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Sustainable production of L-lactic acid from lignocellulosic biomass using an alternative buffer system: Process development and techno-economic and environmental analysis

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ABSTRACT

L-lactic acid (L-LA), a key monomer in biodegradable plastics, is a sustainable alternative that can be derived from LCB. The L-LA production process typically involves various technologies such as fermentation, filtration, and distillation. In the L-LA production process, large amounts of buffers are used to maintain proper pH during fermentation, so conventional buffers (e.g., $CaCO_3$) are often selected because of their low cost. However, these buffers cannot be recycled efficiently, and the potential for alternative buffers remains uncertain. In this work, we aim to develop and evaluate novel processes for sustainable L-LA production using the alternative buffer (i.e., KOH). The processes involve a series of different unit operations such as pretreatment, fermentation, extraction, and electrolysis. An efficient buffer regeneration process using membrane electrolysis is implemented to recycle the buffer with minimal energy input. Then, we evaluated the viability of the proposed processes compared to the conventional process based on minimum selling price (MSP), and global warming potential (GWP). The MSP for L-LA was evaluated to be 0.83 USD /kg L-LA, and the GWP was assessed to be 2.93 kg CO_2-eq/kg L-LA. These results represent a 25% reduction in MSP and a 32% reduction in GWP compared to the conventional process. Additionally, a sensitivity analysis was performed to identify the major cost drivers of MSP, such as interest rate, and the price of biomass. The proposed process, as a cost-effective and eco-friendly process, promotes biotechnology practices for sustainable production of L-LA.

Keywords: L-lactic acid, lignocellulosic biomass, alternative buffer, process development, techno-economic analysis

INTRODUCTION

Climate change and food security remain critical challenges for sustainable development [1]. The global dependence on petroleum-based chemicals continues to drive environmental degradation and climate change [2]. To address these challenges, there is growing interest in producing chemicals and materials from renewable resources. Lignocellulosic biomass (LCB) offers a promising sustainable alternative to produce various bio-based materials [3]. One significant LCB-based chemical is lactic acid (LA), which has emerged as a key platform chemical, particularly important in the production of biodegradable plastics [4]. LA exists in two enantiomeric forms, with L-lactic acid (L-LA) being crucial for industrial applications due to its influence on the mechanical and thermal properties of polylactic acid (PLA) [5]. Consequently, numerous studies on LA microbial fermentation technologies focusing on high enantiomeric purity of L-lactic acid (L-LA) have been published, demonstrating the potential to improve the quality and application potential of LA-based products across various industries.

Microbial fermentation is widely used to produce L-LA with a high enantiomeric purity. As with other fermentation processes, the L-LA fermentation process requires various feedstocks, including fermentation medium and other necessary materials. Buffers are particularly important for maintaining an optimal pH level to ensure the efficiency and yield of the process [6]. Notably, calcium-based buffers (e.g., $Ca(OH)_2$ and $CaCO_3$) are commonly preferred in commercial L-LA production due to their cost-effectiveness. However, using these buffers typically results in solid byproducts, such as gypsum ($CaSO_4$), which require disposal and create waste management challenges [7]. Therefore, an alternative buffer system could potentially address these issues by reducing waste and improving the sustainability of the L-LA production process.

In this work, we aim to develop and evaluate novel approaches for sustainable L-LA production using an alternative buffer (i.e., KOH). To achieve this goal, we first established a conventional L-LA production process as a baseline and developed a KOH recycling-based L-LA production (KRL) system incorporating buffer recycling technologies. We then evaluated the economic and environmental impacts of the proposed KRL systems and compared them with those of the conventional process. Additionally, sensitivity analysis was conducted to identify major cost drivers of proposed processes for cost reduction.

TECHNOLOGY OVERVIEW AND ANALYSIS METHODS

Process configuration

Fig. 1(a) represents the baseline L-LA production process, which uses $Ca(OH)_2$ as a buffer in the fermentation stages. After fermentation, H_2SO_4 is mixed to convert L-lactate to L-LA, and the gypsum is filtered out by centrifugation. Crude L-LA is separated and purified by reactive distillation units coupled with the synthesis and hydrolysis of methyl lactate. This baseline process demonstrates the established methodology and operational simplicity of the purification method. However, the generation of gypsum causes significant waste management problems.

