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Journal of Chemical Engineering Research Progress, 3 (1) 2026, 124-129

Research Article

Improving Operational Energy Efficiency in the Acetaldehyde Production Process Through the Addition of a Heat Exchanger and Optimization of Heat from Reactors' Outlet

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Received: 10th December 2025; Revised: 22nd December 2025; Accepted: 24th December 2025
Available online: 9th January 2026; Published regularly: June 2026

Abstract

Enhancing the energy efficiency of acetaldehyde production is essential for advancing operational performance and supporting sustainable chemical manufacturing. This study investigates the effect of integrating an additional heat exchanger into the ethanol dehydrogenation flowsheet, positioned before the feed stream enters the process unit, on overall thermal efficiency. Thermodynamic simulations were conducted to compare the baseline configuration with the modified design. The added heat exchanger recovers energy from existing process streams, thereby reducing dependence on external heating utilities and minimizing unnecessary heat losses. Simulation results reveal a significant reduction in total energy demand, with overall heat consumption lowered by 507,602.4 kJ/h relative to the original system. These findings highlight the potential of strategic heat integration to markedly enhance the energy performance of acetaldehyde production. In conclusion, incorporating a heat exchanger prior to downstream heating units offers a practical and effective means of optimizing energy use while promoting more efficient and environmentally responsible process designs.

Keywords: Energy efficiency; Acetaldehyde; Heat exchanger; Ethanol dehydrogenation; process design

How to Cite: Nazlia, B., Fahira, F. M., Hapsari, H. N., Putri, P. A. N., Adyawita, K. G. (2026). mproving Operational Energy Efficiency in the Acetaldehyde Production Process Through the Addition of a Heat Exchanger and Optimization of Heat from Reactors' Outlet. *Journal of Chemical Engineering Research Progress*, 3 (1), 124-129 (doi: 10.9767/jcerp.20561)

Permalink/DOI: https://doi.org/10.9767/jcerp.20561

1. Introduction

Acetaldehyde (CH_3CHO), a versatile carbonyl compound, is a key intermediate in the synthesis of numerous industrial chemicals, including acetic acid, pyridine, and various pharmaceuticals. [1]. Its production primarily via ethylene oxidation through the Wacker process or ethanol dehydrogenation remains a cornerstone of the petrochemical industry. [2] with global demand exceeding 1 million metric tons annually. However, conventional methods often suffer from inefficiencies such as low yields, high energy consumption, and the generation of hazardous byproducts, underscoring the need for optimization to enhance both sustainability and economic viability.

In ethanol dehydrogenation, acetaldehyde is produced through the catalytic reaction:

$$C_2H_5OH_{(g)} \rightarrow CH_3CHO_{(g)} + H_{2(g)} \quad \Delta H^\circ_{(298)} = +64 \text{ kJ.mol}^{-1} \quad (1)$$

This endothermic process has a standard enthalpy change of approximately $\Delta H^\circ_{(298)} = +64$ kJ.mol^{-1}. Alongside the main reaction, several side reactions contribute to byproduct formation. Ethyl acetate is generated via ethanol coupling ($2C_2H_5OH \rightarrow CH_3COOC_2H_5 + 2H_2$), which is mildly endothermic ($\Delta H^\circ_{(298)} \approx +24$ kJ.mol^{-1}). In contrast, 2-butanol formation ($2C_2H_5OH \rightarrow C_4H_9OH + H_2O$) is exothermic ($\Delta H^\circ_{(298)} \approx -65$ kJ.mol^{-1}). A minor pathway yields acetic acid ($C_2H_5OH + H_2O \rightarrow$

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$CH_3COOH + 2H_2$), also endothermic with $\Delta H°_{(298)} \approx +44$ kJ.mol^{-1}. The coexistence of endothermic and exothermic reactions within the reactor highlights the critical importance of heat management, making heat integration and recovery from the reactor outlet essential for improving overall energy efficiency.

