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Research Article

Optimizing Energy Efficiency in Acetone Production via Isopropyl Alcohol Dehydrogenation through Feed-Effluent Heat Integration

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Abstract

Acetone production via isopropyl alcohol (IPA) dehydrogenation is an energy-intensive process due to the endothermic nature of the reaction. This study aims to minimize net energy consumption by simulating a modified process design that incorporates a Feed-Effluent Heat Exchanger (FEHE) strategy. The simulation results demonstrate that the modified configuration successfully recovers heat from the reactor effluent to preheat the feed stream to 178 °C, thereby reducing the total energy consumption from 4,695.8 kW to 4,532.0 kW. This energy saving of 163.8 kW confirms that the proposed heat integration is technically feasible and significantly enhances the thermodynamic efficiency of the acetone production process.

Keywords: Acetone production; Isopropyl alcohol dehydrogenation; Heat integration; Net energy minimization

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1. Introduction

The production of acetone has traditionally relied on the cumene process, in which acetone is obtained as a by-product alongside phenol [4]. Although this route has been widely adopted in industry, it suffers from inherent limitations because acetone output is entirely dependent on phenol demand, often leading to supply imbalances in the global market [2]. Moreover, the cumene process is highly energy-intensive and generates considerable emissions and waste, which increasingly conflict with tightening environmental regulations [3]. These challenges have stimulated growing interest in alternative production pathways that can yield acetone as the primary product, improve energy efficiency, and reduce environmental impact [6]. Acetone itself plays a crucial role in both laboratory and industrial applications. It serves as a chemical intermediate in pharmaceuticals and as a solvent for vinyl and acrylic resins. It is also widely used in varnishes, paints, inks, cosmetics, and coatings. In addition, acetone supports the manufacture of paper coatings, adhesives, and heat-seal layers, and it functions as a key base material for synthesizing various chemical compounds [13].

The dehydrogenation of isopropyl alcohol (IPA) has emerged as a promising alternative route for acetone production. This endothermic catalytic reaction directly converts IPA into acetone and hydrogen without the need for additional reactants [7]. In contrast to the cumene process, this pathway provides greater flexibility, as acetone is obtained as the primary product while hydrogen serves as a valuable by-product with significant potential in clean energy and chemical manufacturing. Previous studies have

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demonstrated that metal-based catalysts such as copper, silver, and platinum can achieve high selectivity toward acetone while effectively suppressing undesirable side reactions [1]. More recent research highlights the critical influence of operating conditions, particularly reactor temperature and heat recovery integration, in maximizing conversion efficiency and overall energy performance [4].

Comparative evaluations of acetone production routes indicate that IPA dehydrogenation offers superior efficiency and sustainability compared to acetylene hydration, which requires extreme operating conditions and costly catalysts [15], and the cumene process, which generates phenol as an additional product requiring further treatment [10]. To support industrial adoption, process simulation and modeling serve as essential tools. Validated models enable engineers to assess mass and energy balances, optimize reactor configurations, and evaluate utility requirements prior to implementation [15]. Software such as Aspen HYSYS further enhances design flexibility by facilitating the exploration of alternative process schemes, integration of heat recovery systems, and reduction of emissions, thereby advancing sustainability objectives [11].

Through advanced simulation and innovative reactor design, IPA dehydrogenation can be optimized to achieve high acetone yields, enhanced energy efficiency, and reduced operational costs. Furthermore, sourcing IPA from renewable feedstocks such as bio-IPA amplifies the environmental advantages of this pathway [7]. Taken together, these advancements establish IPA dehydrogenation as a strategic and sustainable alternative for meeting the growing global demand for acetone, while simultaneously supporting the broader transition toward a more energy-efficient and environmentally responsible chemical industry.

Despite these advancements, only a limited number of studies have specifically examined energy minimization strategies in IPA dehydrogenation through systematic heat integration [5,7]. Previous research has primarily concentrated on catalyst development [1,14] and reactor optimization [15], while comparatively little attention has been directed toward the application of Feed-Effluent Heat Exchanger (FEHE) configurations to reduce net energy consumption [8]. To address this gap, the present study evaluates the thermodynamic performance of a modified IPA dehydrogenation process incorporating an FEHE strategy. The objectives are to minimize external energy requirements, demonstrate the feasibility of internal heat recovery, and enhance process sustainability through simulation-based design improvements in Aspen HYSYS [2,3].

