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Journal of Chemical Engineering Research Progress, 2 (2) 2025, 306-315

Research Article

Integrated Optimization of Cyclohexane Production via Benzene Hydrogenation Incorporating Advanced Separation, Extended Distillation, and Heat Exchanger Integration to Enhance Product Purity and Energy Efficiency

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Received: 12th December 2025; Revised: 15th December 2025; Accepted: 17th December 2025
Available online: 24th December 2025; Published regularly: December 2025

Abstract

Cyclohexane is an essential intermediate in the production of nylon-based polymers, yet its industrial synthesis via benzene hydrogenation and subsequent purification remains challenged by thermodynamic limitations and the narrow boiling-point gap between benzene and cyclohexane. This study presents an integrated process optimization strategy aimed at enhancing product purity and net energy efficiency without altering the existing operating conditions. Process simulations were performed to evaluate a modified flowsheet incorporating an additional separator, a second distillation column, and heat-exchanger integration for internal heat recovery. The results show that the modified configuration significantly improves separation performance, raising cyclohexane purity from 57.98% in the basic design to 93.40%. Energy integration through strategic heat-exchanger placement also reduced net energy demand from 910,655,219 kJ/h to 37,151,954 kJ/h, demonstrating substantial thermal-efficiency gains. These findings confirm that equipment-level modifications particularly enhanced separation structures and internal heat-recovery mechanisms can effectively intensify cyclohexane production processes, leading to higher product quality and improved energy sustainability.

Keywords: Cyclohexane; Integrated Optimization; Benzene Hydrogenation; Energy Efficiency

How to Cite: Artha, M. T. M., Rofiq, W. A., Aqilah, M. I., Umar, R. K., Ardelia, N. A. (2025). Integrated Optimization of Cyclohexane Production via Benzene Hydrogenation Incorporating Advanced Separation, Extended Distillation, and Heat Exchanger Integration to Enhance Product Purity and Energy Efficiency. *Journal of Chemical Engineering Research Progress*, 2 (2), 306-315 (doi: 10.9767/jcerp.20581)

Permalink/DOI: https://doi.org/10.9767/jcerp.20581

1. Introduction

Cyclohexane plays a pivotal role in the global chemical industry, primarily serving as the key feedstock to produce nylon 6 and nylon 6.6 which collectively account for approximately 86% of total global nylon consumption. The economic significance of this compound is reflected in the global market projection for cyclohexane derivatives, such as cyclohexanone, which is expected to grow at a compound annual growth rate (CAGR) of 4.5%, reaching a market value of US$8.72 billion by 2023 [1]. Given this massive scale of demand, the development of efficient and sustainable production methods has become an urgent priority in chemical process engineering [2].

The production of cyclohexane and its derivatives face significant technical challenges across both oxidation and hydrogenation routes. In the conventional liquid-phase oxidation pathway, reaction conversion must be strictly limited to below 6% to maintain product selectivity above 80% and prevent excessive by-product formation. In addition to this conversion

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inefficiency, commercial processes often require harsh operating conditions, such as temperatures of 170-230 °C and pressures of 1-2 MPa, which increase operational costs and safety risks [3]. Conversely, the benzene hydrogenation route, while more commonly utilized, encounters thermodynamic constraints due to the highly exothermic nature of the reaction, necessitating strict reactor temperature control to minimize the formation of by-products such as methane and methyl-cyclopentane [4].

However, the primary bottleneck in overall process efficiency often lies in the separation and purification stages. Mixtures of cyclohexane and benzene are notoriously difficult to separate due to their similar molecular structures and a minute boiling point difference of only 0.6 K, which leads to the formation of a homogeneous azeotrope. Conventional distillation methods have proven ineffective for separating this azeotropic mixture, resulting in high energy consumption and substantial operating costs. Furthermore, the presence of specific organic impurities, such as 2-cyclohexen-1-one (CXENONE), in the product stream must be minimized as they can significantly degrade the quality of the resulting nylon fibers [5].

