleftharpoons 4.115CH_{1.64}O_{0.39} + 0.885CO_2 + 1.625H_2O$	-201.1	

steps starting with LA esterification using methanol, followed by fractional distillation of methyl lactate (ML), ML hydrolysis, and recovery of LA via distillation. This traditional LA purification approach is referred to as conventional distillation (CD).

2. The ML hydrolysis is an equilibrium-limited reaction. Therefore, sequential ML hydrolysis and LA purification by CD involves recycling unhydrolyzed ML and multiple distillation columns. This downstream LA separation process is thus energy-intensive. Simultaneous ML hydrolysis and methanol−LA separation in one unit using RD is an amicable solution to overcome the above challenges. This approach also overcomes the equilibrium limitation of ML hydrolysis, making the LA separation simple and energy-efficient. Therefore, this scenario employs LA production from the cofermentation of glucose and xylose (derived by alkali-pretreated SCB), followed by its purification using LA esterification with methanol, ML distillation, and LA recovery using ML RD. This advanced LA separation method is referred to as the RD configuration.
3. The present work additionally compares the technoeconomics of the above alkali pretreatment-RD scenario with dilute acid pretreatment of SCB, followed by LA separation using RD. In this scenario, LA is produced by the separate fermentation of glucose and xylose.

Preprocessing of SCB. Preprocessing of SCB started with size reduction (cutting/chopping) to below 2 mm. In the subsequent step, the carbohydrates of SCB were extracted using two different pretreatment methods: alkali and dilute acid.

Alkali Pretreatment. The alkali pretreatment primarily aimed at the removal of lignin from SCB by adding 0.13 kg of NaOH per kg of biomass using a solid loading of 15% (w/v). The pretreatment was carried out in an autoclave for 30 min at 121 °C. The solid recovery was 73.18 wt % of dry SCB.[24] The recovered solid comprised 54.66 wt % glucan, 29.78 wt % xylan, 11.59 wt % lignin, and 2.47 wt % ash.[24] The experimental results translated to a dissolution of around 1.3 wt % glucans, 20.9 wt % xylans, 64.6 wt % acid-soluble and -insoluble lignin together, and 52.9 wt % ash during alkali pretreatment. The extractives, being nonstructural SCB components like sugar alcohols and organic acids, were assumed to dissolve completely during alkali pretreatment.[27]

Dilute Acid Pretreatment. The dilute sulfuric acid pretreatment was based on the method developed by Nova Pangaea Technology Ltd.[28,29] It was performed at 170 °C and 11 bar (g) pressure with a 15 min residence time using 0.015 L of sulfuric acid per kg of dry SCB. The steam [190 °C and 11 bar (g) pressure] and recycled hot water were added to the pretreatment reactor. The combined mass of water and steam was equivalent to about 5 wt % sulfuric acid. An appropriate steam/water ratio was used to maintain the desired reactor temperature without any external heat duty. This step was assumed to dissolve 90% hemicellulose and entire extractives, retaining the whole cellulose and lignin.[28,29]

Enzymatic Saccharification. The solid recovered from alkali and acid pretreatment was saccharified enzymatically under fed-batch mode with a 20% (7.5 + 7.5 + 5% at 0, 2, and 4 h, respectively) solid loading using the Cellic CTec3 enzyme containing 112.03 mg BSA equivalent protein/g.[24] The enzymatic hydrolysis was operated at 50 °C for 48 h by using a protein loading of 12.5 mg/g glucan. However, the process modeling excluded the enzyme addition in enzymatic hydrolysis for simplicity. Based on our experimental results, the saccharification of 93.26% glucan and 86.25% xylan was considered in enzymatic hydrolysis.[24] The percentage of glucan and xylan hydrolysis was calculated experimentally by measuring sugar concentration in the saccharified broth and compositional analysis of residual biomass (postenzymatic saccharification). A significant amount of sugars remained adsorbed and adhered to the residual biomass. The residual biomass was thus washed with water, which was used for sugar analysis. Following enzymatic hydrolysis, the total sugar yield in the case of alkali pretreatment was ∼417 g per kg of wet SCB, with 305 g of glucan and 111 g of xylose. The glucan and xylose concentrations in the hydrolysate were about 165 and 60 g/L, respectively.

LA Fermentation. Hydrolysate from alkali pretreatment comprised both C6 and C5 sugars, and therefore, cofermentation was considered. The thermophilic *Bacillus coagulans* DSM 2314 was considered in the present work for the cofermentation of glucose and xylose to L(+) LA.[30,31] *B. coagulans* is an acid-sensitive organism and requires pH control around the neutral zone. The dilute sulfuric acid pretreatment generated distinct C6 and C5 sugar-rich streams, and the separate fermentation of xylose and C6 sugar-rich streams was thus performed. The LA fermentation was carried out in batch mode at 50 °C with a fermentation period of 96 h. The neutral pH was maintained by the continuous addition of calcium hydroxide in the fermenter, which neutralized LA to calcium lactate as soon as it formed. The stoichiometry of the fermentation of glucose and xylose to LA is depicted in Scheme 1. A fraction of sugars was also consumed for biomass formation, whose reaction stoichiometry is depicted in Scheme

Scheme 2. Kinetics of Reversible Esterification of LA to ML

Reaction	Kinetics
$C_3H_6O_3 + CH_3OH \rightleftharpoons C_4H_8O_3 + \text{Water}$ Lactic acid Methanol Methyl lactate $\Delta H^0_{298K} = -35.6$ kJ/mol	$-r' = k_e \exp\left(-\frac{E_e}{RT}\right) x_{LA} x_M - k_h \exp\left(-\frac{E_h}{RT}\right) x_{ML} x_W$ $k_e = 1.48 \times 10^6$ kmol/kg.s, $E_e = 48.68$ kJ/mol, $k_h = 6.31 \times 10^5$ kmol/kg.s, $E_h = 49.92$ kJ/mol

Where x_{LA}, x_M, x_{ML}, and x_W represent the mole fraction of LA, methanol, ML, and water, respectively.

Scheme 3. Reaction Stoichiometry for AD of Soluble Organics

Substrate	Stoichiometry	ΔH^0_{298K}, kJ/mol	
Glucose/Mannose	$C_6H_{12}O_6 \rightleftharpoons 3CH_4 + 3CO_2$	-268.61/-249.85	(i)
Xylose	$2C_5H_{10}O_5 \rightleftharpoons 5CH_4 + 5CO_2$	-148.75	(ii)
Extractives	$4C_6H_{12}O_7 \rightleftharpoons 11CH_4 + 13CO_2 + 2H_2O$	-296.24	(iii)
Lactic acid	$2C_3H_6O_3 \rightleftharpoons 3CH_4 + 3CO_2$	-19.4	(iv)

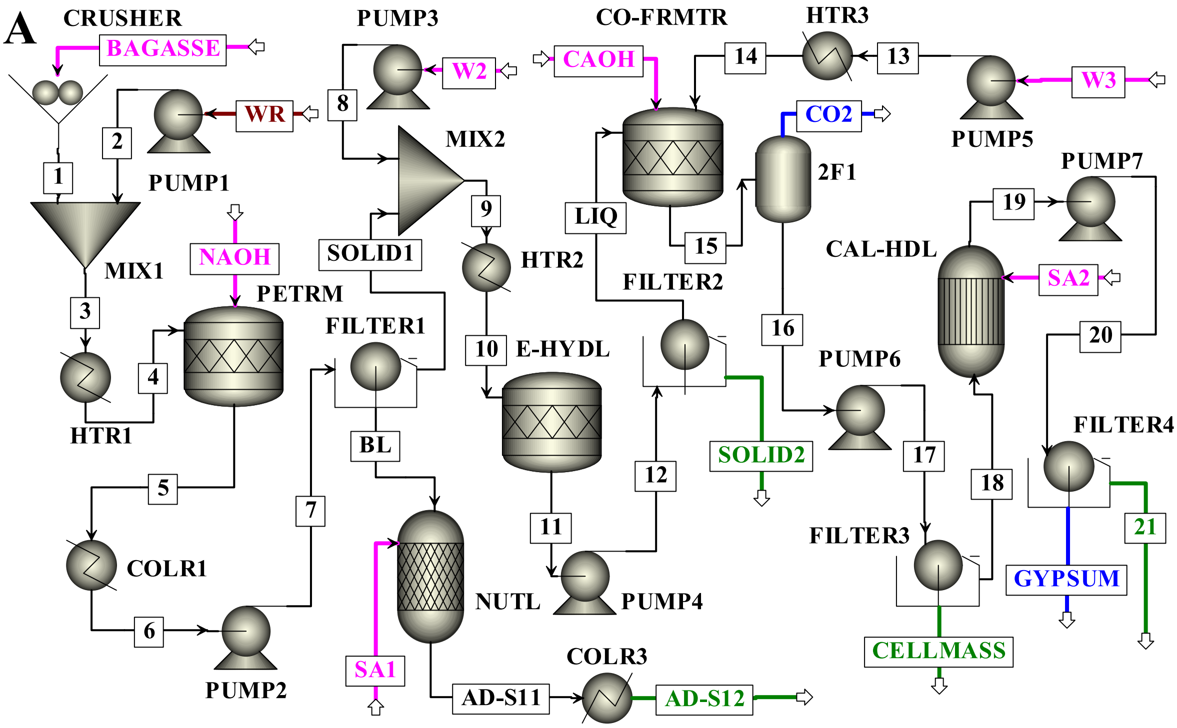
1. In both pretreatment scenarios, the overall conversion of glucans and xylose was taken as 95%.[29] About 90% of consumed sugars were assumed to be utilized for LA production, with the remaining 10% acting as a carbon source for biomass growth. In the present work, sugars were considered the sole carbon source for biomass growth, excluding the other nutrients, for the simplicity of process design. Likewise, the addition of an inoculum in the fermenter was also avoided in the process flowsheet. However, the economic analysis accounted for the suitable costs of nutrients and the inoculum. The LA titer in the fermentation broth after the hydrolysis of calcium lactate was around 100 g/L for the alkali pretreatment. However, for acid pretreatment, the overall LA concentration obtained from the combined C5 and C6 fermentation broth was around 104 g/L. The cell biomass, being a nondatabank component, was represented as a solid containing 64.4 wt % carbon, 8.2 wt % hydrogen, and 31.4 wt % oxygen with a chemical formula of $CH_{1.64}O_{0.39}$. However, sulfur and nitrogen contents were excluded from cell biomass for simplicity. The physical properties of cell biomass were acquired from the NREL database.[25] The calcium lactate in the fermentation broth was hydrolyzed to LA in an RStoic reactor using sulfuric acid, cogenerating gypsum byproduct. The fermenter was represented using an RStoic reactor and a flash drum to remove generated CO_2 during biomass growth.

