Superior Performance in Reactive Distillation Method for Industrial Application: A Case Study of Ethyl Lactate Production

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Abstract. *Ethyl lactate, a biodegradable and environmentally friendly solvent, offers a sustainable alternative to conventional petroleum-based solvents. This study presents a comprehensive evaluation of ethyl lactate production through both conventional and intensified process designs using rigorous process simulation. The reactive distillation column (RDC) was identified as the most efficient configuration, achieving notable reductions in total capital cost (57.3%) and total operating cost (40.2%) compared to traditional setups. The NRTL thermodynamic model was employed to accurately capture non-ideal behavior among reactive components, and kinetic parameters were validated against experimental data. The results demonstrate that RDC-based process intensification significantly enhances economic performance while promoting sustainable chemical manufacturing, positioning it as a promising approach for future green solvent production.*

Keywords: Reactive distillation, Ethyl Lactate, Green Solvent, Process intensification, Aspen Plus.

1. INTRODUCTION

Green solvents are essential for promoting environmentally sustainable and safer chemical processes. Unlike traditional petroleum-based solvents, which are often toxic, volatile, and non-biodegradable, green solvents are typically derived from renewable resources, biodegradable, and exhibit low toxicity [1]. Their use significantly reduces the environmental impact of industrial operations by minimizing air and water pollution, as well as soil contamination. In addition, green solvents enhance workplace safety by lowering exposure to hazardous substances. They also support global efforts toward sustainability by decreasing reliance on finite fossil fuels and aligning with green chemistry principles. As regulatory frameworks become increasingly strict regarding environmental and occupational safety, the adoption of green solvents like ethyl lactate becomes not only beneficial but necessary for compliance and long-term industrial viability [2].

Ethyl lactate is a biodegradable and environmentally friendly solvent derived from renewable resources, making it an attractive alternative to traditional petroleum-based solvents. It is an ester formed through the reaction of lactic acid and ethanol, typically via esterification in the presence of an acid catalyst [3].

Lactic acid can be obtained from fermentation of carbohydrates such as glucose or starch using *Lactobacillus* species, while ethanol is commonly produced from biomass through fermentation [4]. The production of ethyl lactate is of growing interest due to its low toxicity, high solvency power, and biodegradability, making it useful in applications ranging from pharmaceuticals and food processing to industrial cleaning and green chemistry.

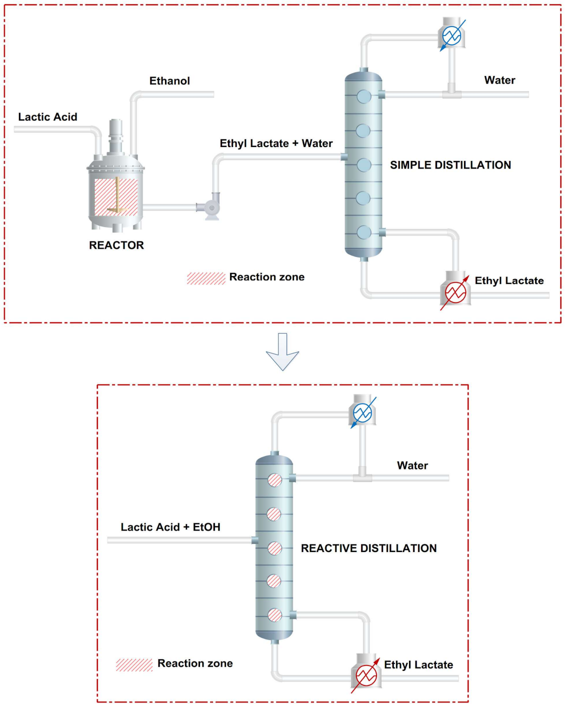

Figure 1. Hierarchy of the process design.

Recent research in this field focuses on optimizing production processes, such as using reactive distillation, enzymatic catalysis, or heterogeneous catalysts, to improve yield, reduce energy consumption, and make the process more sustainable and cost-effective [5], [6].

