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Research Article

Enhancing Ethyl Acetate Conversion from Acetic Acid Esterification by Optimizing Reactant Mole Ratio and Reaction Temperature

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Abstract

Ethyl acetate is among the most widely utilized and produced compounds in the chemical industry, serving as a key solvent in coatings, adhesives, pharmaceuticals, and various synthesis processes. Its production typically occurs through the esterification of acetic acid with ethanol, a reaction that is both exothermic and reversible. These characteristics make the control of operating conditions critically important for achieving high conversion rates and minimizing energy consumption. In this study, the optimization of two primary operating parameters, reactant ratio and temperature, was undertaken to enhance the conversion of ethyl acetate. Simulation results revealed that the optimal conditions were achieved with a reactant mole ratio of 3:1 at a temperature of 135.7 °C, resulting in an ethyl acetate conversion of 97.21%. These findings underscore the significance of systematic parameter optimization in improving process efficiency, reducing costs, and supporting sustainable production practices within the chemical industry.

Keywords: Ethyl Acetate; Conversion; Esterification; Reactant Ratio; Temperature

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1. Introduction

Solvents, such as ethyl acetate, are indispensable in a broad spectrum of industrial applications, particularly within the chemical sector. Their versatility has driven sustained global demand, which continues to expand in response to diverse manufacturing needs [1]. Furthermore, increasingly stringent regulatory frameworks addressing emissions of hazardous pollutants from production activities have underscored the strategic importance of *green chemistry*, a paradigm that promotes the use of substances that are non-toxic to both the environment and living organisms [2]. Within this evolving regulatory and scientific landscape, the imperative for widely utilized solvents to minimize adverse impacts on human health and ecological systems has become critical. Ethyl acetate exemplifies this shift, distinguished by its relatively low toxicity and biodegradability [3]. Consequently, these attributes have not only stimulated substantial market growth but have also positioned ethyl acetate as a benchmark solvent in sustainable industrial practice, serving as a model compound for environmentally responsible solvent design and aligning closely with the principles of green chemistry.

Ethyl acetate is synthesized through the reaction of acetic acid with ethanol, yielding ethyl acetate and water via the Fischer esterification process [4]. This reaction is exothermic, reversible, and generally proceeds at a relatively slow rate, thereby necessitating the use of a catalyst to achieve high ester yields. More broadly,

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esterification refers to the chemical transformation of a carboxylic acid and an alcohol into an ester in the presence of an acid catalyst [5]. The optimization of ethyl acetate production presents distinct challenges due to the reversible nature of the esterification reaction, as well as the need to control by-product formation and energy consumption. Developing an optimal process is therefore critical for improving conversion efficiency, reducing operational costs, and ensuring sustainable production [6].

Several strategies can be employed to enhance the conversion of ethyl acetate, including the selection of an appropriate production pathway, modification of process models and equipment, and optimization of operating conditions [6,7]. Among these, operating conditions exert the most critical influence on process performance. Identifying optimal parameters that maximize conversion while simultaneously minimizing energy consumption and production costs is therefore essential. The key operating variables include the reactant ratio and reaction temperature. Since the esterification of acetic acid with ethanol is both reversible and exothermic, precise control of temperature and reactant ratios is required to shift the equilibrium toward product formation, thereby improving conversion efficiency [7].

This study aims to identify the optimal operating conditions for enhancing the conversion of ethyl acetate. The findings provide valuable insights into process parameter optimization, reactor design improvement, and the advancement of overall efficiency and sustainability in production. In this work, the synthesis of ethyl acetate via esterification in a continuous stirred-tank reactor (CSTR) is examined in detail, with emphasis on improving conversion outcomes. The optimal operating conditions were determined based on established reaction kinetics and subsequently validated through comparison with experimental results.

2. Methods

The production process model for ethyl acetate from esterification of acetic acid was designed using Aspen HYSYS V11 by adding components acetic acid, ethanol, ethyl acetate, and H_2O. The fluid package utilized in the simulation was the Non-Random Two-Liquid (NRTL) model. The choice of NRTL was made deliberately, as this thermodynamic framework is particularly well-suited for systems in which strong non-idealities arise due to molecular interactions. In the present process, the inclusion of water as one of the components introduces significant polarity effects, which can strongly influence phase equilibria and activity coefficients. By employing the NRTL model, the simulation can account for these non-ideal behaviors with greater accuracy, thereby ensuring reliable representation of both liquid-phase interactions and overall system performance [8].