Various process intensification strategies have been proposed in recent literature to address these reaction and separation challenges. In terms of reaction engineering, the use of microreactors has proven effective in enhancing gas-liquid mass transfer rates and operational safety under high-temperature and high-pressure (high T, P) conditions [6]. Green chemistry approaches are also being actively explored, such as the use of Z-type heterojunction photocatalysts (WO_3/C_3N_4) that enable C-H bond activation under ambient conditions using water and oxygen [7], as well as the development of alumina-supported noble metal catalysts (Ru, Pt) to enhance oxidation activity [8].

Regarding separation, alternative technologies, such as selective adsorption using thienothiophene cages (ThT-cages), offer up to 94% selectivity for separating cyclohexane from benzene via non-covalent interactions [9]. Reactive distillation methods have also been developed to remove CXENONE impurities through catalytic condensation reactions [10]. However, for industrial-scale applications, extractive distillation remains the preferred choice; recent studies indicate that utilizing ethylene glycol as a solvent can achieve product purities exceeding 99.91% while reducing CO_2 emissions by 72.38% compared to ionic liquid-based methods [11].

In this study, the modification is carried out specifically on the process equipment configuration without altering the existing operating conditions. The modification involves adding a separator and an additional distillation column to further purify the produced cyclohexane. In addition, heat exchanger integration is implemented to enhance the process's net energy efficiency. Accordingly, this research aims to simulate the process flowsheet using Aspen HYSYS V11 to evaluate the effects of the modification on cyclohexane purity as well as the net energy efficiency of the heat-transfer system.

2. Methods

2.1. Cyclohexane Production Process

Cyclohexane is a saturated hydrocarbon (C_6H_{12}) that plays an essential role in various chemical industries, particularly as a precursor in the production of adipic acid and caprolactam [12]. Cyclohexane can be produced through two primary methods, recovery from petroleum naphtha fractions and synthesis via benzene hydrogenation. Although recovery from naphtha enables the direct extraction of cyclohexane, its natural abundance in the naphtha stream is very limited, typically only around one to three percent, which makes this route insufficient to meet large-scale production demands [13]. Consequently, benzene hydrogenation has become the most dominant and widely utilized method in industrial practice, as it provides high-purity products and allows production capacities to be expanded in an economically feasible manner [14].

The hydrogenation of benzene involves the reaction between benzene (C_6H_6) and molecular hydrogen (H_2) to form cyclohexane (C_6H_{12}) through a highly exothermic transformation. This reaction has been extensively studied due to its energetic nature and its relevance in designing efficient catalytic systems for industrial hydrogenation processes [15]. The formation of cyclohexane through benzene hydrogenation is represented in Equation (1) [16]:

$$C_6H_6 + 3H_2 \rightarrow C_6H_{12} \quad \Delta H^o_{r\,298K} = -206.07 \text{ kJ/mole} \quad (1)$$

The production of cyclohexane begins with the controlled pumping of benzene and its blending with hydrogen gas at a specific molar ratio to ensure hydrogen excess, which enhances conversion and inhibits by-product formation during catalytic hydrogenation. The reactant mixture is then heated using heat exchangers or pre-heaters to reach the required reaction temperature before entering the fixed-bed catalytic reactor. Within the fixed-bed reactor, the reactant stream flows through the catalyst bed, where the hydrogenation reaction proceeds as a

strongly exothermic process, necessitating temperature management strategies such as quench gas injection or inter-bed cooling to avoid overheating of the catalyst bed [17].

The reactor effluent usually consists of cyclohexane, excess hydrogen, unreacted benzene, and minor impurities. Subsequent separation of the gas and liquid phases is achieved through a vapor–liquid separator, with excess hydrogen typically recycled back to the reactor to enhance overall process efficiency [18]. The liquid phase, mainly comprising benzene and cyclohexane, is processed in a distillation column; due to the very small boiling point difference between these compounds, sharp distillation conditions such as high tray numbers or elevated reflux ratios, or the application of advanced separation technologies, may be required to achieve high-purity cyclohexane suitable for chemical industry applications [19].