Ethanol dehydrogenation is among the simplest and most industrially significant methods for acetaldehyde production [3]. Compared to the Wacker oxidation process, it offers advantages such as reliance on renewable feedstocks and potentially lower energy requirements [2]. Moreover, the coupling reactions yield valuable co-products—including acetaldehyde, ethyl acetate, and n-butanol—that enhance the economic value of ethanol while promoting resource efficiency and reducing environmental impact [4].

Despite its simplicity, the process requires careful optimization to achieve commercial feasibility, particularly in the context of sustainable chemistry. Key parameters, such as temperature, pressure, catalyst composition, and reactor design, strongly influence performance. Recent studies have highlighted the benefits of nanostructured catalysts [5] and membrane reactors [6] in boosting efficiency. Nevertheless, comprehensive optimization strategies that simultaneously address yield, energy consumption, and byproduct minimization remain limited. This research seeks to bridge that gap by employing a multi-objective optimization framework that integrates experimental data with computational simulations to improve ethanol dehydrogenation into acetaldehyde.

Building on prior findings that demonstrated improved conversion and selectivity alongside reduced energy use through process optimization [7], our current work introduces a method to minimize both utility and capital costs in acetaldehyde production. This is achieved by integrating heat exchanger equipment and maximizing the recovery of useful energy from reactor outlet streams.

2. Methods

2.1. Property Package

Aspen HYSYS provides a comprehensive suite of thermodynamic models designed to accurately represent phase behavior and calculate the enthalpy of complex mixtures. For simulating the ethanol dehydrogenation process leading to acetaldehyde production, the Non-Random Two-Liquid (NRTL) property package was selected as the thermodynamic foundation, owing to its proven reliability in handling non-ideal liquid systems and vapor–liquid equilibrium calculations.

2.2. Energy Optimization by using a Heat Exchanger

Heat transfer in chemical processes can be optimized using heat exchangers, heaters, and coolers. While heaters and coolers depend on external energy sources to raise or lower fluid temperatures, heat exchangers facilitate thermal energy transfer between process streams without direct mixing, thereby significantly reducing overall energy consumption [8]. In acetaldehyde production, which requires both heating and cooling stages, the integration of heat exchangers is particularly advantageous for enhancing energy efficiency and stabilizing process condition [9].

In the modified process design, an additional heat exchanger is incorporated upstream of the process unit, positioned before the ethanol feed enters the pump. This modification leverages waste heat available within the system. Since ethanol dehydrogenation operates at elevated temperatures, the feed must be preheated before entering the reactor to achieve the desired reaction conditions [10]. Rather than relying exclusively on external heating, the added exchanger recovers heat from a hotter process stream, enabling the ethanol feed to absorb thermal energy earlier in the flowsheet. As a result, the fluid enters the pump and subsequent heater at a higher temperature, thereby reducing the downstream heating load [11].

Placing the heat exchanger before the pump improves heat distribution, minimizes utility consumption, and enhances thermal balance across process units. This strategy not only supports sustainable energy management but also ensures more consistent operating parameters throughout acetaldehyde production [12]. Moreover, the use of recovered heat aligns with widely adopted energy integration principles in the chemical industry, reducing dependence on external utilities and lowering the Specific Energy Consumption (SEC) of acetaldehyde manufacturing [13]. The Specific Energy Consumption (SEC) can be determined using the following equation:

$$SEC\left(\frac{kJ}{ton}\right) = \frac{Energy\ consumption\frac{kJ}{year}}{Production\ quantity\frac{ton}{year}} \tag{2}$$

3. Results and Discussion

3.1. Comparison between Basic and Modified Proces

The production of acetaldehyde via ethanol dehydrogenation is a well-established route in the chemical process industries, valued for its efficiency and industrial relevance. As illustrated in Figure 1, the ethanol feed undergoes pumping and external preheating before entering the dehydrogenation reactor. The reactor operates under isothermal conditions at approximately 340 °C and 300 kPa, providing a stable thermal environment for the inherently endothermic reaction. These operating parameters supply sufficient activation energy to promote C–H bond cleavage in ethanol molecules while simultaneously shifting the equilibrium toward acetaldehyde and hydrogen formation, in accordance with Le Chatelier's principle. The reactor effluent, entirely in the gaseous phase, is subsequently cooled in a condenser to 2 °C and 200 kPa, with an assumed pressure drop of 50 kPa across each unit operation.