The production of ethyl acetate from acetic acid was carried out in a continuous stirred-tank reactor (CSTR). To maximize acetic acid conversion, process modifications were implemented by optimizing the reactant mole ratio and reaction temperature within the reactor. These adjustments significantly enhance the efficiency of ethyl acetate production. Acetic acid conversion can be calculated using Equation (1) [9]:

$$\text{Conversion (\%)} = \frac{\text{mole of acetic acid feed - mole of acetic acid out}}{\text{mole of acetic acid feed}} \quad (1)$$

From Equation (1), we have the result of acetic acid conversion. With this equation, we can compare the result without modification and after modification.

3. Results and Discussion

3.1. Process Description of Basic Process Before Modification

The simulation of ethyl acetate production was conducted using Aspen HYSYS V11, obtaining an acetic acid conversion of 62.12%. The basic (unmodified) process flow diagram is presented in Figure 1, while the corresponding Aspen HYSYS simulation are shown in Figure 2.

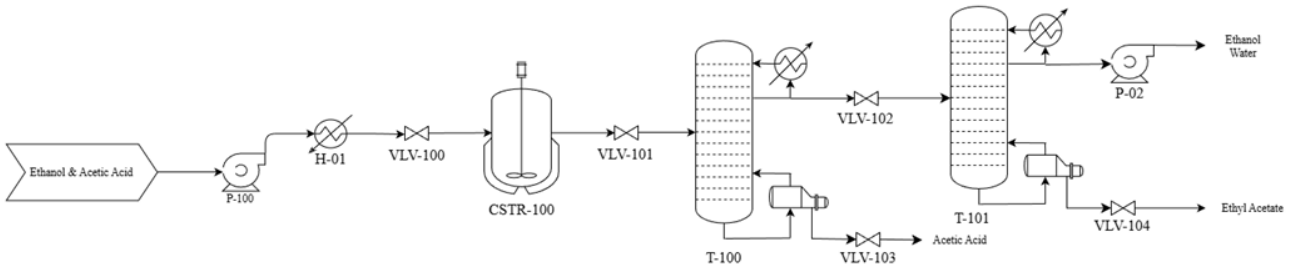

Figure 1. The basic (unmodified) process flow diagram (PFD) of ethyl acetate production [6].

The Non-Random Two-Liquid (NRTL) fluid package was employed to model the vapor–liquid–liquid equilibrium of the system [8]. The feed consisted of liquid ethanol and acetic acid at 25 °C and 1 atm. The reaction chemistry applied in this process is illustrated in Equation (2) [10]:

$$CH_3CH_2OH + CH_3COOH \leftrightarrow CH_3COOCH_2CH_3 + H_2O \quad (2)$$

The raw materials, acetic acid and ethanol, entered the pump at 25 °C and 1 atm. The pump increased the feed pressure from 1 atm to 9.9 atm [11]. The pressurized stream then passed through the heater, which raised the temperature from 25 °C to 70 °C and converted the feed phase from liquid to vapor [12]. The feed stream passed through a valve prior to entering the reactor, where the valve regulated the inlet pressure [13]. A continuous stirred-tank reactor (CSTR) was selected, operating at 70 °C and 1 atm. This reactor was chosen due to its excellent mixing characteristics, uniform heat and mass transfer, continuous operation capability, ease of scale-up, and suitability for liquid-phase reactions requiring stable residence time and consistent product quality [14]. The reactor products consisted of ethyl acetate and water, along with unreacted components in both liquid and vapor phases. The liquid-phase products were directed through valve to control the pressure before entering the distillation column. The distillation process separated compounds based on differences in their boiling points [15]. The first distillation stage operated at 89.6 °C in the condenser and 168.4 °C in the reboiler, primarily separating acetic acid in the bottom stream from the top products. The overhead stream was then fed into a second distillation column, operating at 58.5 °C in the condenser and 172.4 °C in the reboiler, to separate ethyl acetate from the remaining components.

The primary reaction for ethyl acetate production occurs through the interaction of acetic acid and ethanol. To determine whether the reaction is exothermic or endothermic, the standard heat of reaction $(\Delta H^\circ_{298\,K})$ at 1 bar and 298 K must be calculated based on the standard heats of formation of the reactants and products. The value of ΔH_f° used in this calculation are provided in Table 1. Standard heat of reaction at 298 K $(\Delta H^\circ_{298\,K})$ is calculated as follow:

$$(\Delta H^\circ_{298\,K}) = \sum \Delta H_f^\circ \text{ product} - \sum \Delta H_f^\circ \text{ reactant} = (\Delta H_f^\circ\, CH_3COOCH_2CH_3 + \Delta H_f^\circ\, H_2O) - (\Delta H_f^\circ\, CH_3COOH + \Delta H_f^\circ\, CH_2OH) = -19 \text{ kJ/mol}$$

Based on the calculations, we get the value $\Delta H^\circ_{298\,K}$ = -19 kJ/mol. Since the value is negative, the reaction is classified as exothermic.