2. Methods

To enhance the efficiency of acetone production via isopropyl alcohol (IPA) dehydrogenation, Aspen HYSYS V11 is employed for process simulation, design, optimization, and control [5]. The system consists of four main components: isopropyl alcohol (C_3H_8O), acetone (C_3H_6O), hydrogen (H_2), and water (H_2O). The UNIQUAC thermodynamic model is applied to calculate non-ideal mixture properties, and the overall process flow is illustrated in Figure 1. The process begins with 2,401 kg/h of fresh IPA, which is combined with recycled azeotropic streams in a mixer to produce a total feed of 2,585 kg/h. This feed is preheated and then sent to Reactor R-101, operating isothermally at 350 °C and 1.9 bar, achieving an IPA conversion of approximately 90% per pass. Following the reaction, the effluent is cooled to 45 °C to separate the hydrogen-rich vapor from the liquid product. The liquid stream subsequently undergoes purification in a distillation column to recover high-purity acetone, while the unreacted IPA is recycled back to the feed section.

As a modification, a heat integration strategy is implemented by adding heat exchangers downstream of the feed pump and the reactor to evaluate differences in energy consumption between the base and modified processes [7]. Specifically, the reactor effluent heat is utilized to preheat the feed stream, thereby reducing the load on the main heater. Key variables such as stream temperatures and utility duties are compared to assess the net energy savings. This approach minimizes external energy requirements while maintaining product quality. Furthermore, additional improvements in energy efficiency are demonstrated through the significant reduction in heating and cooling duties achieved by the heat recovery system.

3. Results and Discussion

3.1. Differences Between Basic and Modified Process

The simulation of acetone production via isopropyl alcohol (IPA) dehydrogenation was conducted using Aspen HYSYS V11 to evaluate the performance of two approaches: the basic process and the modified process. An overview of the simulation results and the process flow diagram for the basic process is presented in Figures 1 and 2 as well as in Tables S1 and S2 (Supporting Information), while the configuration of the modified process is shown in Figures 3 and 4. The simulation employed the UNIQUAC fluid

package, which has been validated to accurately predict vapor–liquid equilibrium (VLE) data and the formation of the minimum-boiling azeotrope (88 wt% IPA) inherent in this system.

In the basic process, heat management is carried out conventionally. The feed stream is fully heated using an external heater before entering the reactor. The reactor effluent, at a high temperature of 350 °C, is then cooled directly using a cooler before being sent to the flash separator. This configuration is inefficient because it requires substantial utility energy input on the heating side, while valuable sensible heat is wasted on the cooling side.

In contrast, the modified process applies a heat integration strategy by incorporating a heat exchanger into the process stream. In this configuration, the cooler between the reactor and separator is eliminated and replaced by a Feed-Effluent Heat Exchanger (FEHE), which directly utilizes the reactor effluent heat to preheat the feed stream [8]. This modification not only removes the need for a separate cooling unit before the separator but also significantly reduces the load on the main heater. The result is a more energy-efficient consumption profile while maintaining operational effectiveness.

The dehydrogenation of IPA proceeds according to the following reaction:

$$C_3H_9O \rightarrow C_3H_6O_2 + H_2 \quad (1)$$

Thermodynamic evaluation was based on standard enthalpy of formation (ΔH_f) and Gibbs free energy (ΔG_f) at 298 K (Table 1.). The reaction enthalpy was determined to be +55.02 kJ/mol. The positive reaction enthalpy (+55.02 kJ/mol) confirms that the process is endothermic, requiring continuous heat supply. This validates the use of a high-temperature isothermal reactor in the simulation [14]. At 298 K, the Gibbs free energy change was calculated as +20.54 kJ/mol, corresponding to an equilibrium constant of 2.51×10^{-3}. Since $K_{298} < 1$, the reaction is non-spontaneous at room temperature. Using Van't Hoff's equation, the equilibrium constant at the simulation operating temperature (773 K or 350 °C) is $K_{773} \approx 2{,}11 \times 10^{3}$. At elevated temperatures, K >> 1, indicating the equilibrium strongly shifts toward product formation. Consequently, high conversion rates become attainable in acetone production [12].