2.2. Thermodynamic Assessment

Thermodynamic assessment provides a fundamental basis for understanding the chemical reaction characteristics occurring within a process system. This analysis encompasses the determination of the standard enthalpy of formation for each component (ΔH_f^o), the standard Gibbs free energy of formation for each compound (ΔG_f^o), and the equilibrium constant (K), all of which play essential roles in describing the reaction direction, degree of spontaneity, and the operational conditions required to achieve optimal conversion. These parameters are crucial for evaluating the thermodynamic feasibility of a process prior to its design and subsequent operation under actual industrial conditions. The main reaction along with the total enthalpy change in the reactor is obtained according to Equation (2) and the value $\Delta H_{r\,298K}^o$ for the cyclohexane formation reaction is obtained using Equation (3), based on the ΔH_f^o data provided in Table 1 [20].

$$C_6H_6 + 3H_2 \rightarrow C_6H_{12} \quad \Delta H_{r\,298K}^o = -206167 \text{ kJ/kmole} \tag{2}$$

$$\Delta H_{r\,298K}^o = \sum \Delta H_{f\,298K\,product}^o - \sum \Delta H_{f\,298K\,product}^o \tag{3}$$

$$\Delta H_{r\,298K}^o = \Delta H_{f\,298K\,C6H12}^o - \left(\Delta H_{f\,298K\,C6H6}^o + \left(3 \times \Delta H_{f\,298K\,H2}^o\right)\right) = -206.07 \text{ kJ/mole}$$

Based on the calculations performed using Equation (3), the standard enthalpy of reaction $\Delta H_{r\,298\,K}^o$ was determined to be –206.07 kJ/mole. The negative value indicates that the formation of cyclohexane at standard temperature proceeds exothermically. The thermodynamic assessment of the reaction, expressed as the standard Gibbs free energy change (ΔG_r^o) was subsequently evaluated using Equation (4), employing the standard Gibbs free energy of formation data $(\Delta G_{f\,298\,K}^o)$ or each component as listed in Table 1.

$$\Delta G_{r\,298K}^o = \sum \Delta G_{f\,298K\,product}^o - \sum \Delta G_{f\,298K\,product}^o \tag{4}$$

$$\Delta G_{r\,298K}^o = \Delta G_{f\,298K\,C6H12}^o - \left(\Delta G_{f\,298K\,C6H6}^o + \left(3 \times \Delta G_{f\,298K\,H2}^o\right)\right) = -97.9 \text{ kJ/mole}$$

The equilibrium constant (*K*) is determined by applying Equation (5) at the specified temperature of T = 298 K.

$$\Delta G_{r\,298K}^o = -R \times 298\ K \times ln\ K_{298} \tag{5}$$

$$ln\ K_{298} = \frac{\Delta G_{r\,298K}^o}{-R \times 298\ K}$$

$$K_{298} = 1.44 \times 10^{17}$$

At the reactor operating temperature of 300 °C (573 K), the corresponding value is determined by applying Equation (6).

$$ln\ \frac{K_{573}}{K_{298}} = -\frac{\Delta H_{r\,298K}^o}{R} \times \left(\frac{1}{T} - \frac{1}{298\ K}\right) \tag{6}$$

$$K_{573} = 0.59$$

Accordingly, the Gibbs free energy change of the reaction (ΔG) at the reactor operating temperature (573 K) was calculated using Equation (7).

$$\Delta G_{r\,573K}^o = -R \times 573\ K \times ln\ K_{573} = 2.5136\ kJ/mole \tag{7}$$

The calculated value of the equilibrium constant (*K*) approaching 1 signifies that the reaction system is thermodynamically positioned near equilibrium, indicating minimal driving force toward either the forward or reverse direction.

2.3. Methods to Improve Net Energy Efficiency

Enhancement of energy efficiency in the cyclohexane production process via benzene hydrogenation was undertaken through a systematic energy integration strategy implemented in Aspen HYSYS V11. In the

Table 1. Enthalpy formation and Gibbs free energy of compounds [20].