LA Purification. Besides primary metabolites (LA), the fermentation broth contains additional high-boiling-point soluble organics, such as unconverted sugars, nutrients, and byproducts. These factors complicate LA separation from the fermentation broth. The first approach adapted for LA purification from fermentation broth was based on a commercially used CD method. This method involves the conversion of LA into thermally stable and relatively volatile ML by esterification with methanol (Scheme 2), which can be easily distilled from heavy fermentation residues with high purity. The LA was subsequently regenerated from ML by hydrolysis. Both esterification and ML hydrolysis reactions were carried out in a fixed-bed reactor at 80 °C and 3 bar pressure using three moles of methanol (or water) per mole of LA (or ML).[19] The excess methanol for the forward reaction and surplus water for the reverse reaction were used to drive the reaction equilibrium toward the targeted product. Sanz et al. developed an empirical kinetic model for the reversible esterification of LA with methanol.[32] The kinetic parameters of their empirical model, such as pre-exponential factor and activation energy, were used for designing the fixed-bed reactor for both forward and reverse reactions. However, in the CD configuration, per pass conversion during the ML hydrolysis remains low due to equilibrium limitations, with additional costs for downstream unreacted ML separation and recycling. Reactive distillation (RD), where reaction and product separation occur simultaneously in the same equipment, is a promising approach to overcome the equilibrium limitations of the ML hydrolysis reaction. At the same time, this approach avoids the complex separation of the ML−water azeotropic mixture, reduces TCI, and minimizes utility consumption.[33] The efficacy of this RD configuration was thus compared with that of the CD method.

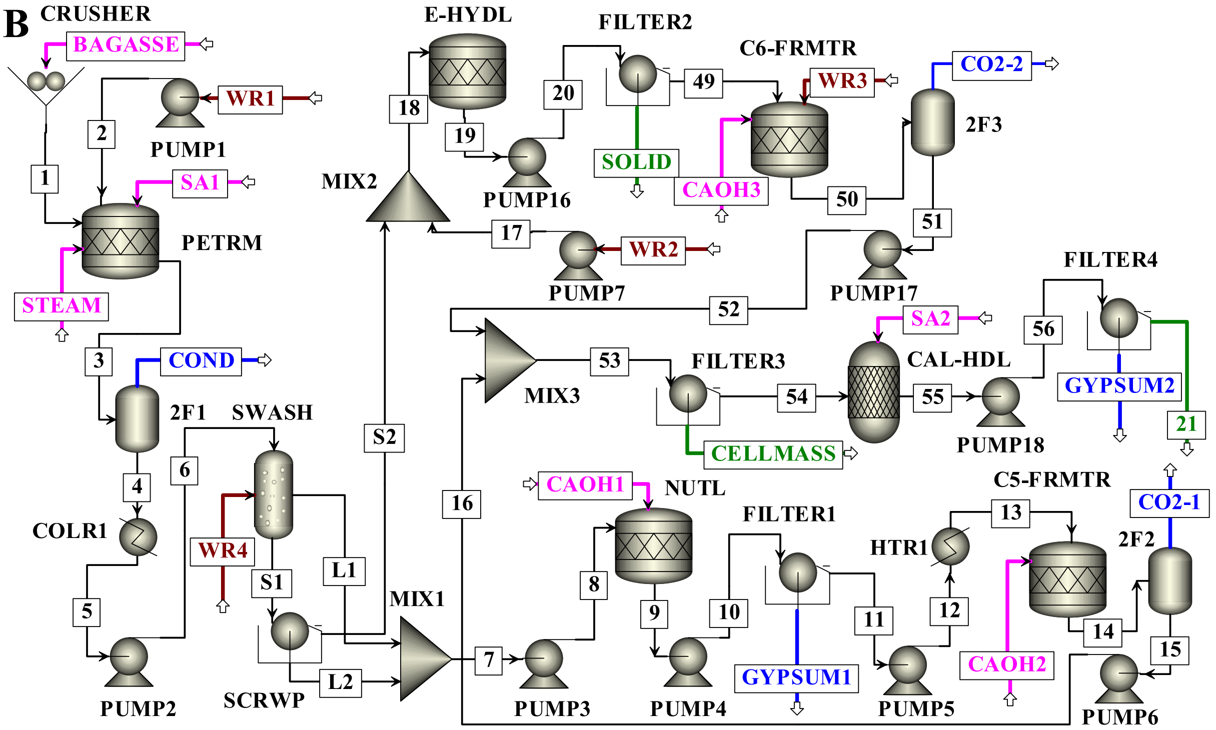
Anaerobic Digestion (AD) and Cogeneration of Steam. The soluble organic-rich stream obtained from alkali pretreatment following neutralization, unconverted sugars from the fermenter, and ML-containing water stream were treated using an anaerobic digestor to generate biogas. However, AD was limited to the latter two streams only for the acid pretreatment scenario. The AD was carried out at 41 °C for a digestion period of 14 days (Scheme 3). AD was represented by a combination of an RStoic reactor and two-phase flash models. The biogas generated from AD and solid residues obtained from various process steps, such as enzymatic hydrolysis and fermenter, were utilized for the cogeneration of high-pressure steam to complement the process heat requirements.

Process Flowsheet. The process starts with a mechanical size reduction of SCB using a cutting mill fitted with a 2 mm mesh (Figure 1).

Alkali Pretreatment. The chopped SCB was first combined with an appropriate quantity of water, heated to 121 °C, and directed to an alkali pretreatment reactor (Figure 1a). The pretreated SCB slurry was cooled to 30 °C, and the undissolved solid was filtered. The separated solid was mixed