Table 1. ΔG_f and ΔH_f for each component at temperature 298 K.

Compound Name	Molecular Formula	$G_{f\,298\,K}$ (kJ/mol)	$H_{f\,298\,K}$ (kJ/mol)
Isopropyl Alcohol	C_3H_8O	-272.59	-173.59
Acetone	C_3H_6O	-217.57	-153.05
Hydrogen	H_2	-	-

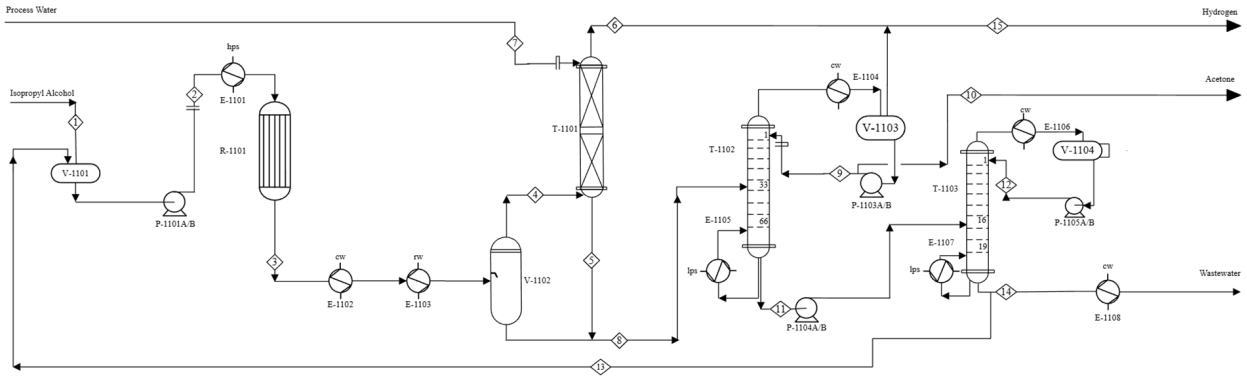

Figure 1. Basic process flow diagram of acetone production [16].

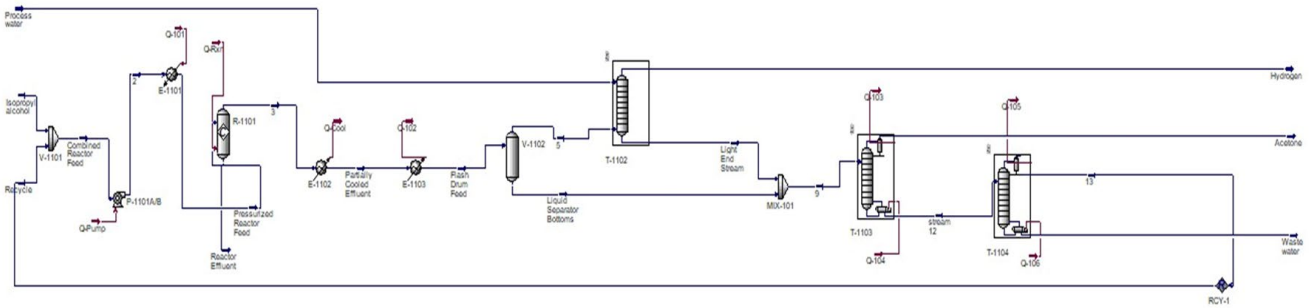

Figure 2. Aspen HYSYS simulation of the basic acetone production.

3.2. Comparison of Energy Efficiency before and after Modified Optimization

The net energy requirements for both the basic and modified processes are summarized in Table 2. In the basic process, the total energy demand of the system is 4,695.8341 kW. The distribution of energy consumption across individual units is as follows: 950.1 kW in Q-101; 688.3 kW in Q-Rxn; 864.6 kW in Q-Cool; 141.4 kW in Q-102; 311.0 kW in Q-103; 659.2 kW in Q-104; 538.0 kW in Q-105; 543.1 kW in Q-106; and 0.1341 kW in the Q-Pump. In contrast, the modified process, where the cooler between the CSTR and the separator is removed, has a total energy consumption of 4,532.0343 kW. The distribution of energy use is as follows: 908.8 kW in Q-101; 688.5 kW in Q-Rxn; 869.7 kW in Q-102; 311.1 kW in Q-103; 658.7 kW in Q-104; 545.0 kW in Q-105; 550.1 kW in Q-106; and 0.1343 kW in the Q-Pump.