Compounds	Molecular Formula	$\Delta H_{f\,298K}^o$	$\Delta G_{f\,298K}^o$
Hydrogen	H_2	0.00	0.00
Benzene	C_6H_6	49.00	129.66
Cyclohexane	C_6H_{12}	–156.40	31.76

preliminary stage of the simulation, benzene, hydrogen gas, cyclohexane, and cooling water were defined within the process flowsheet. The Peng–Robinson (PR) equation of state was selected as the fluid-property model due to its robustness in characterizing thermodynamic behavior of non-polar and mildly polar hydrocarbon systems, particularly with respect to enthalpy, entropy, fugacity, and vapor–liquid equilibrium predictions under moderate-pressure conditions [21]. This thermodynamic foundation ensures accurate heat-duty estimations across all process units, including heaters, coolers, and separation systems [22]. In the baseline configuration (Figure 1) followed by the simulation process design provided in Figure 2, thermal energy is not effectively recovered, resulting in elevated external utility requirements for both heating and cooling. To improve the net energy performance, the modified process configuration (Figure 3) incorporates advanced heat-integration measures through the installation of an additional heat exchanger that employs the high-temperature reactor effluent as a preheating medium for the incoming feed stream prior to entering the hydrogenation reactor. This counter-current heat-recovery mechanism substantially lowers the thermal load imposed on the primary heater, as the feed enters the reactor at an elevated inlet temperature. Furthermore, product cooling is conducted via an auxiliary heat exchanger using cooling water to ensure adequate temperature reduction before the multiphase separation stage. The introduction of these exchangers reduces dependence on external utilities by internally redistributing

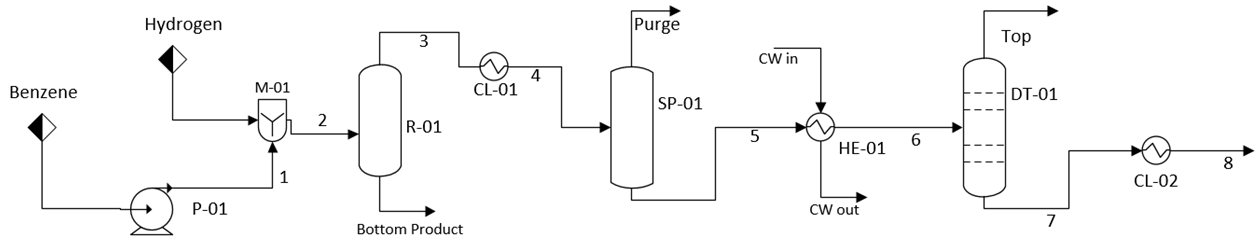

Figure 1. Process Flow Diagram (PFD) of basic (unmodified) cyclohexane production process.

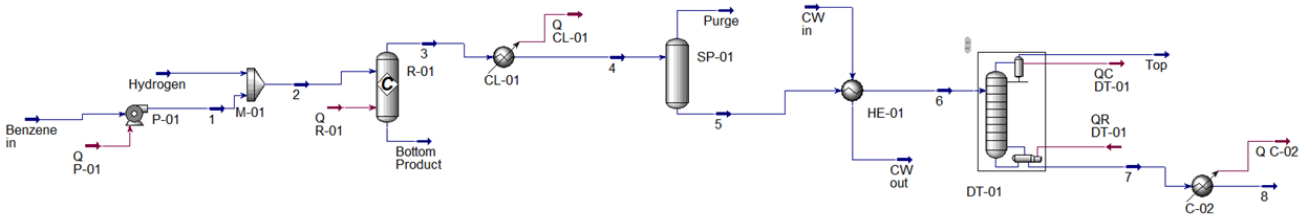

Figure 2. Aspen HYSYS simulation of basic (unmodified) cyclohexane production process [24].