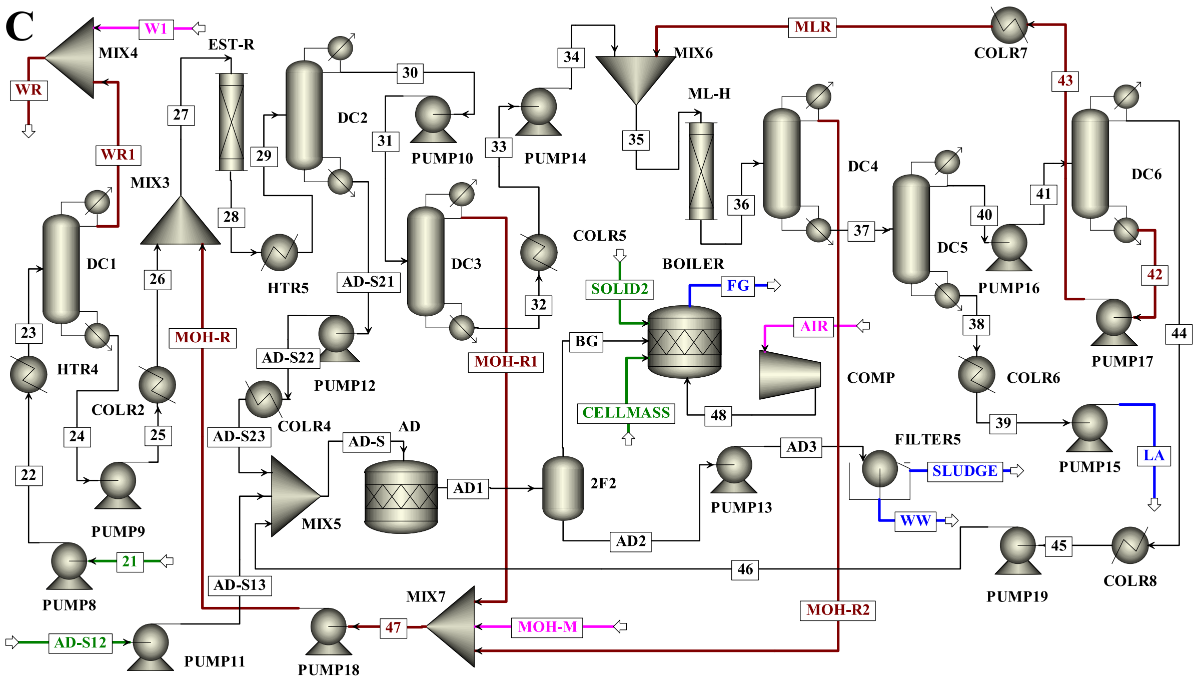


PETRM-Pretreatment, NUTL-Neutralization, E-HYDL-Enzyme hydrolysis, CO-FRMTR-Co-fermentation, HTR-Heater, COLR-Cooler, CAL-HDL-Calcium lactate hydrolysis, MIX-Mixer, 2F-Two-phase flash, W-Process water, WR-Recycled water. Colour code: Pink-Input, Brown-Recycled stream, Blue-Output, Green-Stream for downstream process.

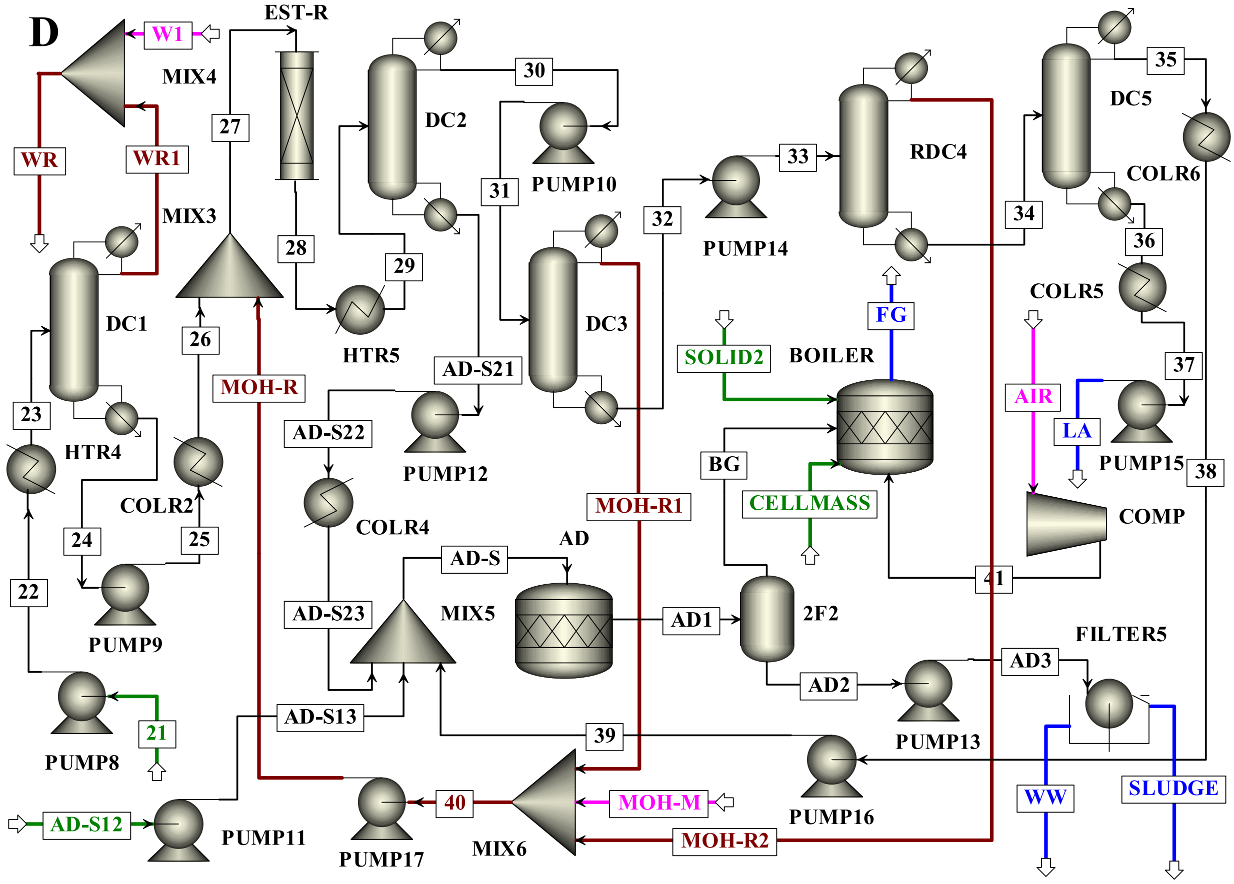


PETRM-Pretreatment, NUTL-Neutralization, E-HYDL-Enzyme hydrolysis, FRMTR-Fermentation, HTR-Heater, COLR-Cooler, CAL-HDL-Calcium lactate hydrolysis, SWASH-Water wash, SCRWP-Screw press, MIX-Mixer, 2F-Two-phase flash, SA-Sulfuric acid Colour code: Pink-Input, Brown-Recycled stream, Blue-Output, Green-Stream for downstream process.

Figure 1. continued



DC-Distillation column, EST-R-Esterification reactor, ML-H-ML hydrolysis, AD-Anaerobic digestion, COMP-Compressor, HTR-Heater, COLR-Cooler, MIX-Mixer, 2F-Two-phase flash.
Colour code: Pink-Input, Brown-Recycled stream, Blue-Output, Green-Stream to/from upstream/downstream process.



DC-Distillation column, RD-Reactive distillation, EST-R-Esterification reactor, AD-Anaerobic digestion, COMP-Compressor, HTR-Heater, COLR-Cooler, MIX-Mixer, 2F-Two-phase flash.
Colour code: Pink-Input, Brown-Recycled stream, Blue-Output, Green-Stream to/from upstream/downstream process.

Figure 1. Process flowsheet for the fermentative production of LA from SCB without process integration using (A) alkali pretreatment and (B) acid pretreatment. Downstream separation of LA (C) by CD and (D) RD for alkali pretreatment.

with water and directed to a fed-batch enzymatic hydrolysis reactor after the solid slurry was heated to 50 °C. The hydrolysate from the enzymatic hydrolysis reactor was filtered from the unconverted solid. The concentrated hydrolysate was then diluted with a proper amount of water to maintain a 100 g/L equivalent LA titer in the fermenter. The cell biomass was separated from the fermenter by filtration and directed to the boiler for the cogeneration of steam. The cell biomass-free fermentation broth was sent to the sulfuric acid-mediated calcium lactate hydrolysis reactor operated at 50 °C to regenerate LA with the cogeneration of gypsum, which was separated by filtration. The yield of LA after cofermentation was 0.356 kg (0.548 kg) per kg wet (dry) SCB.

Acid Pretreatment. The size-reduced SCB was pretreated with a suitable quantity of steam, recycled hot water, and sulfuric acid (Figure 1b). The SCB slurry was then sent to a two-phase flash drum, where around 9% of the condensate was separated. The SCB slurry obtained from the flash drum was afterward cooled to room temperature and sent for water washing, where the quantity of water used was equivalent to 50 wt % of the SCB slurry. Around 50% of the soluble fraction was removed in the washer as a washed stream containing about 137 g/L of sugar. However, the solid recovered from the washer still contained around 50% of the xylose sugars. This solid was then sent to a screw press, where around 47% of the liquid was removed. The xylose-rich liquid streams obtained from the washer and screw press were combined and neutralized by calcium hydroxide with the cogeneration of gypsum, which was separated by filtration. The filtrate stream was heated to 50 °C and sent to xylose fermentation. Likewise, the solid fraction obtained from the screw press was mixed with recycled hot water to attain 50 °C and sent to enzymatic hydrolysis. The undissolved solids were filtered and sent to the boiler, while the sugar-containing liquid stream was sent to the C6 fermentation reactor. Both C5 and C6 fermentation broths were mixed, and the cell biomass was filtered and sent to the boiler. The calcium lactate-containing fermentation broth was finally hydrolyzed using sulfuric acid to regenerate LA with the cogeneration of gypsum. After the filtration of gypsum, the fermentation broth was directed to downstream separation. The LA yield in the case of acid pretreatment [0.336 kg (0.517 kg) per kg wet (dry) SCB] was slightly less than alkali pretreatment due to the relatively lower utilization of sugars in separate C5 and C6 fermentation.