In this study, we propose two novel KOH recycling-based L-LA production (KRL) configurations that incorporate advanced buffer recovery and regeneration technologies, as shown in Fig. 1(b) and (c). In the fermentation steps, KOH is used as a buffer to maintain the optimal condition for microbials. H_2SO_4 is substituted with HCl to convert L-lactate to L-LA. The use of HCl allows the KOH to be regenerated using alternative downstream processes. Solvent extraction and back-extraction units are employed for buffer recovery, L-LA separation, and purification. Solvent extraction effectively separates the impurities from the L-LA, while KCl releases the salts. The distillation unit purifies L-LA to high concentration by removing water and residual impurities while operating under vacuum conditions. The stream containing KCl is subjected to membrane filtration for conditioning. Alkaline water electrolysis decomposes KCl and water to regenerate KOH. This reaction also produces hydrogen (H_2) and chlorine (Cl_2) gases as byproducts. In addition, the first alternative configuration (KRL #1) employs gas treatment units to clean the byproduct gases. The purified byproduct gases can be sold, contributing to the economic potential of the process.

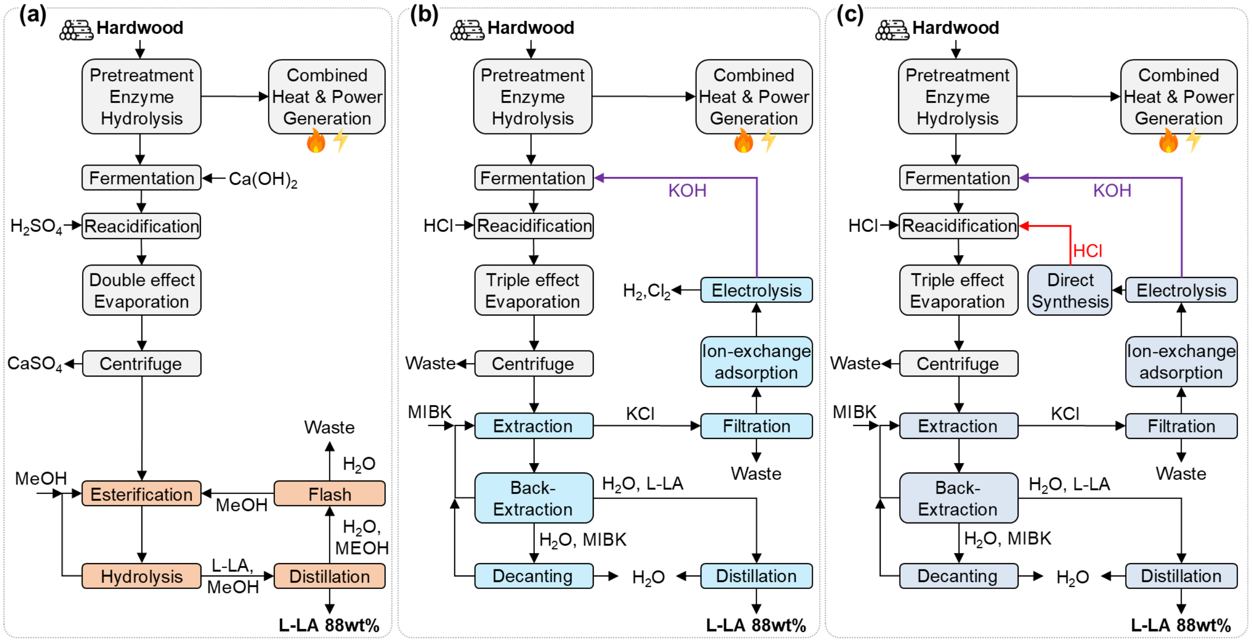

Figure 1: Block diagrams of the L-lactic acid production from lignocellulosic biomass. (a) baseline process; (b) KRL #1: KOH recycling-based process; (c) KRL #2: KOH and HCl recycling-based process.