Several studies have explored ethyl lactate production using various reactor setups. Pereira et al. [7] used a batch reactor focusing on kinetics and adsorption, without detailed process modeling. Delgado et al. [2] combined a batch reactor with a pervaporation unit but only at the experimental scale. Daengpradab and Rattanaphanee [8] investigated small-scale synthesis via esterification of magnesium lactate using one reactive distillation column (RDC) and three separation units, considering only the primary reaction. Adams and Seider [9] proposed semicontinuous, continuous (PFR and CSTR), and batch (RBatch) processes, but ignored oligomeric reactions. Tusson-Pizzon et al. [1] analyzed the process using the LHHW kinetic model, addressing economic, safety, and sustainability aspects but excluding oligomers. Dai et al. [3] evaluated a process using RDC and pervaporation, yet no study has compared conventional and intensified designs in terms of capital and operating costs. This work addresses that gap by simulating a conventional PFR-based design and comparing it with RDC-based intensified processes using direct and extractive distillation strategies. Fig. 1 shows the conceptual design of conventional design transforms to RDC. Residue curve map analysis is also conducted, followed by a comprehensive economic evaluation of all designs.

2. MODEL VALIDATION

2.1. Thermodynamic Model

In the production of ethyl lactate, accurate thermodynamic modeling is essential for simulating reaction and separation processes, particularly when using reactive distillation or extractive distillation systems. The choice of a thermodynamic model depends on the phase behavior, polarity, and non-ideality of the components involved, namely lactic acid, ethanol, ethyl lactate, and water.

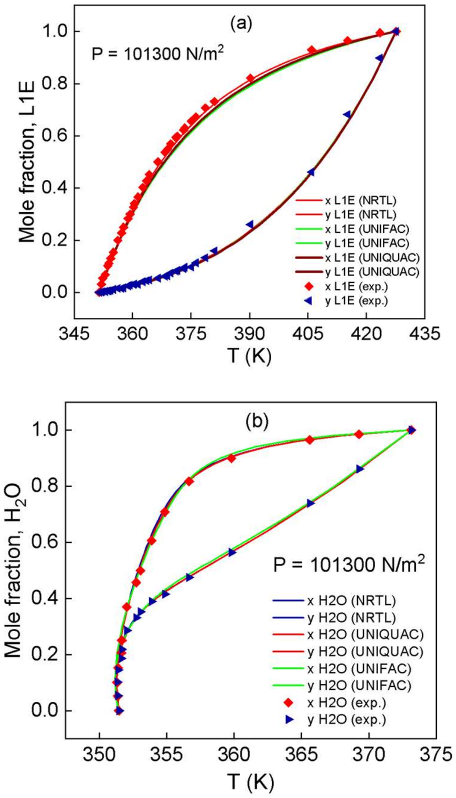

Figure 2. Thermodynamic models validation: (a) L1E-ETOH with the experimental data by Pena-Tejedor et al. [10]; (b) H_2O-ETOH with the experimental data by Lai et al. [11].

For ethyl lactate production involving esterification and separation (e.g., reactive distillation), the NRTL model is most commonly recommended due to its ability to handle non-ideal interactions, particularly in aqueous-organic polar mixtures like those involving lactic acid, ethanol, ethyl lactate, and water [10], [12]. Fig. 2 shows the accurate prediction of the component interaction by several thermodynamic models. Althiugh all three models are qualified for the model prediction, NRTL is more suitable once the separation process by extractive distillation is cosidered [6].

2.2. Kinetic Model

The primary reaction involved in ethyl lactate production is the esterification process (Eq. (1)). Nonetheless, several side reactions may also take place, as shown in Eqs. (2) to (8). Among these, oligomerization reactions are represented by Eqs. (2) and (3). Due to the relatively low equilibrium constants for L_2E and L_3E [19] and the limited availability of kinetic data for the esterification reactions in Eqs. (4) to (8), these side reactions are excluded to simplify the model. As a result, only the kinetic parameters for Eqs. (1) through (3) are considered. Amberlyst-15 is used as the catalyst, with kinetic data sourced from existing literature [20]. Although heterogeneous catalysts derived from materials such as empty fruit bunch, montmorillonite, and diatomaceous earth have demonstrated excellent reusability, their kinetic parameters have not yet been reported [21].