Downstream LA Separation. The polymer-grade LA was recovered using the esterification-based reactive separation method from the fermentation broth. After LA regeneration from calcium lactate, the LA-containing fermentation broth was concentrated by evaporating about 99% water, which was essential to favor equilibrium LA conversion to ML in the subsequent esterification step. The water removal from fermentation broth was modeled using a combination of a preheater (HTR4) and RadFrac atmospheric distillation column (DC1), with a recovery of more than 99.5% of LA. The water was partially vaporized in HTR4 with a molar vapor fraction of 0.5. Though this preheating increased the condenser duty by 0.3%, it reduced the expensive reboiler steam duty by around 59%. Besides, the preheater heating duty could be partially obtained from various hot streams, thereby enhancing the thermal efficiency. The reboiler temperature in DC1 was around 135 °C, which was well below the LA thermal decomposition temperature of 180 °C. The liquid hot water (around 100 °C) obtained from DC1 was less than the required amount for alkali pretreatment. The recovered hot water was thus entirely utilized for alkali pretreatment after the makeup amount was added, thereby reducing the necessary preheating duty for pretreatment. On the contrary, in the case of dilute acid pretreatment, the recovered hot water from DC1 was in excess of the combined requirement for pretreatment, enzymatic hydrolysis, and fermentation. Therefore, the required amounts were directed to the corresponding sections after purging the excess quantity. The LA-rich stream from DC1 was cooled to a temperature (96 °C) in such a way that after mixing with recycled methanol (64 °C), the mixed stream attained the desired inlet temperature for the esterification reactor (80 °C). In the fixed-bed esterification reactor, about 85% of LA was converted to ML. The product mixture from the LA esterification reactor was sent to the distillation column DC2 to distill excess methanol, water, and ML from unreacted LA and unfermented sugars. The DC2 feed stream was also preheated to 95 °C to reduce the reboiler duty. This distillation column was designed at 0.2 bar pressure to uphold the reboiler temperature of 181 °C to circumvent operational challenges due to possible thermal decomposition of unesterified LA at a high reboiler temperature under atmospheric pressure distillation. The DC2 distillate stream containing methanol, water, and ML was directed to DC3, where excess methanol was distilled.

CD Configuration. In this configuration, LA was regenerated by the hydrolysis of ML in a fixed-bed reactor (Figure 1c). For this purpose, the water and ML-containing stream from DC3 were cooled from 101 to 80 °C, mixed with recycled ML + water stream at 80 °C, and directed to a fixed-bed ML hydrolysis reactor. The per pass ML conversion was around 55.3% in the hydrolysis reactor. The reactor outlet stream comprised around 28 wt % water, 32 wt % LA, 11 wt % methanol, and 29 wt % ML. The most volatile methanol was first distilled from this mixture in DC4. The methanol recovered from DC3 and DC4 was reused for the esterification after adding a small amount of makeup corresponding to the loss during the separation. Conversely, the high-boiling and thermally sensitive LA was separated by vacuum distillation (DC5, 0.2 bar) with an acceptable reboiler temperature of 178 °C. The hot LA was sent to the storage tank after cooling it to room temperature. The distillate from DC5 comprised unconverted ML and water. However, the amount of water was more than the required quantity for maintaining a 3:1 water/ML mole ratio. The excess water was thus separated before recycling this stream to the ML hydrolysis reactor. However, ML forms a low-boiling azeotrope with water at around 5 mol % ML (Figure S1).[34] Therefore, the excess water accompanied by an azeotropic amount of ML was separated in DC6 and directed to AD. The ML stream obtained from DC6 was cooled from 99.5 to 80 °C and recycled to the ML hydrolysis reactor.

RD Configuration. The DC3 bottom stream was composed of 61 mol % water and 29 mol % ML (Figure 1d). This stream contained more water than required for the complete hydrolysis of ML. The stream was, thus, directly sent to the RD column (RDC4). The temperature and composition profile in the RD column are shown in Figure S2. Almost complete hydrolysis of ML was achieved in the RD column, with the recovery of methanol as a distillate and LA accompanied by excess water from the bottom. The excess water in the feed helped to maintain the reboiler temperature at ~134 °C under atmospheric pressure. The recovered

Table 1. Optimum Design Parameters of Distillation Columns

		number of stages	reflux ratio	feed stage	reactive stages	diameter, m		height, m
						alkali	acid	
common	DC1	10	0.0055 (mass)	8		16.15	16.76	10.97
	DC2	10	0.0071 (mole)	4		7.01	7.77	10.97
	DC3	23	2 (mole)	14		4.42	4.42	22.56
CD	DC4	27	2.9 (mole)	13		2.90		25.60
	DC5	11	0.01 (mole)	5		7.16		11.58
	DC6	10	1.5 (mole)	9		1.83		10.97
RD	RDC4	26	2.2 (Mass)	17	16–25	3.20	3.20	24.99
	DC5	11	0.05 (mole)	5		2.90	2.59	11.58

Table 2. Raw Material/Chemical Consumptions and Product/Coproduct Yields in MT per Annum along with Cost

	alkali pretreatment	acid pretreatment	cost
NaOH	6.17×10^4		0.184 US$/kg[27]
$Ca(OH)_2$	1.07×10^5	1.08×10^5	0.126 US$/kg[19]
H_2SO_4	2.17×10^5	1.43×10^5	0.29 US$/kg[19]
gypsum	2.49×10^5	2.51×10^5	12 US$/MT[40]
process water	4.19×10^6		0.00072 US$/kg[27]
lactic acid	2.21×10^5	2.09×10^5	
sludge	8.33×10^4		0.075 US$/kg[27]
steam, 165 psi	1.87×10^5 (D), 1.50×10^5 (RD)	1.34×10^5	0.021 US$/kg[41]
cooling water	4.30×10^8 (D), 3.94×10^8 (RD)	3.35×10^8	0.037 US$/cum[41]
SCB			50 US$/MT[42]
electricity	2896 kW-h/h (D), 2859 kW-h/h (RD)		0.0775 US$/kW-h
enzyme	1.15×10^4	7.87×10^3	3.55 US$/kg[19]
inoculum	3.16×10^5	2.17×10^5	0.0081 US$/kg[19]
nutrients	6.0×10^4	4.13×10^4	0.27 US$/kg[19]

methanol was reused for the esterification. The LA was subsequently separated from water by vacuum distillation. The water recovered as a distillate contained a small quantity of ML and was sent for AD. All distillation and RD columns were designed using the RadFrac model and NRTL property method. Their optimal design parameters with column diameter and height are displayed in Table 1. All of the columns were considered as sieve trays with a 0.61 m tray spacing. The reflux ratio for DC5 in the RD configuration was slightly higher than that of the CD configuration due to a relatively lower distillate rate. The overall flowsheets and block diagrams displaying mass flow rates for the SCB-to-LA conversion processes for all three scenarios are shown in Figures S3 and S4, respectively. The LA yields were identical for both CD and RD configurations. For alkali pretreatment, the overall yield of polymer-grade LA (99.99%) was 0.30 kg (0.47 kg) per kilogram of wet (dry) SCB. However, it was slightly less in acid pretreatment 0.29 kg (0.44 kg) per kilogram of wet (dry) SCB.

Anaerobic Digestion (AD). The neutralized black liquor obtained from alkali pretreatment, unesterified LA and soluble organics recovered from the bottom of the DC2, and ML-containing water stream from DC6 (in CD configuration) or DC5 (in RD configuration) were separately cooled to 41 °C and utilized for generating biogas by AD.[35] For alkali pretreatment, total digestible organics in AD were 12.13 and 11.64 MT/h for CD and RD configurations, respectively. The biogas generated per hour from these organics was about 12.08 MT for the CD configuration and 11.53 MT for the RD configuration for alkali pretreatment, with a CH_4/CO_2 mole ratio of 0.98. However, total digestible organics in AD were 13.94 MT/h for acid pretreatment with an RD configuration that generated about 13.84 MT biogas per hour. The lignin is not generally digested in AD, and the lignin and ash were separated by filtration following AD in alkali pretreatment, which could be used as a fertilizer.[27] The biogas produced in AD, unconverted solids recovered after enzymatic hydrolysis, and the cell biomass separated from the fermenter were used as fuel for the boiler to cogenerate steam. The overall raw material/chemical consumptions and product/coproducts obtained are shown in Table 2.