On the other hand, as shown in Fig. 1(c), the second alternative configuration (KRL #2) includes HCl regeneration steps where H_2 and Cl_2 gases are reacted to produce an HCl solution. This HCl solution is then used in the reacidification unit to enhance the recycling loop. Accordingly, the novel KRL system offers key advantages over the conventional process through integrated recycling technologies. These improvements minimize raw material consumption and waste generation, thereby enhancing both economic viability and environmental sustainability.

Technology overview

Pretreatment and enzymatic hydrolysis

Pretreatment converts hemicellulose to sugars, degrading LCB for efficient enzymatic hydrolysis. In this area, LCB is treated in high-temperature dilute H_2SO_4 for degradation. It is then neutralized with ammonia to pH 5 for optimal enzymatic hydrolysis. This technique directly conditions the entire hydrolysate slurry without the need for solid-liquid separation, thereby improving sugar recovery [8]. Table S1 in Digital Supplementary Information (SI) presents the major reactions and process conditions.

In this study, the feedstock for the process is 1000 dry tons/day of Eastern cottonwood, a hardwood species. Hardwoods are widely used in bioprocessing due to their high cellulose and hemicellulose content and low inhibitor content compared to other biomass species. The composition of Eastern cottonwood is provided in Table S2 in SI. This composition is implemented in Aspen Plus V12.0 software using an in-house physical property NREL database to ensure an accurate representation of the biomass components [9].

L-LA fermentation

Microbial fermentation is a preferred method for L-LA production due to its ability to achieve high optical purity. In this process, sugars derived from LCB are converted to L-LA by microbial metabolism. As a microbial strain, thermophilic Bacillus coagulans was used in this study due to its capability to co-utilize hexose and pentose sugars efficiently [10,11]. This co-utilization of carbon sources minimizes by-product formation and maximizes L-LA yield. The fermentation process uses $Ca(OH)_2$ or KOH as a buffer to maintain optimal pH levels. The buffer reacts with the L-LA released by the microbes to form L-lactate. This ensures stable microbial activity and improves L-LA productivity.

Separation and purification

After fermentation, insoluble cellular material is first separated from the broth by centrifugation. Then, the crude L-lactate mixture is treated with a strong acid to convert L-lactate to L-LA in the acidification reactor. The crude L-LA stream is concentrated via a multi-effect evaporator unit. The conventional process employs the reactive distillation units to separate other impurities and purify L-LA. L-LA in the concentrated stream is converted into methyl L-lactate by esterification coupled with a distillation. Then, another reactive distillation unit for hydrolysis is used to decompose methyl L-lactate into L-LA and purify L-LA. The raw L-LA is purified to over 88wt% in the distillation column.

The novel configurations (KRL #1 and KRL #2) employ liquid-liquid extraction units with methyl isobutyl ketone (MIBK) as the extraction solvent to effectively remove heavy impurities from the concentrated stream. The extracted solution is back-extracted with water to transfer the L-LA and ions to the aqueous phase, leaving the light impurities to remain in the solvent. The MIBK solvent is then recovered by decanting and distillation. Finally, the aqueous L-LA stream is further concentrated and purified by evaporation and distillation to achieve the L-LA product of over 88wt% purity.

Alkaline water electrolysis and acid gas synthesis

The regeneration of KOH is achieved through an integrated system involving the electrolysis of KCl. In the alkaline water electrolysis step, a fluorinated cation exchange membrane was used to decompose water and KCl. The membrane enables high current efficiency and low voltage operation, achieved through its selective ion transport properties and enhanced chemical stability under alkaline conditions [12]. Additionally, the electrolysis reaction also generates H_2 and Cl_2 gases as byproducts. In KRL #1, these by-product gases are purified and prepared for sale as chemical products. The H_2 gas from the alkaline water electrolysis achieves 99.97% purity through pressure swing adsorption using a molecular sieve hierarchical adsorbent. The adsorption columns operate at 30°C-35°C with pressure cycling up to 34 bar, resulting in the H_2 recovery of 91.9% [13]. The chlorine gas is dried through desorption using concentrated sulfuric acid, which effectively removes moisture to achieve a final purity of 99.99%. These high-purity byproducts provide a significant source of revenue. By contrast, KRL #2 uses these gases directly in the acid gas synthesis unit. The H_2 and Cl_2 gases react to form dry HCl gas. This gas is absorbed into deionized water to make an aqueous HCl solution, which is used in the reacidification unit.