By eliminating the recycle cooler, the total energy requirement of the modified process is reduced by 163.7998 kW. This reduction represents a significant improvement in energy efficiency, as the modified configuration achieves lower utility consumption, while maintaining system performance. The modification demonstrates a more efficient process by redistributing the thermal load, eliminating the need for an additional cooling unit, and streamlining energy use across the system. As a result, the modified process achieves superior energy efficiency, aligning more closely with the ideal of minimizing unnecessary energy consumption, thereby enhancing both sustainability and cost-effectiveness compared to the basic process.

3.3. Net Energy Minimization Analysis

The primary objective of this process modification is to minimize external energy requirements by applying the principles of process intensification. The effectiveness of the modification is quantitatively assessed through

Table 2. Comparison of energy required for basic and modified process.

Energy stream	Energy required (kW)	
	Basic process	Modified process
Q-101	950.1	908.8
Q-Rxn	688.3	688.5
Q-Cool	864.6	-
Q-102	141.4	869.7
Q-103	311.0	311.1
Q-104	659.2	658.7
Q-105	538.0	545.0
Q-106	543.1	550.1
Q-Pump	0.1341	0.1343
Total	4695.8341	4532.0343

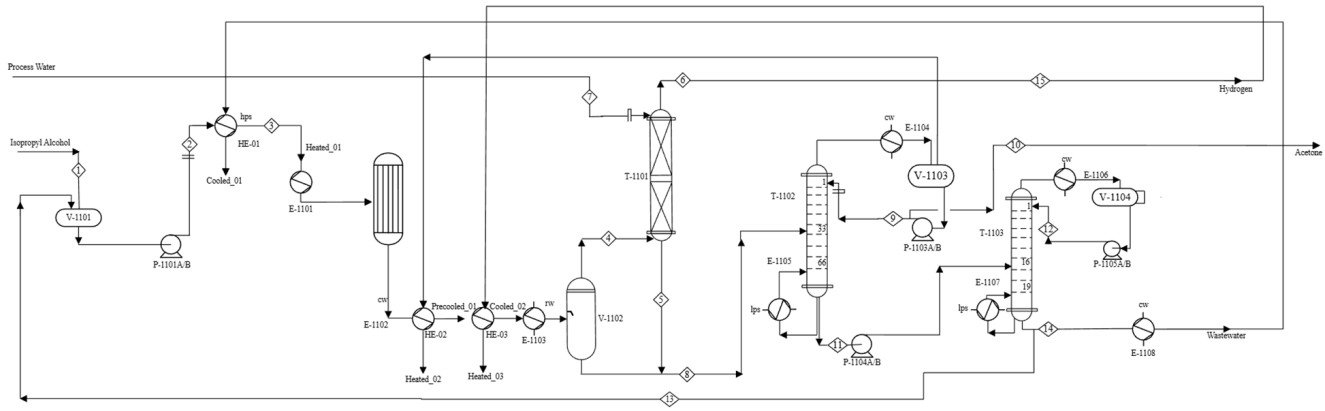

Figure 3. Process flow diagram (PFD) of modified acetone production process.

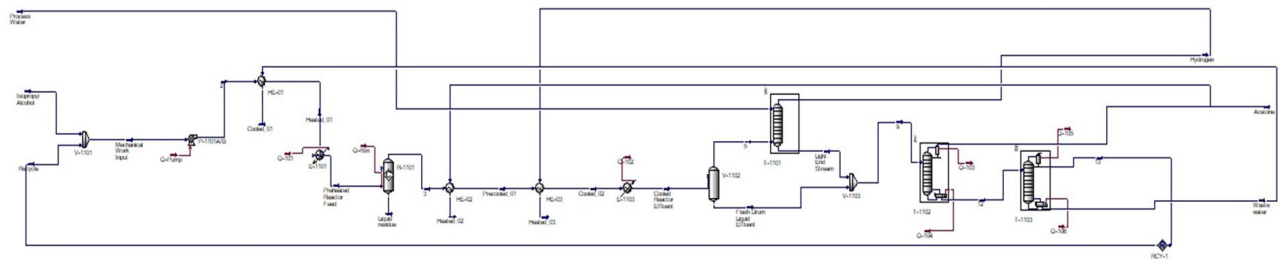

Figure 4. Aspen HYSYS simulation of the modified acetone production.