Economic Analysis. The equipment costs were calculated based on the Chemical Engineering Plant Cost Index 816 for 2022 using the following equation.[36] The number and costs of fermenters and saccharification reactor were calculated considering 500 cum stirred reactor with 3/4th as the working volume. The enzymatic hydrolysis involved 25 and 22 reactors for alkali and acid pretreatments, respectively. The number of fermenters was 86 and 82 for alkali and acid pretreatments, respectively. The storage cost was calculated based on the volume requirement considering 12 and 25 day stocks of LA and sulfuric acid, respectively.[36] The retail price of chemicals acquired from different sources was also converted to the cost for the year 2022 by using the above cost index (Table 2). The operating labor cost was calculated based on total employee hours using the plant capacity and number of processing steps.[36] The proportion of employee hours for the common and skilled labor was taken as 75% and 25%, with their hourly salary of US$25 and US$35, respectively. The economics was evaluated considering 0.052 kg enzymes, 0.273 kg nutrients, and 1.43 kg inoculum consumption per kg of LA produced[19]

$$\text{cost of equipment} = \text{cost of known equipment} \times \left(\frac{\text{size of equipment}}{\text{size of known equipment}}\right)^{0.6} \times \left(\frac{\text{cost index of 2022}}{\text{reference cost index}}\right) \quad (1)$$

RESULTS AND DISCUSSION

Pinch Analysis. The heat duty of various process streams with their inlet and outlet temperatures is shown in Figure S5. These stream data and mass flow rates of different streams formed the basis of pinch analysis, which was done using 10 °C

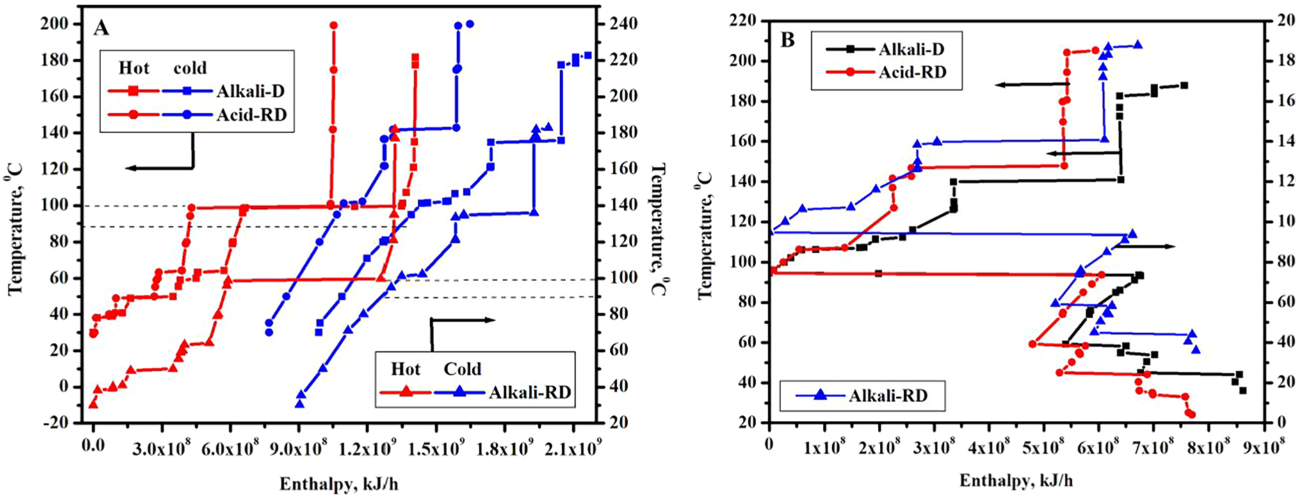


Figure 2. Pinch analysis for alkali and acid pretreatment processes. (A) composite and (B) grand composite curves.

as ΔT_{min}. All scenarios demonstrated identical cold (89.65 °C) and hot (99.65 °C) pinch point temperatures (Figure 2).

Alkali Pretreatment. The cooling and heating duties without pinch analysis were 1.41×10^9 and 1.18×10^9 kJ/h, respectively, for the CD configuration. However, the pinch analysis for this configuration reduced the minimum cooling duty by around 29.8% (9.88×10^8 kJ/h) and heating duty by 39.7% (7.56×10^8 kJ/h). Nevertheless, the minimum duties involved in the CD configuration were much higher than those in the RD configuration (6.72×10^8 kJ/h heating and 9.04×10^8 kJ/h cooling). However, the cumulative heat exchange potential was marginally lower in the RD configuration (4.15×10^8 kJ/h) than in the CD (4.20×10^8 kJ/h). Despite lower process heat exchange, the RD configuration offered 11.1% heating and 9.3% cooling energy savings as compared with the CD configuration. The AD of organic waste streams cogenerated 3.72×10^8 kJ/h and 3.64×10^8 kJ/h equivalent steams in CD and RD configurations, respectively. Therefore, the net heating duty for these configurations was 3.84×10^8 kJ/h and 3.08×10^8 kJ/h, respectively.

The heat exchanger networks of alkali pretreatment with CD and RD configurations are shown in Figure 3. In the CD configuration, HTR1 was first heated to pinch temperature using the condenser of DC1, followed by further heating to around 110 °C using COLR1 and then by steam to 121 °C. The temperature of COLR1 was simultaneously reduced to the pinch point in the heat exchanger. The heat energy of COLR1 below the pinch point was partially exploited for heating HTR2 and HTR3 using two equal split fractions. The temperature of COLR1 was further reduced using cooling water. Similarly, the heat energy demand of the HTR4, HTR5, and ML hydrolysis reactors below the pinch point was obtained from the DC1 and DC6 condensers. However, above the pinch point, HTR4 was divided into four streams with split fractions of 0.3, 0.1, 0.5, and 0.1. The heating duties of these split fractions were partially accomplished from four different hot streams, namely, COLR2, COLR4, COLR6, and COLR7, respectively. The remaining heating energy of HTR4 was achieved from steam. The heating demand of HTR5 above the pinch point was acquired from COLR5 partly, with the balance being endured from steam. Below the pinch point, COLR2, COLR4, COLR5, COLR6, and COLR7 were cooled to their desired temperatures by cooling water. The heat duty of all other hot streams below the pinch and cold streams above the pinch was attained by using cooling water and steam, respectively. The heat exchanger network for the RD configuration is quite similar to the CD configuration, as shown in Figure 3b.

Acid Pretreatment. This configuration showed much lower minimum cooling (7.70×10^{08} kJ/h) and heating (5.95×10^{08} kJ/h) duties than the corresponding configuration of alkali pretreatment despite lesser process heat exchange potential (2.85×10^{08} kJ/h) (Figure 2 and Table 2). This configuration showed around 11.5 and 14.8% lower heating and cooling duty consumption than alkali pretreatment with RD. The higher minimum heating duty in alkali pretreatment was due to additional preheating duties before pretreatment, enzyme hydrolysis, and fermentation. However, the acid pretreatment bypassed these heating needs due to the use of recycled hot water or high-pressure steam (only for pretreatment). Conversely, the deviation in the minimum cooling duty originated from the excessive cooling duty involved for the hot pretreatment stream in alkali pretreatment. In this scenario, the process integration reduced around 27% cooling and 32% heating duty, slightly lower than alkali pretreatment with RD. Besides, the steam generated in this configuration (5.81×10^{08} kJ/h) was much higher than alkali pretreatment. The higher steam generation potential of this configuration originated from the utilization of lignin additionally in the boiler. The net heating duty in this scenario was thus reduced to merely 1.34×10^{07} kJ/h. However, this configuration involved the direct addition of an additional 8700 kg/h of high-pressure steam in the pretreatment step. Below the pinch temperature, the heat duty of COLR3 and COLR7 was used to heat the HTR1 and HTR5, respectively, with further cooling by cooling water (Figure 3c). Above the pinch, the heat duty of COLR1 was used to heat HTR4 partially, with further cooling by cold water below the pinch temperature. The HTR4 was heated by the DC1 condenser below the pinch. However, above the pinch, HTR4 was partially heated by COLR2, COLR4, and COLR5 using split fractions of 0.36, 0.24, and 0.4, respectively. These coolers were cooled further using cold water, while the remaining heat energy of HTR4 was managed from the hot utility. The integrated processes with the heat exchanger network are shown in Figure S6.