Hydrogen, produced as a byproduct, is separated downstream in a gas–liquid separator, while acetaldehyde undergoes further purification in a distillation column to meet industrial purity requirements. This separation strategy leverages the distinct solubility differences between acetaldehyde and hydrogen in water: acetaldehyde exhibits significantly higher solubility, enabling effective absorption into the aqueous phase, whereas hydrogen remains in the gas phase. Consequently, the process achieves selective absorption and efficient gas–liquid separation, improving the quality of the primary product while facilitating the utilization of hydrogen as a secondary product.

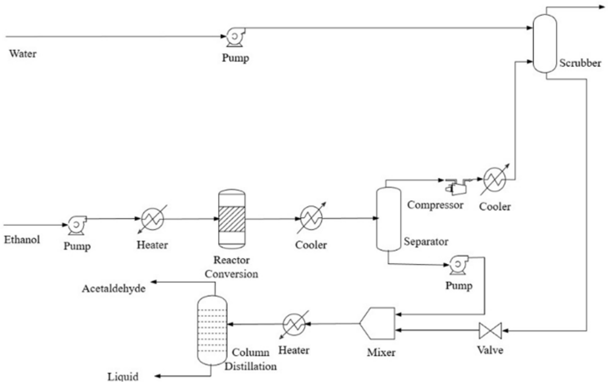

Figure 1. Unmodified process flow diagram of acetaldehyde to be simulated [14].

Although the unmodified system successfully produces acetaldehyde, its energy consumption remains relatively high due to the absence of integrated energy recovery. To overcome this limitation, a modified configuration was developed by incorporating a heat exchanger (HE) immediately after the feed stream, as shown in Figure 2. In this design, the HE is strategically positioned upstream of the pump, enabling recovery of thermal energy from high-temperature process streams. The recovered heat is used to preheat the incoming feed, thereby reducing reliance on external heating and enhancing overall process efficiency.

A comparative evaluation of the unmodified and modified systems demonstrates that the integration of a heat exchanger yields substantial energy optimization. The modified configuration achieves lower energy consumption, improved thermal efficiency, and greater process sustainability. These enhancements not only reduce operational costs but also mitigate environmental impacts associated with excessive energy use.

3.2 Thermodynamics Review

The evaluation of thermodynamic parameters, particularly enthalpy change (ΔH) and Gibbs free energy (ΔG), is fundamental to chemical process design. Analysis of ΔH reveals whether a reaction is exothermic or endothermic, providing critical insight for heat management, equipment specification, and the optimization of energy utilization within the system [15]. A clear understanding of the thermal characteristics also informs decisions related to process control, operational safety, and overall efficiency. In parallel, the assessment of ΔG establishes the