3.2. Process Modification

To maximize acetic acid conversion, operational modifications were implemented by varying the reactant mole ratio (ethanol to acetic acid) and adjusting the reaction temperature, as these parameters represent the most critical factors influencing esterification performance. The efficiency of esterification is strongly dependent on both the reactant ratio and temperature control, which govern the evaporation of volatile components and continuously drive the reversible reaction toward ethyl acetate formation [17]. In the continuous stirred-tank reactor (CSTR), precise temperature regulation enhances the reaction rate in accordance with the Arrhenius equation, while avoiding the promotion of excessive side reactions [5]. The modified process flow diagram for ethyl acetate production is presented in Figure 3, and the corresponding Aspen HYSYS simulation results are shown in Figure 4.

The production process was carried out by varying ethanol-to-acetic acid mole ratios of 1:1, 2:1, and 3:1 within a temperature range of 70–140 °C, while maintaining a total feed flow rate of

Table 1. The value of ΔH_f° [16].

Compound	Molecular Formula	ΔH_f° (kJ/mol)
Acetic acid	CH_3COOH	-432.3
Ethanol	CH_3CH_2OH	-235
Ethyl acetate	$CH_3COOCH_2CH_3$	-444.5
Water	H_2O	-241.8

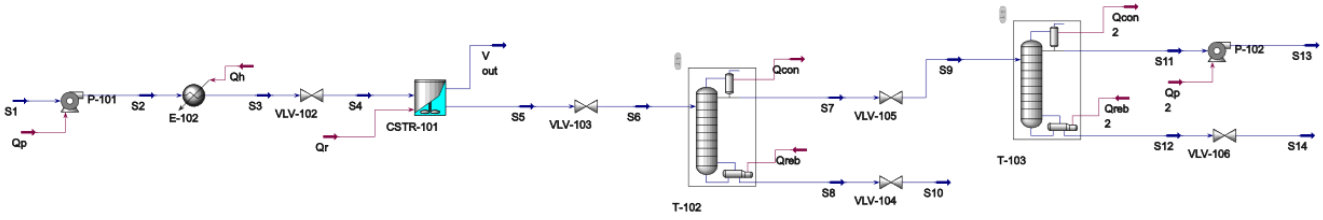

Figure 2. Process simulation using Aspen HYSYS for the basic (unmodified) process of ethyl acetate production.

388 kgmol/h. The SET feature was applied prior to mixing to adjust the reactant ratio, whereas the ADJ feature ensured that the total molar feed flow at the mixer outlet remained constant at 388 kgmol/h [18]. These adjustments established consistent inlet conditions across all simulation runs, thereby enabling reliable comparison of process performance under different operating scenarios.

The results demonstrated that the combined influence of reactant ratio and temperature had a significant effect on ethyl acetate conversion. At a 1:1 ethanol-to-acetic acid ratio, conversion reached 73.32% at 152.1 °C, exceeding the initial operating range due to the pronounced temperature sensitivity of the esterification reaction. Consequently, Aspen HYSYS adjusted the system to steady state in order to satisfy conversion specifications, even at temperatures beyond the predefined limits [18]. This outcome indicates that a 1:1 ratio was insufficient to shift the equilibrium toward product formation within the specified range. At a 2:1 ratio, conversion increased to 94.12% at 138.3 °C, confirming that excess ethanol effectively promoted product formation. At a 3:1 ratio, the highest conversion of 97.21% was achieved at 135.7 °C. This condition represents the optimal operating parameters, as it successfully shifted the equilibrium toward product formation while simultaneously enhancing reaction kinetics in the continuous system.

3.3. Improvement of Acetic Acid Conversion Due to the Process Modification

Increasing conversion of acetic acid in esterification process is carried out by optimizing reaction temperature and ethanol:acetic acid ratio. The reactant ratio is being adjusted by using SET, while ADJ is used to keep the molar flow remain constant at 388 kgmole/h to keep the inlet consistency while running the simulation [8]. Then, the increasing temperature accelerates the rate of esterification reaction according to Arrhenius equation, allowing acetic acid to react more quickly with ethanol [7]. In the unmodified design, the acetic acid conversion reached 62.12%, while after process modification the acetic acid conversion (Equation (1)) reached 97.21%. To determine the conversion percentage of modified process, calculations were carried out using Equation (3). Table 2 compares the conversion percentage in process without modification and with modification.

Table 2. Comparison process without modification and with modification (Equation (1)).