Capital Expenditure (CAPEX). The capital expenditure (CAPEX) and contribution of individual equipment to CAPEX

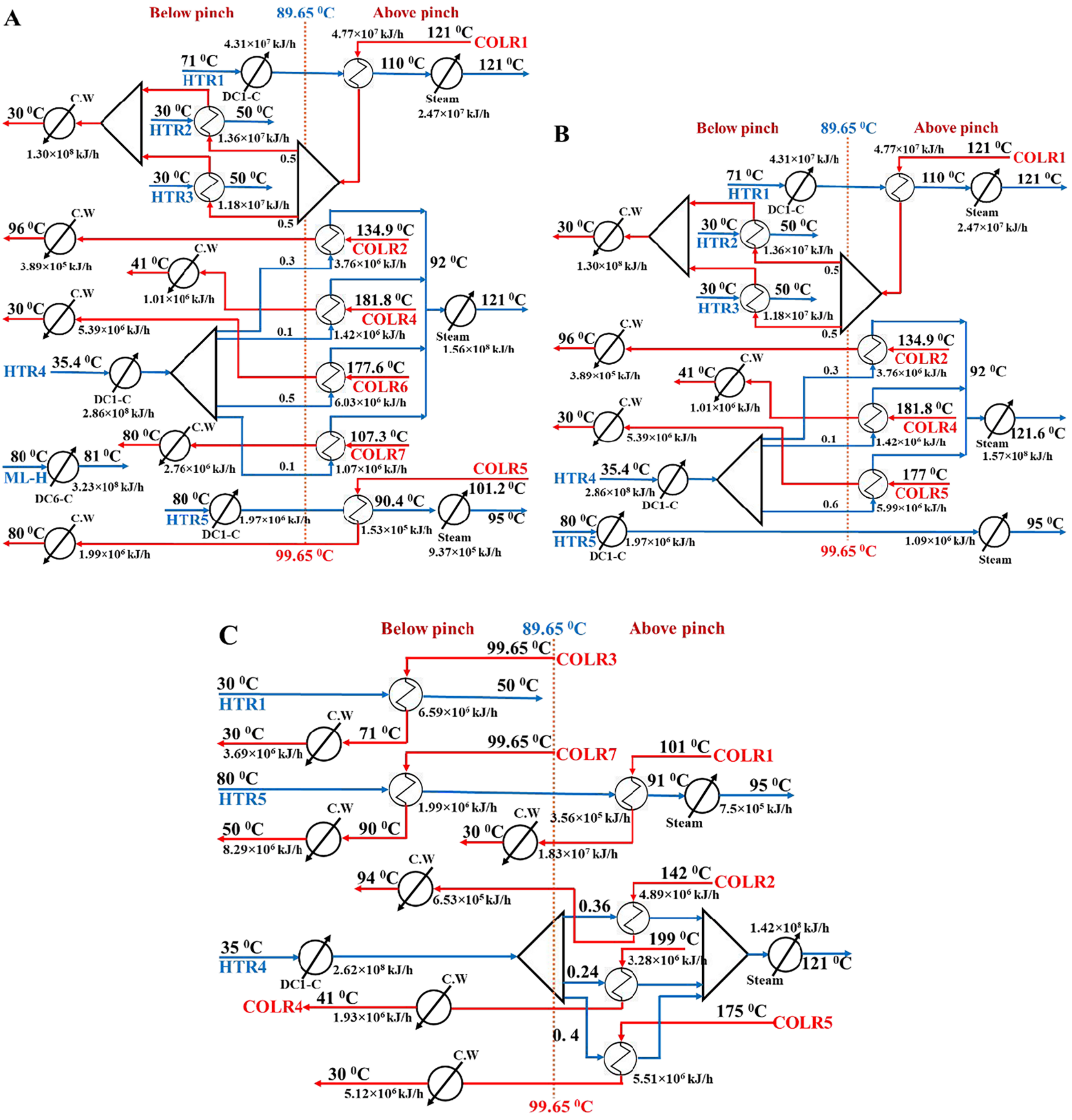


Figure 3. Heat exchanger network for alkali pretreatment with (A) CD and (B) RD configurations and (C) acid pretreatment with the RD configuration.

for the three process scenarios are shown in Table 3 and Figure 4a. The reactors for fermentation and enzymatic hydrolysis were the expensive process equipment involved in these bioprocesses, contributing 56−57 and 15−17% of TCI (Figure 4a). It was due to the low sugar/solid loading with huge processing volume and long fermentation and saccharification time. However, the CAPEX for fermentation and enzyme hydrolysis was slightly lower for acid pretreatment than for alkali one due to the relatively lower processing volume with a lesser number of reactors. The distillation columns were capital-intensive downstream LA separation equipment, with a 7−9% contribution of TCI. The CAPEX for the distillation columns was higher in the CD configuration than downstream LA separation by RD. The RD configuration comprised four distillation columns and one RD column compared to six distillation columns in the CD scenario. Besides, the RD configuration avoided a separate ML hydrolysis reactor with reduced process complexity. On the other hand, acid pretreatment involved lower CAPEX for distillation columns than alkali pretreatment due to reduced processing volume. The compressor involved in discharging air to the boiler contributed around 9−14% of TCI. The capital cost for the compressor was higher in acid pretreatment due to the larger volume of biogas and greater amount of solids, with more air

Table 3. Capital Expenditure in Million US$

	alkali pretreatment		
	CD	RD	acid pretreatment with RD
crusher	1.707	1.707	1.707
autoclaves	1.280	1.280	0.670
enzymatic hydrolysis	18.444	18.444	16.231
fermenters	63.448	63.448	60.497
reactors	0.051	0.026	0.026
distillation columns	8.924	7.371	6.581
anaerobic digestor	3.044	3.045	0.470
filters	0.306	0.306	0.460
boiler	2.890	2.849	3.775
compressor	10.159	9.986	15.566
heat exchangers	1.793	1.726	0.786
pumps	0.204	0.190	0.184
storage tanks	1.665	1.665	1.456
total equipment cost	**113.915**	**112.041**	**108.409**
installation	56.957	56.021	54.204
instrumentation and controls	29.618	29.131	28.186
piping	77.462	76.188	73.718
electricals	17.087	16.806	16.261
building	51.262	50.418	48.784
yard improvements	12.531	12.325	11.925
service facilities	62.653	61.623	59.625
land	5.696	5.602	5.420
direct fixed cost (A)	**427.180**	**420.154**	**406.533**
engineering and supervision	34.174	33.612	32.523
construction expenses	42.718	42.015	40.653
legal expenses	8.544	8.403	8.131
contractor fees	25.631	25.209	24.392
contingency	51.262	50.418	48.784
indirect fixed cost (B)	**162.328**	**159.659**	**154.483**
fixed capital cost (C = A + B)	589.508	579.813	561.016
working capital (D)	29.475	28.991	28.051
total capital investment (C + D)	**618.983**	**608.803**	**589.067**

flow for the boiler. The CAPEX values for AD (0.4−3.0%) and boiler (3.0−4.0%) were moderate in these processes. The acid pretreatment involved a lower CAPEX for AD than the alkali pretreatment due to the reduced volumetric flow rate and the lower reactor volume. However, the CAPEX for the boiler was much higher in acid pretreatment than in alkali one due to the combustion of a greater quantity of biogas and solids. The costs of heat exchangers were slightly lower in acid pretreatment than in alkali due to the lesser number of heat exchangers with reduced heat exchange duty. The TCI was highest in the alkali pretreatment plus CD configuration, while it was lowest for acid pretreatment with the RD configuration. The TCI in the current study was 589.06 million US$ for dilute acid pretreatment with LA separation by RD.

The TCI depends on many factors, including plant capacity and processing technology, which make it difficult to compare our results with those of the literature. When Pachón et al. conducted a feasibility study with the intent to develop a multiproduct biorefinery concept in the South African sugar industry (7200 MT/day), the lowest TCI (196.1 million US$) was accredited to the base scenario with sugar as the sole product, followed by coproduction of sugar and LA (509.7 million US$).[37] The latter scenario involved a dilute acid pretreatment of SCB, where 50% of SCB was diverted to LA production. Later, glucose-rich hydrolysate postenzymatic saccharification along with pretreated molasses C was mixed and subjected to LA fermentation using recombinant *Escherichia coli*.[37] Earlier, Daful and Görgens evaluated six different scenarios for LA production from steam-exploded SCB and brown leaves (200 MT/day).[15] The lowest TCI (160.9 million US$) was reported when an acid-tolerant and thermophilic *B. coagulans* was used to produce L (+) LA from the hydrolyzed hemicellulose fraction and later purified using RD. However, Mandegari et al. reported a TCI of 377.9 million US$ for a scenario in which the glucose and xylose derived from 936 MT/day SCB and brown leaves were valorized to LA.[20]

Operating Expenditure. The price of SCB was the major operating cost factor, contributing 15−24% of the total cost of chemicals and utility (Table 4 and Figure 4b). However, there are a number of prior studies wherein the authors have considered SCB as free by annexing the LA production to a sugar mill.[20−22,37] The utility was another dominant running cost and contributed 18−21% for alkali pretreatment and 8% for acid pretreatment. The reduced utility cost in acid pretreatment was due to lower heating and cooling duties