$$L_1 + ETOH \Leftrightarrow L_1E + H_2O \tag{1}$$

$$L_1 + L_1 \Leftrightarrow L_2 + H_2O \tag{2}$$

$$L_2 + L_1 \Leftrightarrow L_3 + H_2O \tag{3}$$

$$L_2 + ETOH \Leftrightarrow L_2E + H_2O \tag{4}$$

$$L_3 + ETOH \Leftrightarrow L_3E + H_2O \tag{5}$$

$$L_2E + ETOH \Leftrightarrow 2\ L_1E \tag{6}$$

$$L_3E + 2\ ETOH \Leftrightarrow 3\ L_1E \tag{7}$$

$$L_3E + ETOH \Leftrightarrow L_1E + L_2E \tag{8}$$

The kinetic parameters were validated using experimental data from Asthana et al. [19], under the following reaction conditions: a feed composed of 50 mol% lactic acid solution (0.152 L1, 0.843 H_2O, 0.005 L2), an ethanol-to-lactic acid molar ratio (ETOH/L1) of 3, and a reaction temperature of 80°C. The reaction was simulated in a batch reactor using the RBatch module in Aspen Plus. As shown in Fig. 5, the model results (solid line) closely match the experimental data (dots), confirming that the model accurately represents the experimental behavior.

3. PROCESS DESIGN

3.1. Conventional Process

Before designing RDC for ethyl lactate production, a conventional setup using a Plug Flow Reactor (PFR) in Aspen Plus is first developed for comparison. Operating conditions are listed in Table 1, and the conversion of lactic acid (L1) and yield of ethyl lactate (L1E) are calculated using Eqs. (9) and (10).

$$L_1 conversion = \frac{F_{L1,in} - F_{L1,out}}{F_{L1,in}}\ x\ 100\% \tag{9}$$

$$L_1E\ yield = \frac{F_{L_1E,out}}{F_{L_{1,in}}}\ x\ 100\% \tag{10}$$

Table 1. Operating conditions and design specifications of conventional design [6].

Parameter		Value
Operating pressure (atm)	PFR	1
	DC-1	1
	DC-2	1
	DC-3	1
Feed flow rate L_1 (kg/h)	-	175.79
Feed flow rate ETOH (kg/h)	-	321.882
Feed composition L_1 50% (mass fraction)	L_1	0.461
	L_2	0.027
	H_2O	0.512
Feed composition ETOH 90 % (mass fraction)	ETOH	0.958
	H_2O	0.042
Product specification (mole fraction)	L_1E	0.99
Number of stages	DC-1	15
	DC-2	12
	DC-3	26
Feed stage	DC-1	13
	DC-2	25
	DC-3	4

In this study, the conventional reactor refers to a plug flow reactor (PFR), with four key design variables analyzed for their impact on ethyl lactate (L1E) production: ethanol flow rate, reactor temperature, diameter, and length.

The results show that the L1 conversion and L1E yield reach 69.37% and 66.1%, respectively, with a final L1E yield of 60.92% after separation losses. In comparison, a CSTR setup yields around 65%

conversion [13], while Tusson-Pinzón et al. [11] reported a higher conversion of 83%, likely due to their model excluding oligomerization reactions and using pure L1 feed, which simplifies the reaction environment. In contrast, this study uses a 50 wt% L1 feed and includes oligomer formation, making the model more representative but less idealized. Additionally, Amberlyst 15 resin, used as a catalyst, selectively absorbs water and swells, adding unpredictability to the reaction phase [14].

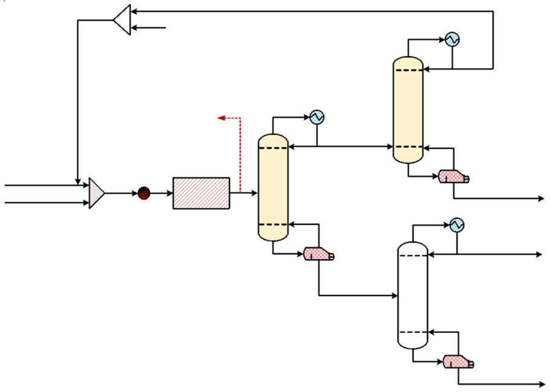

Figure 3. Conventional design of ethyl lactate production combined with direct separation. The make-up streams are required to meet the fresh feed compositions.