Process analysis method

The proposed processes were simulated and modeled using Aspen Plus V.12 software. We evaluated the economic and environmental impacts of the developed process with mass and energy balances obtained from the process simulation. In this study, the viability of the proposed process was evaluated against the conventional process based on minimum selling price (MSP), and global warming potential (GWP).

For the economic evaluation of the L-LA production processes, the MSP was used as a primary indicator of economic viability. The MSP represents the product's sale price at the break-even point, where total revenue matches total expenses. The total revenue is generated from the sales of L-LA, while the total expenses include the annualized return on investment (ROI), fixed operating costs, and taxes.

The ROI was determined based on the total project investment (TPI), the interest rate, and the process lifetime, as in Eq. (1).

$$ROI = TPI \times \frac{i \times (1+i)^r}{(1+i)^r - 1} \tag{1}$$

where i represents the interest rate, and r denotes the lifetime of the process. The TPI, which includes both direct and indirect costs, was determined using cost estimation and scaling methods applied to simulation results. In addition, mass and energy balance data obtained from the process simulation were used to estimate the fixed and variable operating costs. Depreciation was calculated using Eq. (2). Income tax was determined based on the net income and applicable tax rate, as detailed in Eq. (3).

$$Depreciation = \frac{TPI}{Lifetime} \tag{2}$$

$$Tax = (Profit - Depreciation) \times Tax\ rate \tag{3}$$

Finally, the MSP was calculated by dividing the sum of the annualized ROI, total operating expenses, and taxes by the total amount of L-LA produced annually, as shown in Eq. (4).

$$MSP = \frac{ROI + Expense + Tax}{The\ amount\ of\ L{-}LA} [\$/kg_{L-LA}] \tag{4}$$

The GWP was assessed as an environmental performance metric through life cycle assessment (LCA) methodology, representing the total CO_2 equivalent emissions per unit of L-LA produced. The system boundary encompasses raw material extraction, transportation, utility, and waste treatment from manufacturing operations. The GWP analysis quantifies direct CO_{2eq} emissions from process vent streams and indirect CO_{2eq} emissions from utility consumption. It also takes account of emissions associated with waste disposal, input material production, and transport. The assessment followed ISO 14040 and 14044 standards, with inventory factors sourced from the Greenhouse gases, Regulated Emissions, and Energy use in Technologies (GREET) model [14].

RESULTS AND DISCUSSION

Simulation results

In this section, key operational parameters are discussed to provide a detailed understanding of the performance of each process. The operability of the proposed processes was assumed to be 7980 h operation per year. The baseline L-LA production process can produce 88wt% L-LA of 178,752 tons/year. The supplied amount of $Ca(OH)_2$ is 78,204 tons/year on a dry basis and then gypsum waste of 152,418 tons/year is removed via centrifugation after the reacidification unit. The downstream esterification and hydrolysis steps demonstrated a recovery efficiency of 94.9%.

Both KRL #1 and KRL #2 processes achieved an annual production of 197,673 tons/year of 88wt% L-LA. The supplied amount of KOH is 11,387 tons/year on a dry basis. The liquid-liquid extraction steps efficiently removed impurities, with an L-LA recovery efficiency of 85.7%. Separation and electrolysis units regenerated over 96.5% of the KOH supplied to the fermenters. The electrolysis units in KRL #1 produced byproduct gases, H_2 and Cl_2, at rates of 2,394 tons/year and 84,588 tons/year, respectively. In KRL #2, the HCl recovery rate exceeded 87.0% of the HCl supplied to the reacidification reactor,