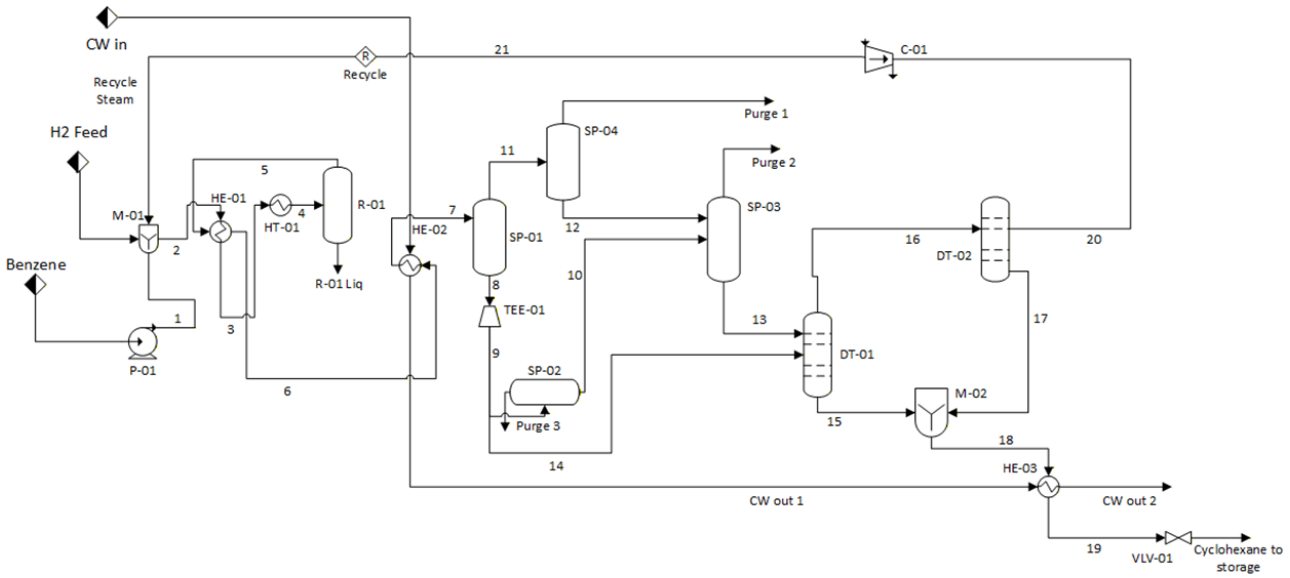

Figure 3. Process Flow Diagram (PFD) of modified cyclohexane production process.

process heat, thereby minimizing exergy losses. The degree of improvement in thermal performance and overall energy efficiency is quantitatively assessed using Equation (8) [23].

$$Q_{net} = Q_{in} - Q_{out} \quad (8)$$

Equation (8) expresses the overall heat balance of a thermodynamic system by quantifying the net amount of heat retained after accounting for both heat input and heat removal. In this formulation, Q_{in} represents all sources of heat supplied to the system such as external heaters or exothermic reaction heat while Q_{out} reflects the heat extracted through cooling utilities, heat exchangers, or other dissipative mechanisms. The resulting Q_{net} indicates whether the system experiences a net thermal gain or loss, thereby providing a direct measure of its thermal efficiency and stability. A positive signifies that the system accumulates heat, whereas a negative value denotes net heat dissipation. When Q_{net} approaches zero, the system is in a near-thermal equilibrium state, reflecting an effective balance between heat input and heat removal.

2.4. Methods to Improve the Purity of Cyclohexane

Product purity optimization was achieved through a series of modifications to the separation units. In the unmodified design, the separation of cyclohexane from hydrogen and benzene relied solely on a single separator followed by a single distillation column (DT-01). However, because benzene and cyclohexane exhibit a very narrow boiling point difference of approximately 0.6 °C. This minimal boiling point gap renders the liquid fractions of both components difficult to separate, resulting in distillate streams that still contain residual benzene impurities [25]. Theoretically, compounds with such close boiling points necessitate advanced separation techniques, such as azeotropic distillation, extractive distillation, or adsorption distillation, which are both technically complex and economically demanding [26]. Therefore, a modification of the flowsheet was required to enhance separation performance without introducing prohibitively expensive separation technologies.

In the modified design (Figure 3), an additional separator was installed downstream of SP-01 to maximize hydrogen removal from the liquid mixture, thereby ensuring that the liquid phase entering the distillation column contains a reduced gas fraction. Moreover, a second distillation column (DT-02) was incorporated to separate benzene from the distillate of the first column. This second column allows the partial benzene fraction that was not completely separated in the initial distillation to be recovered and recycled back to the reactor (M-01). The recycle system not only improves the purity of cyclohexane in the final product but also enhances reactor efficiency by reutilizing unreacted feedstock. Both distillation columns employ 60 trays and a reflux ratio of 10 to maintain consistency between the two designs. Product purity was calculated on a mass basis according to Equation (9) [27].

$$Purity\ (\%) = \frac{Total\ mole\ main\ product}{Total\ mole\ all\ product} \times 100\% \quad (9)$$

Equation (9) quantifies the composition quality of the cyclohexane product in terms of its mole fraction relative to the total product stream. In this expression, the numerator represents the total number of moles of the target compound (cyclohexane) contained in the final product stream, whereas the denominator corresponds to the total moles of all species present, including unreacted benzene, hydrogen, and any minor impurities.