Fig. 3 summarizes the conventional design, which includes a PFR and three distillation columns. Operating conditions were selected based on prior sensitivity analysis, though full process optimization was not performed. With a reaction temperature of 80°C, preheating is required with a heating duty of 27.56 kW. Based on boiling points, distillation is suitable for separating products and unreacted components. In contrast to Tusson-Pinzón's design, which used 100 wt% L1 and allowed DC-2 bottoms recycling due to high purity (99.99%), this study's 50 wt% L1 feed leads to more complex behavior. During separation in DC-1, water removal changes the composition significantly (e.g., to XL1 = 0.877), making control difficult. If recycling is intended, extra treatment—such as water addition—would be necessary.

Fig. 5 presents the composition profiles for ethyl lactate production using direct separation in the conventional design. In DC-1, ETOH/H_2O is separated from heavier components (L1/L2/L3/L1E) using 15 stages and 226.7 kW of reboiler duty (Fig. 5a). This is more energy-efficient than DC-3, which separates ETOH and H_2O directly with 26 stages and 283.6 kW due to their small boiling point difference (22°C) (Fig. 5b). DC-2, with only 14.33 kW of reboiler duty, benefits from a larger boiling point gap (62°C) between L1 and L1E and a lower feed flow (0.56 kmol/h). L1E is obtained at the top of DC-2 with 99% purity (Fig. 5c), while the bottom stream, mainly L1 (0.877 mol fraction), is not recycled.

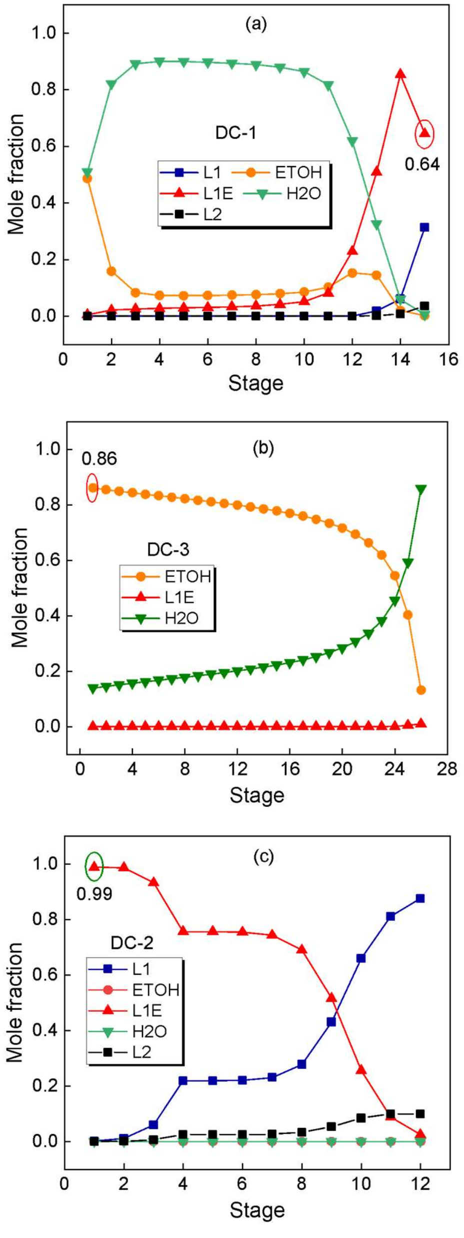

Figure 5. Composition profile of ethyl lactate production: (a) DC-1 separates ETOH/H_2O mixture and $L_1E/L_1/L_2$ mixture; (b) DC-2 separates L_1E and L_1/L_2 mixture; (c) DC-3 separates ETOH and H_2O.

3.2. Reactive Distillation

The RDC offers a process intensification alternative to conventional designs. This study proposes an RDC-based process for ethyl lactate production, combined with various separation strategies, followed by an economic evaluation. The initial RDC setup is adapted from Miller et al. [15] and Da'an et al. [16], and simulations are performed on a mole basis for easier comparison. As shown in Fig. 6, the top product stream closely matches reference data, while the bottom stream shows minor deviations but maintains a similar trend (Figs. 7). A high mole fraction of ethyl lactate (L1E) is observed at stage 56, suggesting the use of a side stream for improved product withdrawal. This side stream approach enhances separation efficiency, reduces CO_2 emissions, and lowers total annual costs [17].