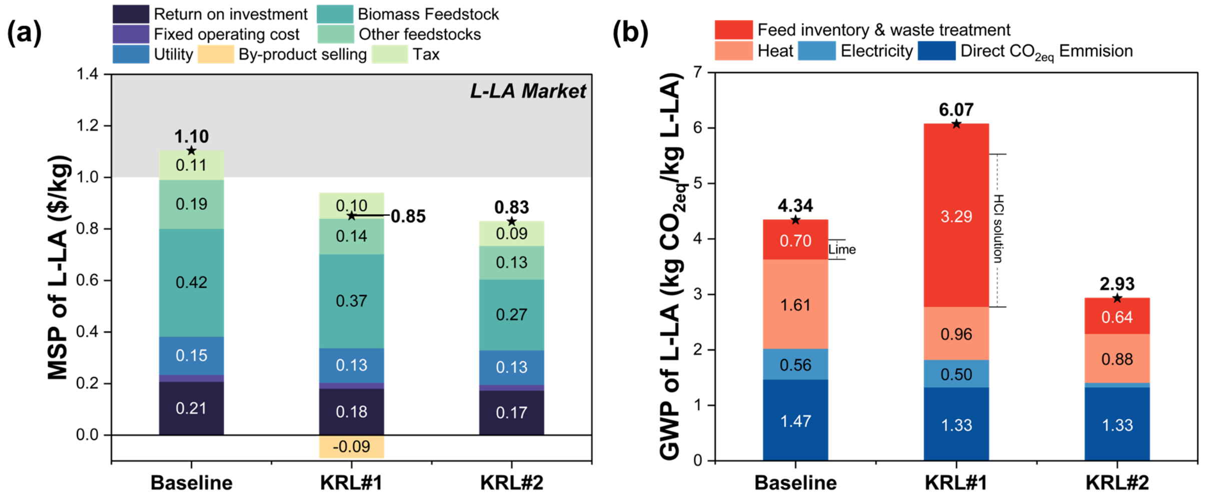

Figure 2. (a) MSP and (b) NCE of produced L-LA via the baseline and proposed processes

reducing the reliance on external inputs.

Techno-economic and environmental analysis

The economic and environmental performance of the developed processes were evaluated using the MSP and GWP as key indicators. As shown in Fig. 2, the proposed KRL system leads to a decrease in the MSP of L-LA. One of the major drivers of this cost reduction was the higher L-LA production rate in the KRL processes compared to the baseline process. Additionally, the introduction of KOH, together with the implementation of advanced buffer recycling technologies, reduced the cost of buffer materials and waste disposal. The favorable results of KRL #2 can be attributed to the integration of effective regeneration and reuse of KOH, which are also present. These elements were further enhanced in KRL #2 through the integration of the HCl recycling loop, optimizing material utilization and reducing production costs. As a result, KRL #2 achieved an MSP of 0.83 \$/kg, representing a 25% reduction compared to the baseline MSP of 1.10 \$/kg.

In terms of environmental performance, the baseline process demonstrated a relatively higher GWP compared to KRL #2, attributed to the substantial use of Ca(OH)$_2$ and the indirect emissions from utility consumption. KRL #1 exhibited a GWP of 3.45 kg CO$_{2\text{-eq}}$/kg L-LA, which represents an increase of 40% compared to the baseline process. This is due to the energy-intensive electrolysis and high consumption of HCl. Conversely, KRL #2 exhibited the lowest GWP of 2.93 kg CO$_{2\text{-eq}}$/kg L-LA, showing a reduction of 51% relative to the baseline process. The recycling of HCl in KRL #2 significantly reduced material consumption, reducing the CO$_{2eq}$ inventory of raw materials.

Sensitivity analysis

A sensitivity analysis was performed to identify the key economic parameters influencing the MSP of L-LA. The sensitivity analysis evaluated how much MSP of L-LA would change if the economic parameters varied by ±20%, as presented in Fig. 3. The detailed values of major economic parameters used in the sensitivity analysis are provided in Table S3 in SI. For the baseline process, the interest rate was the most sensitive factor on MSP, affecting a change of up to +4.69%. The biomass feedstock price was the second largest influential factor, with a ±2.63% variation. For the KRL processes, the interest rate was also the most sensitive factor, with a change of up to 5.20%. Biomass feedstock is another sensitive factor, causing a variation of ±3.08% and ±3.17% in KRL #1 in KRL #2, respectively. Consequently, we identified the interest rate and biomass feedstock price as the main cost drivers influencing the MSP of the developed processes. These results indicate the importance of optimizing these parameters to improve the economic viability of L-LA production.