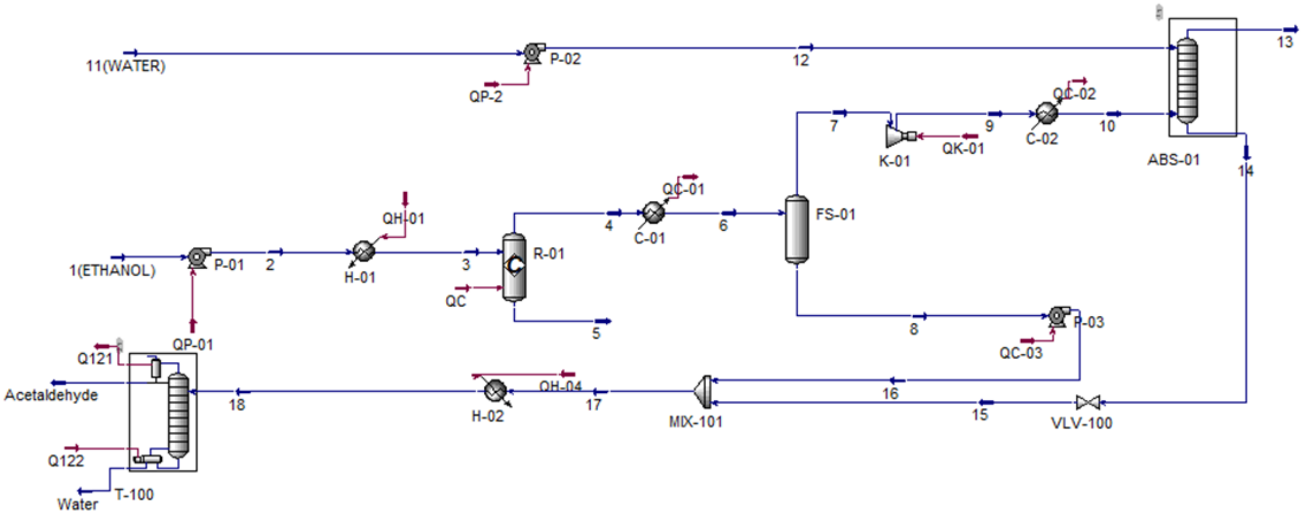

Figure 2. Unmodified process flow diagram of acetaldehyde using ASPEN HYSYS simulation.

spontaneity and thermodynamic feasibility of a reaction under specified conditions. This parameter enables engineers to evaluate reaction reversibility and predict equilibrium behavior [16]. Such knowledge is indispensable for selecting appropriate operating conditions, designing catalytic and separation units, and ensuring that the process achieves its performance targets. The dehydrogenation of ethanol can be represented as Equation (1) [10].

Standard heat of reaction at 298 K (ΔH^{o}_{298K}) (Table 1):

$\Delta H^{o}_{298K} = \Sigma\Delta H_f^{o}$ product – $\Sigma\Delta H_f^{o}$ reactant

$\Delta H^{o}_{298K} = (\Delta H_f^{o}\ CH_3CHO + \Delta H_f^{o}\ H_2) - (\Delta H_f^{o}\ C_2H_5OH) = 68.8$ kJ/mol

Based on the calculations, the result is determined to be positive, indicating that the reaction is endothermic.

Gibbs free energy (ΔG^{o}_{298K}):

$\Delta G^{o}_{298K} = \Sigma\Delta G_f^{o}$ product – $\Sigma\Delta G_f^{o}$ reactant

$\Delta G^{o}_{298K} = (\Delta G_f^{o}\ CH_3CHO + \Delta G_f^{o}\ H_2) - (\Delta G_f^{o}\ C_2H_5OH) = 34.7$ kJ/mol

Equilibrium constant (K_2) in the standard state:

$\Delta G^{o}_{298K} = -RT \ln K$; $K_2 = 8.2688 \times 10^{-7}$

Equilibrium constant (K_1) at reactor temperature T = 340 °C:

$$ln\frac{K_1}{K_2} = \frac{-\Delta H_R{}^{o}}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)$$

ΔH^{o}_{298K} = Standard heat of reaction at 25 °C

So that, $K_1 = 8.3879 \times 10^{-7}$

Table 1. The value of ΔH_f^{o} and ΔG_f^{o} of compounds.

Compounds	Molecular Formula	ΔH_f^{o} (kJ/mol)	ΔG_f^{o} (kJ/mol)
Ethanol	C_2H_5OH	-235	-167.7
Acetaldehyde	CH_3CHO	-166.2	-133
Hydrogen	H_2	0	0

Due to the low equilibrium constant, the dehydrogenation of ethanol is reversible.

Gibbs energy (ΔG^{o}_{613K}):

$\Delta G^{o}_{613K} = -RT \ln K_1 = 71.31\,\frac{\text{kJ}}{\text{mol}}$

The Gibbs free energy change at the reactor temperature of 340 °C is +71.31 kJ/mol, indicating that the reaction is non-spontaneous under the given operating conditions.