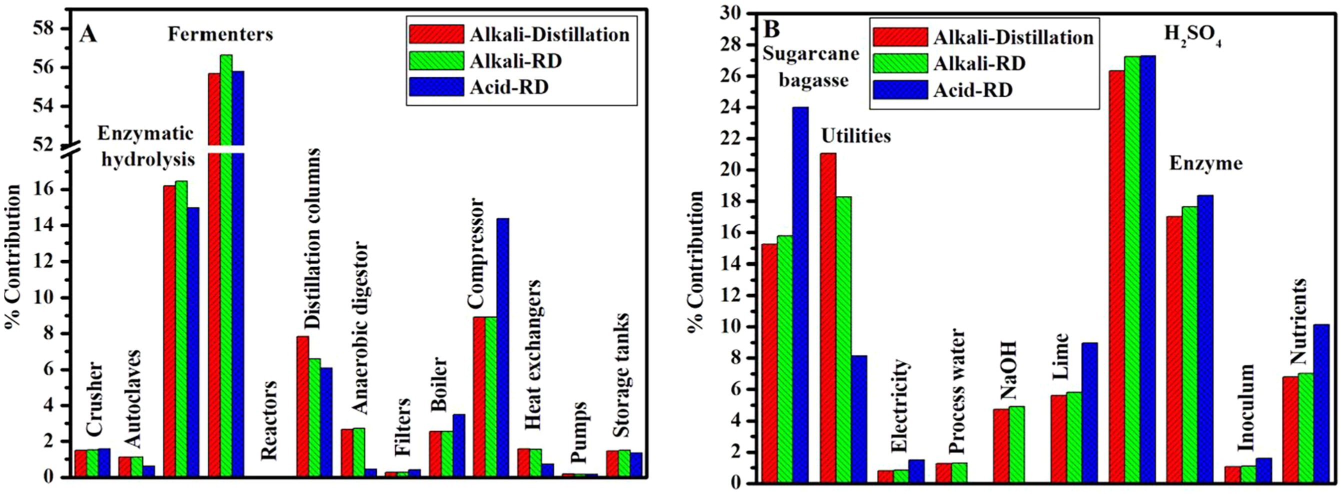


Figure 4. Contribution of individual (A) equipment to total capital expenditure and (B) chemical to total raw material, chemical, and utility cost.

Table 4. Operating and Production Cost in Million US$ per Annum

	alkali pretreatment		
	CD	RD	acid pretreatment with RD
direct cost			
operating labor	10.731	9.198	10.731
supervisory and clerical labor	1.610	1.380	1.610
maintenance and repairs	43.329	42.616	41.235
operating supplies	6.499	6.392	6.185
laboratory charges	1.610	1.380	1.610
plant overhead charges	27.835	26.597	26.788
SCB	36.500	36.500	36.500
utilities (cooling water and steam)	50.414	42.240	12.404
electricity	1.966	1.941	2.279
process water	3.016	3.016	0.000
NaOH	11.350	11.350	0.000
lime	13.482	13.482	13.627
H_2SO_4	63.009	63.009	41.517
enzymes	40.763	40.763	27.949
inoculum	2.558	2.558	2.423
nutrients	16.277	16.277	15.420
indirect costs			
insurance and taxes	1.709	1.681	1.626
depreciation	4.557	4.482	4.336
interest	34.044	33.484	32.399
general and administration expenses	7.329	7.005	7.053
total operating cost (A)	378.586	365.350	285.691
coproduct credit (B)	9.232	9.232	3.015
net production costs (C = A − B)	**369.354**	**356.118**	**282.675**
LA produced, kg/annum (D)	2.21×10^{08}	2.21×10^{08}	2.09×10^{08}
production cost, US$ per kg (C/D)	**1.67**	**1.61**	**1.35**
Without Pinch Analysis			
additional utility costs (B′)	44.002	44.002	30.191
production cost, US$ per kg (C′/D)	**1.87**	**1.81**	**1.50**

involved in the process and the cogeneration of a greater amount of steam in the boiler. On the other hand, the RD configuration in alkali pretreatment diminished heating and cooling duties significantly compared to the CD configuration, with slightly lower costs for utilities. The expensive enzyme price contributed around 17−18% of the total running costs. In acid pretreatment, the quantity of the solid carbohydrate fraction directed to enzyme hydrolysis was significantly lower than in alkali pretreatment, with reduced operating costs for the enzyme (Table 4). Besides, the acid pretreatment evaded the process water and NaOH. However, sulfuric acid consumption in alkali pretreatment was much higher in comparison to the acid pretreatment due to the additional quantity needed for neutralizing NaOH after pretreatment. The contribution of sulfuric acid to the total cost of chemicals and utilities was thus slightly higher in acid pretreatment than in alkali. The nutrients, lime, and NaOH (for alkali pretreatment only) were other significant operating cost factors, contributing around 7−10, 6−9, and 5% of the total costs of chemicals and utilities. However, electricity, inoculum, and process water (for alkali pretreatment only) were minor operating cost factors, with less than 2% of the cost of chemicals and utilities.

The acid pretreatment involved lower coproduct credit due to the utilization of lignin fraction for the boiler. The total operating cost was lower in the acid pretreatment than in the alkali one due to lower TCI and operating costs for chemicals and utilities. Therefore, LA manufacturing cost was slightly lower for acid pretreatment (1.35 US$/kg) than for alkali one despite a slightly lower LA production rate (Table 4). On the other hand, for alkali pretreatment, the operating cost was slightly lower for LA separation by RD than CD due to a reduction in TCI and utility demands. Therefore, the LA manufacturing cost was somewhat lower in the RD configuration (1.61 US$/kg) than in the CD configuration (1.67 US$/kg). The pinch analysis lowered around 10−11% of the LA manufacturing costs.

Production Cost Factors. The direct cost stemming from TCI and operating labor was the dominant factor, contributing around 25% for alkali pretreatment and 31% for acid pretreatment of the LA manufacturing cost (Figure 5a). On the other hand, the indirect cost, which was directly related to TCI, contributed about 11 and 14% of the production cost for alkali and acid pretreatments, respectively. The chemicals were another prominent cost-contributing factor. However, the contribution of chemicals to the LA production cost was lower for acid pretreatment (20%) as compared to that for alkali one (25−26%) due to the reduced sulfuric acid consumption and no consumption of process water and NaOH. However, SCB presented around 10−13% of the manufacturing cost. The enzyme consumption was lower in acid pretreatment, with only around 10% share of the production cost compared to 11−12% for alkali pretreatment. The inoculum and nutrients contributed around 5−6% of the production costs. The utilities were the most significant operating cost. The utility consumption was significantly higher in alkali pretreatment, with around 13−14% share of the production cost, compared to only 5% in acid pretreatment. The quantum of coproduct was lesser in acid pretreatment, sharing merely 1% of the production cost compared to 3% in alkali pretreatment. The above discussion evidenced the dominancy of the price of SCB, utilities, chemicals, and enzymes in the LA manufacturing cost. Consequently, the fluctuation of their price will directly affect the LA production cost. Therefore, the sensitivity study was performed to understand the effect of a ± 50% change in their retail price on the LA manufacturing cost (Figure 5b). However, the LA production cost remained below 2.0 US $/kg despite a 50% increase in the individual retail price of the above dominant cost-contributing factors.

Profitability Analysis. The profitability analysis was performed considering 20 years of plant life. The minimum LA selling price (MLSP) was calculated using a 34% income tax and a price escalation of 3.5% for chemicals, operating labor, and utilities and 3% for products. The MLSP was calculated using 8.5, 10, and 15% discount factors and 5, 8, and 10 year payback periods (Figure 6a). The MLSP was lowest for acid pretreatment with the RD configuration due to both lower TCI and operating expenditure. Similarly, the RD configuration in alkali pretreatment showed lower MLSP than the LA separation by CD due to lower TCI and utility demand with reduced operating expenditure. For a 5 year payback period and an 8.5% discount factor, the MLSP was estimated as 2.32

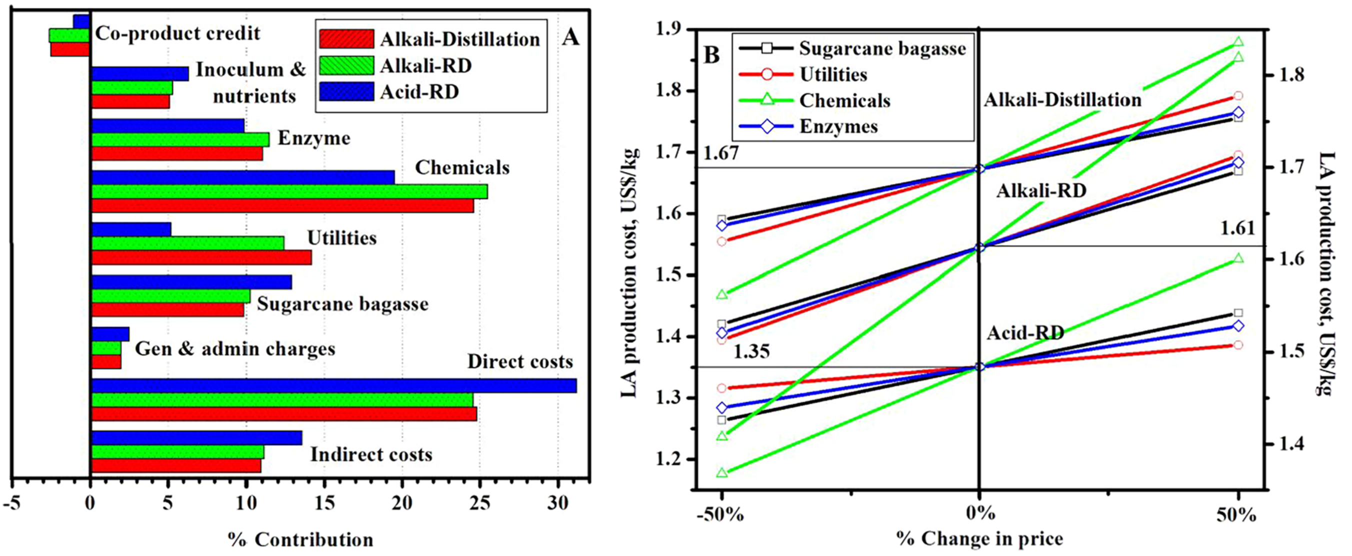


Figure 5. (A) Cost-contributing factors and (B) sensitivity of dominating factors to LA production cost.