Process	Conversion (%)
Without modification	62.12%
With modification	97.21%

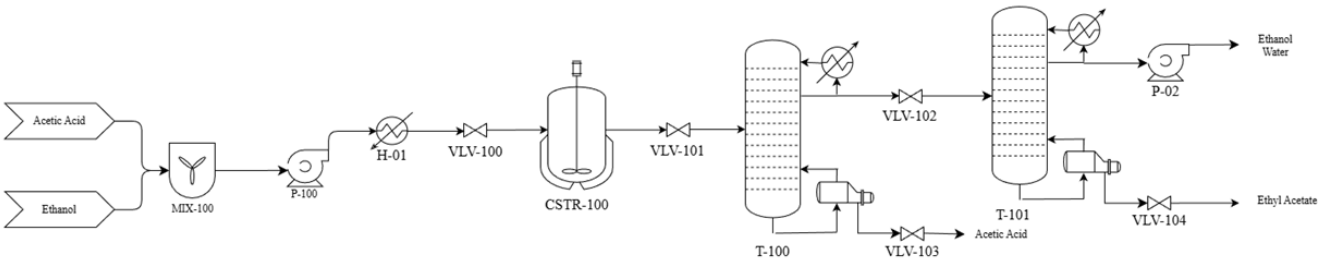

Figure 3. Modified process flow diagram of ethyl acetate production.

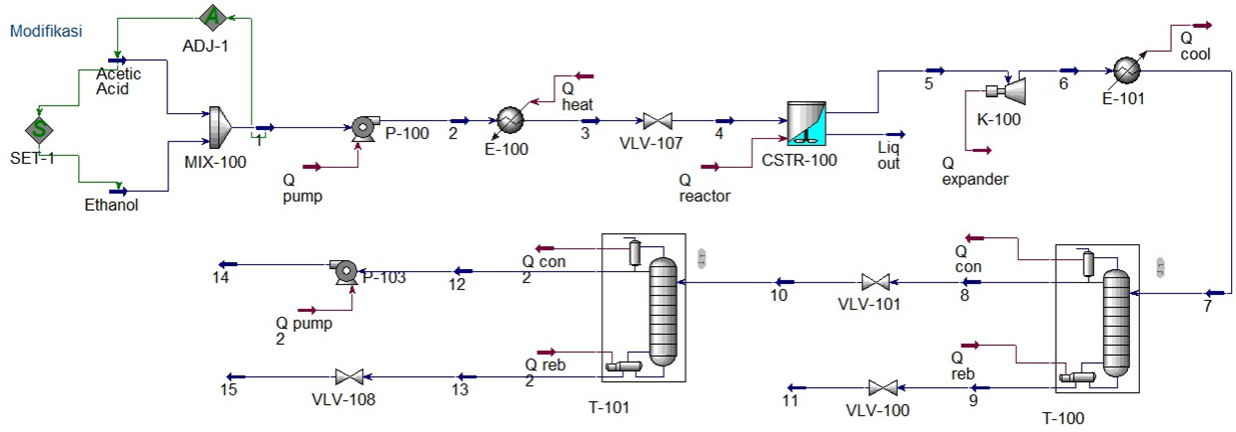

Figure 4. Aspen HYSYS simulation of the modified process of ethyl acetate production.

4. Conclusion

Temperature and reactant ratio are critical parameters that strongly influence the conversion of ethyl acetate during the esterification of acetic acid. Optimizing these operating conditions can substantially improve the efficiency of ethyl acetate synthesis. In reversible reactions, employing an excess of one reactant shifts the equilibrium toward product formation, thereby enhancing conversion. Moreover, precise temperature regulation plays a pivotal role in controlling the reaction rate, which ultimately governs the extent of conversion achieved. Experimental results demonstrate that a reactant mole ratio of 3:1 at 135.7 °C yields an exceptionally high conversion of 97.21%. Achieving conversion levels above 90% indicates that these conditions are close to the process optimum, providing a valuable benchmark for the design, optimization, and control of esterification processes aimed at sustainable and efficient ethyl acetate production

CRedit Author Statement

Author Contributions: F.K. Azizi: Conceptualization, Methodology, Investigation, Resources, Data Curation, Writing, Review and Editing, Supervision; M.S. Arumi: Formal Analysis, Investigation, Writing, Review and Editing; P. Hidayat: Software, Resources, Methodology, Review and Editing; R.D. Nurahman: Conceptualization, Methodology, Formal Analysis, Resources, Validation, Writing; S.N. Anggawijaya: Investigation, Resources, Writing, Review and Editing, Validation. All authors have read and agreed to the published version of the manuscript.

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