3. Results and Discussion

3.1. Process Description of the Basic (unmodified) Simulation Design

The cyclohexane production process is carried out in accordance with the process flow diagram shown in Figure 1. Initially, a liquid benzene stream with a flow rate of 25,000 kg/h at 101.3 kPa is pressurized to 3000 kPa by pump P-01 before entering the mixing unit. The pressurized benzene stream is then combined with a gaseous hydrogen feed at M-01, where both streams are mixed under ambient temperature conditions at a pressure of 3000 kPa. The resulting reactant mixture is subsequently directed to R-01, a conversion reactor operated at 300 °C, where benzene is converted to cyclohexane with a conversion of 80% (Analogous to a catalytic reactor operating at 80% conversion of benzene). Hydrogenation of benzene to cyclohexane is a strongly exothermic catalytic reaction, consistent with thermodynamic theory that elevated temperature and hydrogen pressure enhance reaction rates in metal-catalyzed hydrogenation systems [28]. Because the reaction is strongly exothermic, the hot reactor effluent (stream 3) is routed to CL-01, a heat exchanger used to reduce the stream temperature prior to entering the gas-liquid separation unit. Heat exchangers operate based on the second law of thermodynamics [29]. Transferring energy from a hot stream to a cooler medium to achieve temperature reduction before phase separation [30]. Following initial cooling, the two-phase mixture enters SP-01, a separator that divides the gas fraction comprising unreacted

hydrogen and purge gases from the liquid fraction containing cyclohexane, unconverted benzene, and minor by-products. A portion of the unreacted hydrogen is removed as purge to prevent inert buildup, while the remaining fraction may be recycled to the reactor when desired. Purge stream control is required in recycle systems to avoid inert accumulation that would otherwise diminish reaction efficiency by diluting reactive species [31]. The liquid phase from the separator is subsequently sent to HE-01, a cooler employing cooling water (CW) to further reduce the stream temperature for efficient downstream distillation. The cooled stream is then distributed into DT-01, a distillation column designed to separate cyclohexane from residual benzene and other higher-boiling components. The overhead stream contains light components, whereas the bottoms stream (stream 7) yields high-purity cyclohexane as the primary product. This bottoms product is further cooled in CL-02 to 30 °C before exiting as the final product (stream 8), meeting the specification criteria established through simulation results shown in Figure 3.

The process sequence in the PFD consists of pumping, mixing, catalytic hydrogenation, primary cooling, gas liquid separation, secondary cooling, and distillation collectively enabling the production of high-purity cyclohexane from benzene via catalytic hydrogenation. Comparative simulation results between the unmodified process (Figure 2) and the modified configuration (Figure 4) highlight the integration of additional process units to enhance net energy performance and product purity. Accordingly, several independent variables were defined for both process configurations, including reactant feed conditions, reaction temperature, reaction pressure, reactant conversion, cooling temperature, adiabatic operation of all separators, and distillation column specifications consisting of 60 trays and a reflux ratio of 10. The complete set of process conditions, including mass and energy balances for each design component is provided in the Supporting Information.