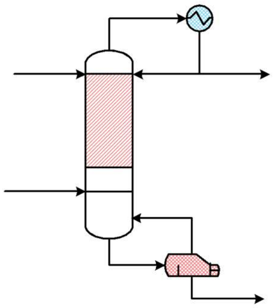

Figure 6. Comparison results of RDC for ethyl lactate production in the present work and the reference [16].

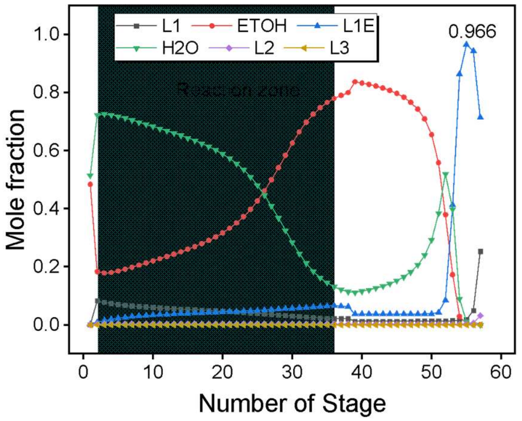

Figure 7. Composition profile of RDC: (a) Present study; (b) Reference by Dai et al. [16].

The RDC design with a side stream is shown in Fig. 8, with product composition closely matching the reference. After optimizing operating conditions, product purity increased to 96.7% at stage 50 (Fig. 9). L1E yields were 88.43% and 91.63% for the current study and reference, respectively—both higher than those from the RDC without a side stream, which gave 72.06% and 93.64%.

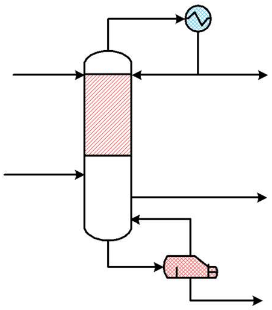

Figure 8. RDC for ethyl lactate production with side stream product. The reference referred to studied by Dai et al. [16].

The top RDC product was an ETOH/H_2O mix (0.47/0.52 mole fraction), while the bottom contained unreacted L1 (0.678) and oligomer L2 (0.321). RDC’s key advantage is simultaneous reaction and separation, allowing product separation by boiling points. Fig. 10 shows the RDC with direct separation setup, where ETOH/H_2O is separated in a single column, but unreacted L1 is not recycled due to high L2 content (32.1 mol%). Recycling in the process design helps reduce material costs. With an ETOH-to-feed (L1, 50 mol%) molar ratio of 1.3 and an L1 mole fraction of 0.152 (0.899 kmol/h), only 0.899 kmol/h of ETOH reacts based on stoichiometry. This means about 6 kmol/h of the 7.44 kmol/h ETOH feed must be recycled. However, the recycled ETOH has a lower purity (86.1 mol%) than the fresh feed (90 mol%), so a 1.19 kmol/h make-up stream of high-purity ETOH (95 mol%) is added to restore the desired composition.

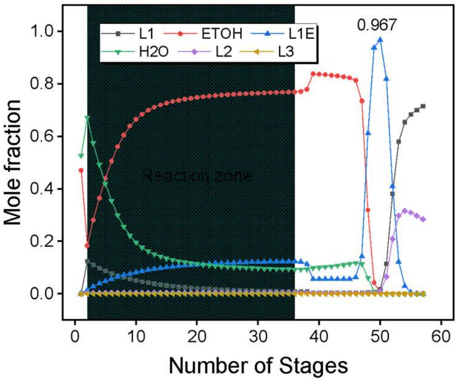

Figure 9. Composition profile of RDC with side stream.

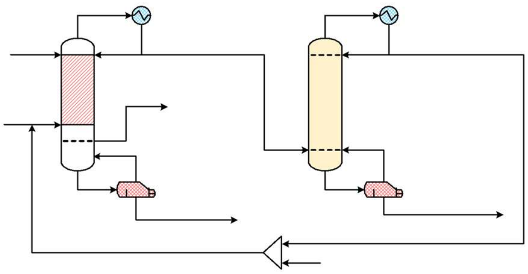

Figure 10. RDC design: using side steam combined with direct separation 1.