thermal load reduction and the calculation of net energy savings. In the basic process design, the main heater carries a substantial sensible heating load to raise the feed temperature from ambient conditions to the reaction temperature, leading to high specific energy consumption. By contrast, the modified design incorporating a Feed-Effluent Heat Exchanger (FEHE) achieves significant internal heat recovery. In this configuration, the sensible heat from the high-temperature reactor effluent (Stream 3) is directly utilized to preheat the incoming feed stream, thereby reducing external heating requirements. Simulation of temperature profiles indicate that this strategy effectively raises the feed temperature (Stream 2) from 26.85 °C to 178.0 °C (Stream Heated_2) prior to entering the main heater. From a thermodynamic perspective, this heat recovery proportionally reduces the heater's workload, thereby lowering external energy demand.

Energy efficiency was evaluated by comparing the total energy consumption of the basic and modified processes, as summarized in Table 2. The basic process requires 4,695.8 kW, while the modified process consumes 4,532 kW. This corresponds to a net energy saving of 163.8 kW. The reduction of 163.8 kW confirms the effectiveness of heat integration within the system. On the cooling side, the reactor effluent temperature decreases from 350.0 °C to 300.0 °C (Stream Precooled_3) solely through heat exchange, thereby eliminating the cooling load in the pre-separation stage.

The thermal efficiency achieved in this simulation aligns with previous studies on acetone production facilities based on IPA dehydrogenation, where reactor configuration optimization and heat management are recognized as critical factors in enhancing overall plant performance [3]. The importance of reducing utility loads is further emphasized by earlier analyses, which identified energy minimization in key operating units as a dominant parameter in sustainability assessments conducted with process simulation tools [2]. Furthermore, the integration of process simulation and energy efficiency strategies has been established as a fundamental pillar of modern industrial practice, supporting the achievement of global sustainability standards [9].

Although the incorporation of a heat exchanger unit in the modified design entails a higher initial capital investment (fixed CAPEX), the resulting improvement in thermodynamic efficiency provides strong technical justification for this approach. As emphasized in pinch analysis studies, the application of heat recovery techniques to minimize external energy demand has proven effective in developing resilient and resource-efficient process systems [13]. Consequently, the reduction in net energy consumption achieved through this modification establishes the configuration as a superior solution, well-suited to the challenges of energy transition in the chemical industry.

4. Conclusion

In conclusion, the modification of the cumene oxidation process by eliminating the cooler between the reactor and the separator demonstrates substantial improvements in both energy efficiency and cost savings. The total energy demand of the modified process is 4,532.0343 kW, which is 163.7998 kW lower than that of the basic process (4,695.8341 kW). This reduction in energy consumption results directly from the removal of the cooler, thereby lowering overall utility requirements while maintaining system performance. From a thermal perspective, the integration of the Feed-Effluent Heat Exchanger (FEHE) proved highly effective in optimizing process thermodynamics. The modification successfully recovered high-grade sensible heat from the reactor effluent, reducing its temperature from 350 °C to 300 °C without reliance on external cooling utilities. This recovered energy was subsequently utilized to preheat the feed stream from ambient conditions, shifting a significant portion of the vaporization load away from the main heater. Overall, this internal heat exchange mechanism validates the effectiveness of the process intensification strategy, demonstrating superior thermodynamic efficiency and resource conservation by minimizing the loss of valuable thermal energy.

CRedit Author Statement

Author Contributions: R. Aditasya: Conceptualization, Methodology, Software, Formal Analysis, Investigation, Data Curation, Writing, Review and Editing, Project Administration; M. Taslim: Conceptualization, Formal Analysis, Investigation, Writing, Review and Editing, Vizualitation; S. F. Azzahra: ; B. B. Narendro: Writing; I. A. Prantindoe: Writing; K. S. Seng: Conceptualization, Methodology, Validation, Investigation, Supervision.. All authors have read and agreed to the published version of the manuscript.

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