3.2. Process Description of the Simulation Design After Modification

The modified process simulation is conducted based on the process flow diagram presented in Figure 3. Liquid benzene, serving as the feed initially pressurized by pump P-01 and directed to the mixer (M-01), like the basic design configuration, where it is combined with a pressurized hydrogen gas stream. The resulting mixture is subsequently heated using the heat exchanger HE-01 and further elevated in temperature by the heater HT-01 to reach the required operating temperature of 300 °C before entering reactor R-01. Pre-heating the feed stream is essential because reaction rates in catalytic hydrogenation increase significantly with temperature according to Arrhenius-based kinetics [32]. Within the reactor, the hydrogenation of benzene to cyclohexane proceeds as a highly exothermic reaction. Therefore, the reactor effluent must be cooled via HE-02 prior to entering the separation section. The cooled product stream is then routed through a series of separators, SP-01 through SP-04, which function to remove unreacted hydrogen and other light gases from the hydrocarbon liquid phase. Gas-liquid separators rely on density differences and vapor–liquid equilibrium, where lighter gases disengage from heavier liquid phases under reduced temperature [33]. A portion of the gaseous stream is purged at designated purge points to prevent inert buildup within the system.

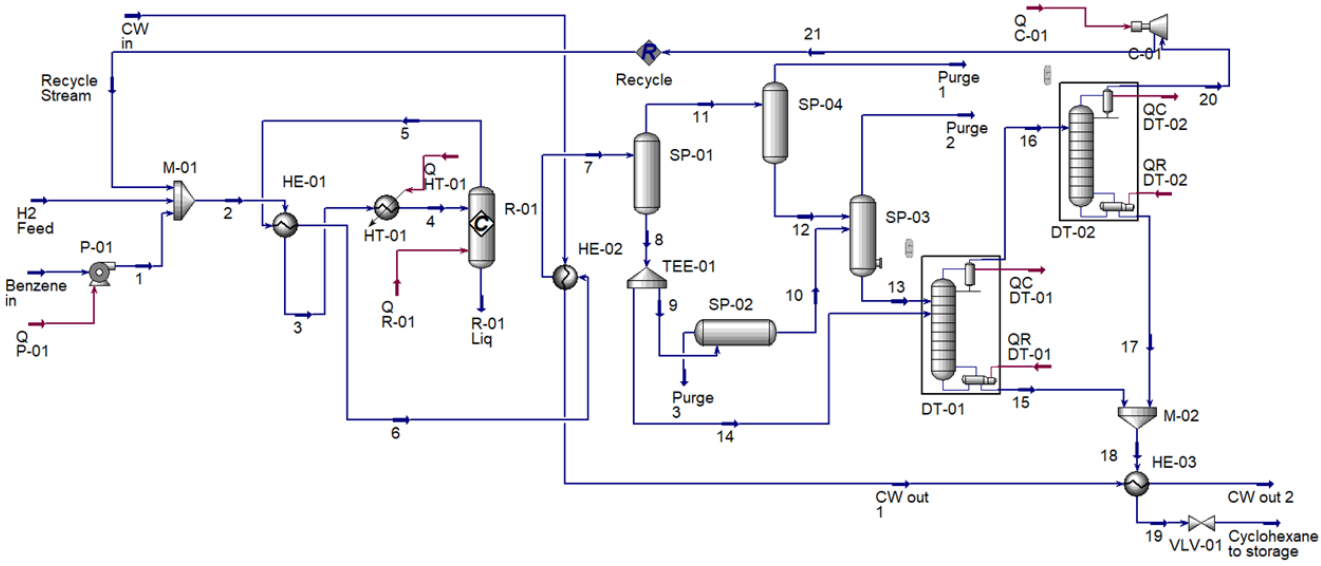

Figure 4. Aspen HYSYS simulation of modified cyclohexane production process.

The liquid hydrocarbon stream, consisting primarily of cyclohexane and residual benzene, is subsequently directed to the distillation columns DT-01 and DT-02 to further separate cyclohexane from benzene. The benzene-rich vapor from the overhead stream of DT-02 is recompressed using compressor C-01 and recycled back into the system. Meanwhile, the final product obtained from DT-01 is cooled using HE-03 before being transferred to storage through valve VLV-01. The entire system employs three purge points and multiple cooling units to maintain operational stability, minimize inert accumulation, and enhance benzene utilization efficiency. Such process modifications are consistent with chemical process optimization strategies aimed at improving reactant utilization, reducing energy losses, and increasing overall process efficiency.