3.3 Improving Energy Efficiency by adding Heat Exchanger

The simulation enables quantification of the total energy demand of the process, expressed as the heat duty (kJ/h) associated with each unit operation. These values provide the basis for evaluating potential energy savings when comparing the modified flowsheet featuring the added heat exchanger with the original configuration (Figures 3 and 4). This approach allows the numerical calculation of energy reduction, thereby facilitating an assessment of

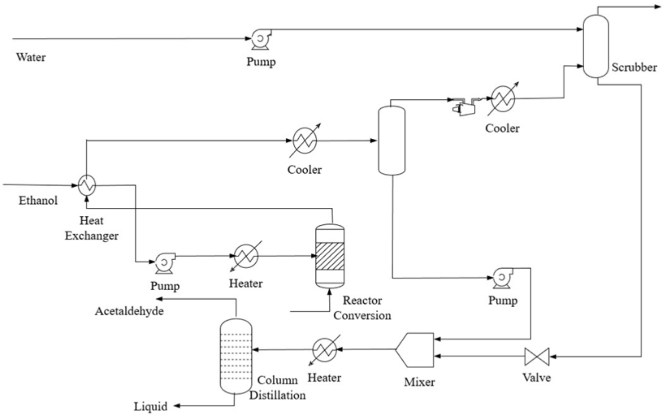

Figure 3. Modified process flow diagram to be simulated.

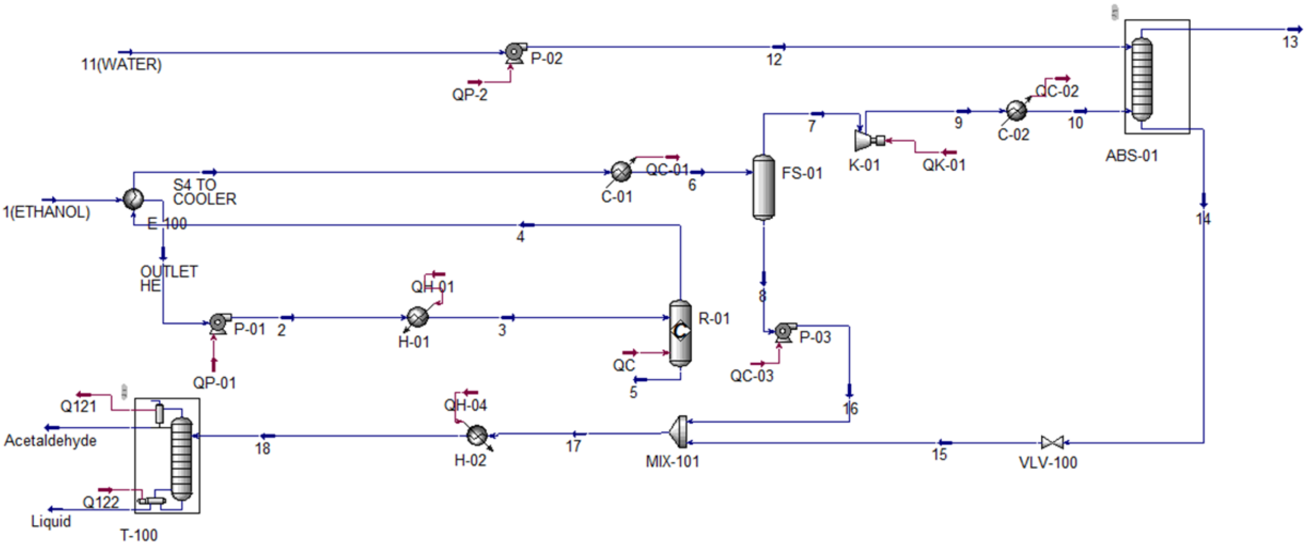

Figure 4. Modified process flow diagram of acetaldehyde using ASPEN HYSYS simulation.

improvements in process efficiency. The heat duty results generated by Aspen HYSYS are compiled and summarized in Table 2 to support further interpretation.