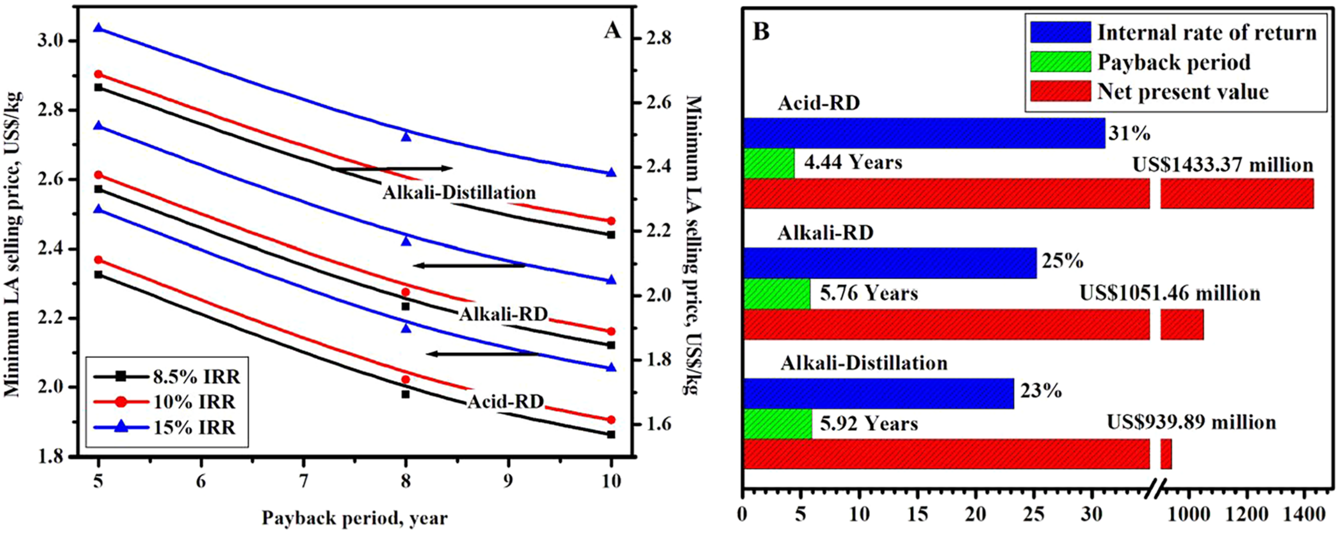


Figure 6. (A) Minimum LA selling price for different payback periods and (B) profitability indicators of the processes.

US$/kg for acid-RD, 2.57 US$/kg for alkali-RD, and 2.65 US $/kg for alkali-CD scenarios. Earlier, Munagala et al. reported the MLSP as 3.20 US$/kg with a payback period of 6 years.[21] The higher MLSP compared to the present study was attributed to the fact that only the glucose fraction of enzymatic hydrolysate from alkali-pretreated SCB was used for LA production, while LA purification was done using RD. State-of-the-art revealed that the LA production cost was merely 1.947 US$/kg when the cellulosic fraction of acid-pretreated SCB after enzymatic hydrolysis was valorized to LA by mixing it with molasses using engineered recombinant *E. coli*.[37] They considered SCB as free and made wise use of molasses to attain higher LA concentrations. Earlier, in the year 2021, Baral et al. reported LA production cost being 2.64 US $/kg wherein SCB was considered free of cost as the authors opted for a configuration annexed to sugar mill. The study involved high-solids alkali pretreatment and high-solids enzymatic saccharification, while the hydrolyzed cellulose fraction was subjected to batch fermentation using thermophilic *B. coagulans* NCIM 5648.[22]

The profitability analysis was further extended to calculate the net present value, payback period, and internal rate of return (IRR), considering an 8.5% discount rate and 2.5 US $/kg as the factory-gate LA selling price for the entire plant life (Figure 6b). The market price of LA varies with country and purity, and it has been reported as 1.874 US$/kg for 80% L(+) LA.[18] However, polymer-grade LA market price has been reported as 1.536 US$/kg in China, 2.793 US$/kg in Germany, and 2.858 US$/kg in the USA.[38] The payback period was quite reasonable for all scenarios, i.e., 5.9 years for alkali-CD, 5.8 years for alkali-RD, and 4.4 years for acid-RD. On the other hand, the IRR (23−31%) and net present value (US$940−1433 million) of these processes were quite high, demonstrating a high return on investment potential. The results of the present study are also comparable with the recent technoeconomic feasibility analysis for the food-waste biorefinery. Among the three products, namely, LA, lactide, and PLA, LA emerged as the most profitable product, with the highest IRR of 31.1% and the shortest payback period of 5.1 years at a discount rate of 5%.[18] Earlier, Farzad et al. also evaluated six scenarios wherein multiple products were targeted from SCB. Their analysis revealed that a maximum IRR of 20.5% could be obtained when ethanol and LA were coproduced from the hydrolyzed fraction of cellulose and hemicellulose.[39] However, when the same group evaluated six different scenarios using LA as the sole product in a sugar cane-based biorefinery, the highest IRR of 21.28% was reported when SCB and brown leaves were subjected to steam explosion and the cellulo-lignin-rich biomass was valorized to LA employing simultaneous saccharification and fermentation. In this gypsum-free process, $Ca(OH)_2$ was replaced with $Mg(OH)_2$ as a neutralizing agent, and triethylamine was used for $Mg(OH)_2$ recovery from Mg-lactate.[15] Further, when the group assessed four different scenarios annexed to a sugar mill, LA production from glucose and xylose derived from SCB, along with electricity production, was the most lucrative option from the economic viewpoint with an impressive IRR of 31.1%.[20] The pretreatment method considered was steam explosion, and later the entire pretreatment slurry was subjected to separate hydrolysis and fermentation.

CONCLUSIONS

The present study demonstrated the technoeconomic viability of stand-alone SCB-to-LA conversion processes involving two pretreatment scenarios (dilute acid and alkali) and two LA separation methods (CD and RD). All processing scenarios were economically viable, with an MLSP of 1.86–2.19 US$/kg and a high IRR (23–31%). However, dilute acid pretreatment with LA separation by RD appeared to be the most cost-effective, with the highest return on investment. The process integration by the pinch method lowered 10–11% of LA manufacturing costs. For alkali pretreatment, the RD configuration involved a lower TCI and utility demand than the LA separation by CD, which was further dropped in acid pretreatment with the RD configuration. The RD configuration in the alkali pretreatment saved 11% heating and 9% cooling energy consumption. The acid pretreatment with LA separation by RD thus showed the lowest LA manufacturing cost (1.35 US$/kg), followed by alkali pretreatment with RD (1.61 US$/kg) and CD (1.67 US$/kg) configurations. Fermenters and hydrolysis reactors were the major capital-intensive equipment, contributing 56–57 and 15–17% of TCI, respectively. For dilute acid pretreatment with RD-based LA separation, SCB (13%), chemicals (20%), enzymes (10%), and utilities (5%) were the major operating costs, besides direct (31%) and indirect (14%) costs. This scenario exhibited an MLSP of 2.32 US$/kg for a 5 year payback period and an 8.5% discount factor. Furthermore, for 20 years of plant life with a factory-gate LA selling price of 2.5 US$/kg, this process demonstrated an IRR of 31% and a net present value of 1433 million US$ for an 8.5% discount rate.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acssuschemeng.5c00223.

> TXY diagram of ML–water; profiles in the RD column; flowsheets with and without process integration; block diagram; and stream data (PDF)

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Notes

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NOMENCLATURE

AD, anaerobic digestion; CAPEX, capital expenditure; CD, conventional distillation; IRR, internal rate of return; LA, lactic acid; ML, methyl lactate; MLSP, minimum LA selling price; MT, metric tons; RD, reactive distillation; SCB, sugar cane bagasse; TCI, total capital investment

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