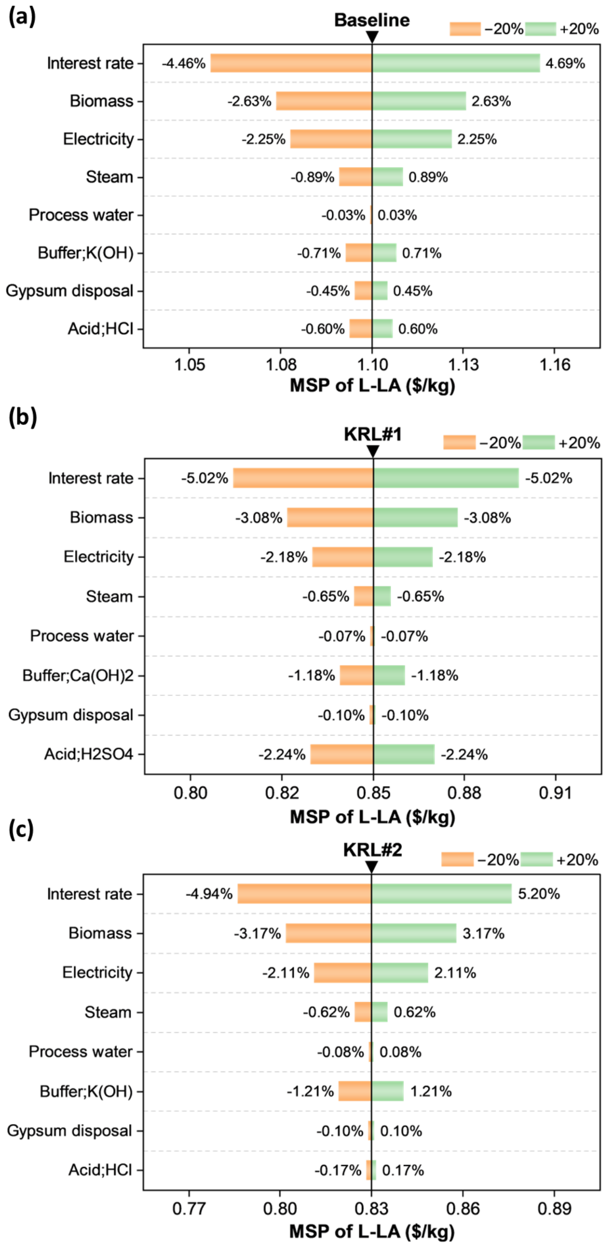

Figure 3. Sensitivity of the major economic parameters on the MSP

CONCLUSIONS

This study developed the conventional L-LA production process and the novel KOH recycling-based L-LA production system for producing high enantiomeric purity of L-LA from LCB. Then we evaluated the economic and environmental performances of the developed processes. Then we evaluated the economic and environmental performances of the developed processes. In economic evaluation, KRL #1 exhibited improved economics due to cost reduction from buffer recycling and byproduct utilization. KRL #2 demonstrated the best improvements in economic performance by incorporating HCl solution synthesis units. The MSP of L-LA was 0.83 $/kg for KRL #2 and 0.89 $/kg for KRL #1, representing cost reductions of 23% and 25%, respectively, compared to the baseline process. However, the environmental performance of KRL #1 was limited by the significant electricity demand and the extensive use of HCl. Conversely, the GWP of L-LA via KRL #2 was 2.93 kg $CO_{2\text{-eq}}$/kg, representing a 51% reduction compared to the baseline process. Furthermore, the sensitivity analysis revealed that the interest rate and biomass feedstock price are the main cost drivers. Addressing these key economic drivers will be essential to further enhance the viability of the developed L-LA production processes. This study highlights the potential of integrating advanced recycling technologies to achieve both economic and environmental benefits, promoting biotechnology practices for sustainable production of L-LA.

DIGITAL SUPPLEMENTARY MATERIAL

The following materials are available in the Living Archive for Process Systems Engineering (LAPSE:2025.0021): These materials provide comprehensive information for reproducing the results presented in this study.

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