4. ECONOMIC ANALYSIS

For a fair comparison of process performance, all designs use the same feed flow rate and composition. The lactic acid (50%) feed is set at 5.921 kmol/hr (175.792 kg/hr), and ethanol (90%) at 7.44 kmol/hr (321.882 kg/hr). Feed material costs are excluded from the cost analysis. Fig. 11 presents the total reboiler duty for each design, with energy consumption in the conventional process covering the heater (HT), DC-1, DC-2, and DC-3.

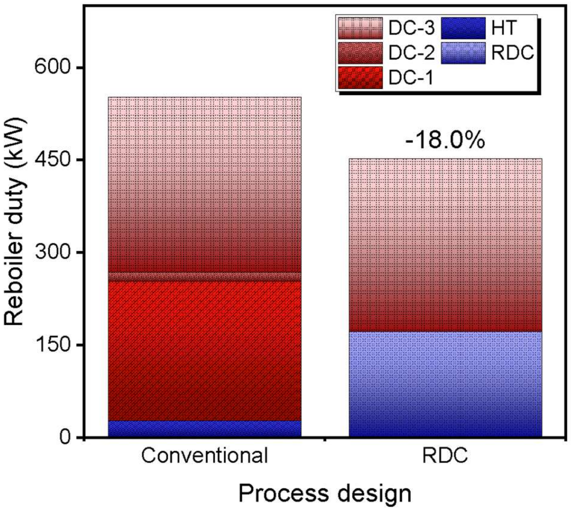

Figure 11. Reboiler duty comparison.

The total annual cost (TAC) in this study is the sum of the total operating cost (TOC) and total capital cost (TCC). TOC covers steam, cooling water, and electricity, while TCC includes equipment, installation, and catalyst costs. TAC is calculated using Eq. (21) [18], [19] with an 8-year payback period [34]. Cost estimation is performed using Aspen Plus Economic Analyzer (APEA), which provides capital and operating cost estimates, investment analysis, and visual process comparisons [60].

$$TAC = TOC + \frac{TCC}{payback\ period} \tag{11}$$

Fig. 12 presents a comparative analysis of total costs across two process designs. The conventional design incurs the highest equipment costs, with DC-3 being the most expensive unit at 820.1 kUSD, followed by the PFR (698.1 kUSD), DC-1 (641.5 kUSD), DC-2 (500.4 kUSD), and the heater (60.8 kUSD) (Fig. 12a). These capital costs reflect the larger number of equipment units required. The total capital cost (TCC) for the conventional process is higher than that of the RDC designs, primarily because the reactor is separate from the separation units, necessitating at least one standalone reactor and three distillation columns. In contrast, the RDC design significantly reduces TCC by 57.3%, requiring only two main units: the RDC and DC-3. This reduction is achievable because the product is withdrawn as a side stream, leaving only the ethanol/water mixture to be separated.

Although the RDC offers a substantial reduction in total capital cost (TCC), achieving savings of 57.3%, its impact on the TOC is comparatively modest, with a savings of only 7.27% as illustrated in Fig. 12b. Additionally, the reduction in reboiler duty—a key factor influencing energy consumption—is limited to just 18%. This suggests that while RDC-based designs are highly effective in minimizing capital investment due to process intensification and equipment integration, they do not provide equally significant reductions in ongoing operational expenses or energy usage [20]. Consequently, further optimization or hybrid process strategies may be needed to enhance overall efficiency.

Based on the TCC and TOC analyses, the most significant cost reduction in terms of TAC was observed in the RDC design. Specifically, the RDC configuration achieved the highest savings in TCC, reducing capital investment by 57.3% compared to the conventional design. Furthermore, the RDC also demonstrated superior economic performance in terms of operating cost, with a TOC reduction of up to 40.2%, as illustrated in Fig. 12c. These findings highlight the economic advantages of process intensification using RDC, offering a more cost-effective and efficient alternative for ethyl lactate production by minimizing both equipment investment and long-term operational expenses.