Beyond quantification, the simulation plays a critical role in assessing the effectiveness of the modified design. By contrasting the heat duties of the modified and unmodified systems, opportunities for reducing utility consumption become evident, guiding process enhancement. This comparison highlights not only the direct benefits of energy recovery but also broader contributions to sustainability and operational performance.

$$\begin{aligned}\Delta H_{Unmodified} = {} & Q_{p-01} + Q_{H-01} + Q_{C-01} + Q_{K-01} \\ & + Q_{C-02} + Q_{P-02} + Q_{C-03} + Q_{H-04} \\ & + Q_{C} + Q_{121} + Q_{122}\end{aligned}$$

$$\Delta H_{Unmodified} = 7{,}178{,}601.5 \text{ kJ/h}$$

$$\begin{aligned}\Delta H_{Modified} = {} & Q_{p-01} + Q_{H-01} + Q_{C-01} + Q_{K-01} \\ & + Q_{C-02} + Q_{P-02} + Q_{C-03} + Q_{H-04} \\ & + Q_{C} + Q_{121} + Q_{122}\end{aligned}$$

$$\Delta H_{Modified} = 6{,}670{,}999.1 \text{ kJ/h}$$

$$Energy\ Reduction = \Delta H_{Unmodified} - \Delta H_{Modified}$$

$$Energy\ Reduction = 507{,}602.4 \text{ kJ/h}$$

The energy efficiency improvements were achieved by incorporating an additional heat exchanger upstream of the downstream heating units. This integration reduced the thermal duty required by the process. In the unmodified flowsheet, the total energy demand reached 7,178,601.51 kJ/h. Following implementation of the modified design, the total energy requirement decreased to 6,670,999.1 kJ/h a reduction of 507,602.41 kJ/h. This demonstrates that the added heat exchanger significantly enhances heat recovery and lowers overall utility usage.

Correspondingly, the Specific Energy Consumption (SEC) for the unmodified design was 1,148,576.2 kJ/ton. After integrating the heat exchanger, the SEC decreased to 1,067,359.9 kJ/ton, representing an energy efficiency improvement of approximately 7.07%.

4. Conclusion

The simulation results demonstrate that integrating a heat exchanger into the acetaldehyde production flowsheet substantially reduces the overall energy demand of the process. The total heat duty decreases from 7,178,601.5 kJ/h in the unmodified configuration to 6,670,999.1 kJ/h in the modified design, yielding an energy saving of 507,602.4 kJ/h. This reduction is primarily achieved through enhanced internal heat recovery, as the added heat exchanger preheats the feed stream before it enters the process unit, thereby lowering the requirement for external heating.

As a direct consequence of this reduced energy demand, the Specific Energy Consumption (SEC) decreases from 1,148,576.2 kJ/ton to 1,067,359.9 kJ/ton, corresponding to an energy efficiency improvement of approximately 7.07%. The decline in SEC confirms that the modified process configuration operates more efficiently on a per-unit-production basis. Collectively, these findings highlight that strategic heat integration via the addition of a heat exchanger is an effective means of improving thermal efficiency, reducing utility consumption, and advancing the sustainability of acetaldehyde production.

CRedit Author Statement

Author Contributions: B. Nazlia: Software, Conceptualization, Methodology, Investigation, Resources, Data Curation, Review and Editing, Supervision; F.M. Fahira: Conceptualization, Methodology, Formal Analysis, Data Curation, Writing Draft Preparation, Visualization, Software, Project Administration; H.N. Hapsari:

Table 2. Energy comparison of unmodified and modified processes.

Unmodified Process		Modified Process	
Heat Streams Items	Heat Flow (kJ/h)	Heat Streams Items	Heat Flow (kJ/h)
QP-01	142.0	QP-01	142.0
QH-01	1,311,000	QH-01	1,311,000
QC-01	685,000	QC-01	685,000
QK-01	351,200	QK-01	243,900
QC-02	821,100	QC-02	415,900
QP-02	114.9	QP-02	114.9
QC-03	44.61	QC-03	242.2
QH-04	421,000	QH-04	426,700
QC	1,178,000	QC	1,178,000
Q121	1,307,000	Q121	1,305,000
Q122	1,104,000	Q122	1,105,000
Total Heat Flow (kJ/h)	7,178,601.5	Total Heat Flow (kJ/h)	6,670,999.1

Validation, Writing, Review and Editing, Data Curation; P.A.N. Putri: Investigation, Software, Resources, Writing, Review and Editing; K.G. Adyawita: Investigation, Resources, Writing, Review and Editing, Validation. All authors have read and agreed to the published version of the manuscript.

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