3.3. Assessment of Net Energy in Cyclohexane Production Process

Based on the cyclohexane production process simulation design presented in Figure 4, heat transfer in the modified configuration is facilitated using a heat exchanger (HE-01) to reduce the thermal load on the heater (HT-01), along with the incorporation of an additional heat exchanger (HE-03) for product cooling. The comparison of net energy efficiency between the two process configurations is summarized in Table 2 and Table 3. The results indicate a significant improvement in energy performance, which is consistent with heat integration theory indicating that effective recovery and reuse of heat in process systems can significantly reduce overall energy consumption [34]. Consequently, the integration of additional heat exchangers reduces the overall energy demand of the system, thereby enhancing the operational efficiency of the process. This phenomenon aligns with pinch analysis principles, which demonstrate that targeted placement of heat exchangers can minimize energy utilities and maximize thermal recovery in complex flowsheets [35].

Table 2. Q_{net} calculation for the basic unmodified process.

Stream	Q_{in} (kJ/h)	Q_{out} (kJ/h)
Q P-01	8,653,408	
Q R-01	572,859,435	
QR DT-01	6,175,191,481	
Q CL-01		952,101,616
Q CL-02		3,673,919
QC DT-01		4,890,273,569
Subtotal	6,756,704,325	5,846,049,105
Q_{net}	910,655,219	

3.4. Assessment of Cyclohexane Purity

The evaluation of the process simulation was conducted by comparing the product purity achieved in the basic process configuration (Figure 2) with that obtained in the modified design (Figure 4). The final product flowrate at the outlet stream (Cyclohexane to storage) was quantified and subsequently assessed using the correlation expressed in Equation (9). The corresponding results are summarized in Table 4. The analysis reveals a marked enhancement in cyclohexane purity within the modified configuration, which can be attributed to the integration of additional separation units and a dual-distillation arrangement. This finding aligns with the principle that incorporating intensified separation structures enhances component resolution by improving mass transfer efficiency and reducing remixing [36,37]. This intensified separation strategy improves the removal of impurity components and thereby facilitates a more effective isolation of the targeted product.

4. Conclusion

The modifications applied to the process equipment configuration including the addition of a separator and an auxiliary distillation column demonstrated a substantial enhancement in product purification performance without requiring any alteration to the existing operating conditions. The cyclohexane purity obtained in the basic unmodified design, initially measured at 57.98%, increased markedly to 93.40% in the modified configuration. Furthermore, the

Table 3. Q_{net} calculation for the modified process.

Stream	Q_{in} (kJ/h)	Q_{out} (kJ/h)
Q P-01	110,784	
Q R-01	-63,286,149	
Q HT-01	87,724,653	
QR DT-01	93,816,340	
QR DT-02	36,004,896	
QC DT-01		78,445,525
QC DT-02		38,773,046
Q C-01		895,284
Subtotal	154,370,525	117,218,571
Q_{net}	37,151,954	

Table 4. Cyclohexane purity on unmodified and modified process.

Parameter	Unmodified	Modified
Purity (%)	57.98	93.40

integration of heat exchangers contributed to an improvement in the system's net energy efficiency. The net energy demand of the basic unmodified design was calculated to be 910,655,219 kJ/h, whereas the modified system exhibited a significantly lower value of 37,151,954 kJ/h. This reduction in net energy indicates a more favorable balance between the energy supplied to and released from the system, thereby enabling a more efficient heat-transfer process. Simulation results confirm that the modifications introduced yielded notable improvements in both cyclohexane purity and overall energy efficiency. Hence, the implemented process enhancements can be considered effective in optimizing the performance of the cyclohexane production system.

CRedit Author Statement

Author Contributions: M.T.M. Artha: Conceptualization, Methodology, Investigations, Software, Writing, Supervision, Data Curation, Project Administration, Formal Analysis, Review & Editing; W.A. Rofiq: Conceptualization, Methodology, Investigations, Software, Writing, Review & Editing, Supervision; M.I. Aqilah: Investigations, Writing, Review & Editing, Validation, Resources, Data Curation; R.K. Umar: Investigations, Writing, Review & Editing, Validation, Resources, Data Curation; N.A. Ardelia: Software, Visualization, Writing, Resources, Review & Editing. All authors have read and agreed to the published version of the manuscript.

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