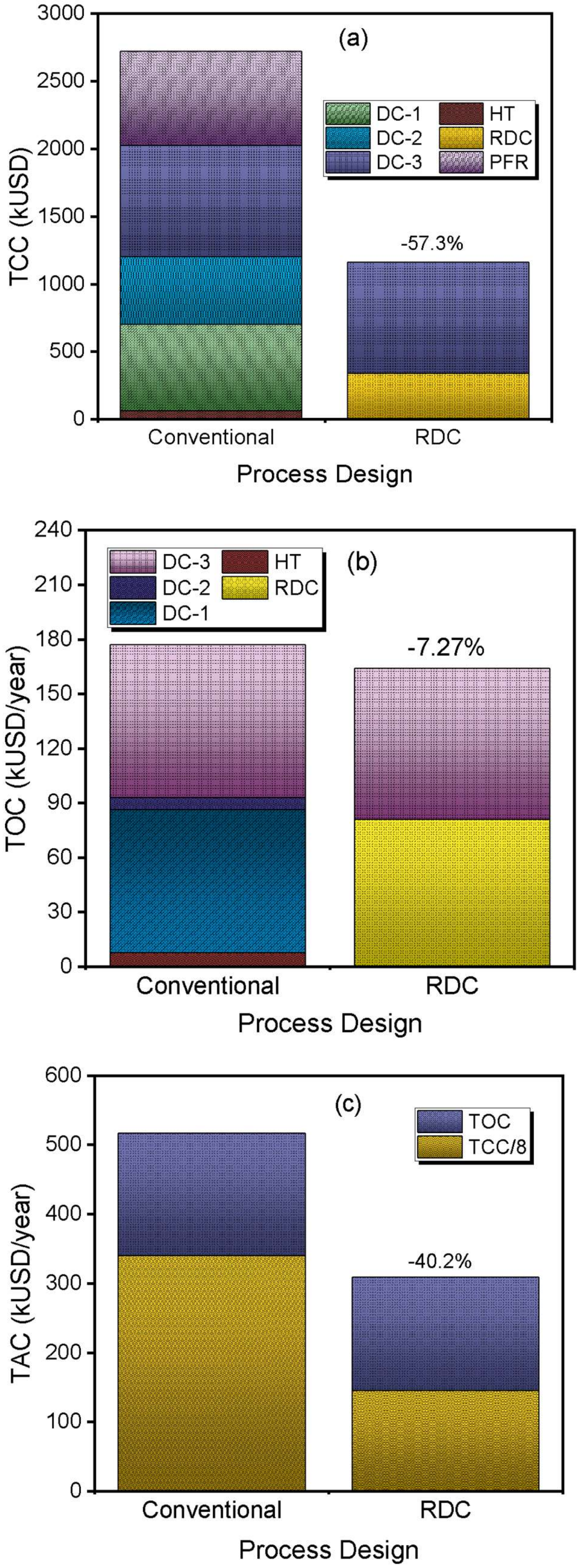

Figure 12. Total comparison cost analysis: (a) Total capital cost, TCC; (b) Total operating cost, TOC; (c) Total annual cost, TAC. Noted: the payback period is set to 8 years.

5. CONCLUSION

The production of ethyl lactate, a green and biodegradable solvent, presents a sustainable alternative to conventional petroleum-based solvents, aligning with global efforts toward environmentally friendly chemical processes. The adoption of green solvents is increasingly important due to their lower toxicity, renewable origins, and reduced environmental impact. In this study, a comprehensive evaluation was conducted, comparing conventional and intensified process designs using rigorous simulation. Among the alternatives, the reactive distillation column (RDC) emerged as the most promising, offering significant reductions in both total capital cost (TCC) and total operating cost (TOC)—by 57.3% and 40.2%, respectively. The use of the NRTL thermodynamic model enabled accurate representation of the non-ideal interactions among components, while kinetic parameters were successfully validated against experimental data from the literature.

Overall, the findings confirm that process intensification through RDC not only improves economic feasibility but also supports the broader goal of sustainable chemical manufacturing. This positions RDC-based ethyl lactate production as a viable and efficient solution for future green solvent applications.

ACKNOWLEDGE

The author gratefully acknowledges that this research was fully supported through self-funding. The dedication and commitment to advancing sustainable chemical processes were made possible by personal resources and independent effort.

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