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Research Article

Process Optimization of Cumene Production: Energy Efficiency Optimization and Conversion Enhancement through Heat Integration and Recycle Strategies

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Abstract

Cumene production via benzene–propylene alkylation is a highly exothermic process that requires effective thermal management. This study aims to optimize energy efficiency and enhance conversion performance in cumene production through the integration of reactor heat recovery and recycle strategies. To improve heat utilization efficiency, the process was modified by integrating a circulating heat transfer fluid system that captures reactor heat and reuses it for feed preheating, thereby reducing external utility demand. Additional heat released during effluent cooling is recovered to supply the mechanical energy required for pumping. The modified and baseline configurations were modeled using chemical process simulator and evaluated using a net energy (NE) framework. Results show that the basic process yields an NE of 3,119,682.58 kJ/h, while the modified process achieves 2,055,114.79 kJ/h, with 21,294,605.8 kJ/h of internal energy successfully recovered and reused. This demonstrates a substantial improvement in thermal integration and reduced reliance on external heating. Furthermore, the introduction of a vapor phase benzene recycle stream enhances benzene conversion, suppresses secondary alkylation, and increases cumene yield. Overall, the integrated heat recovery and recycle strategy significantly improves energy efficiency, conversion performance, and sustainability in cumene production.

Keywords: Cumene; Alkylation; Conversion; Process modifications; Heat efficiency

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1. Introduction

Cumene (isopropylbenzene) is a critical intermediate in the petrochemical value chain and the dominant precursor for phenol and acetone, key building blocks for bisphenol A, epoxy resins, polycarbonates, and numerous engineering polymers. Industrial records indicate that virtually all globally produced cumene is directed toward phenol synthesis, underscoring its strategic importance in aromatic chemicals manufacturing [1]. With continued growth in phenol and acetone demand, particularly across Asia, where large-scale aromatic complexes are rapidly expanding, cumene production capacity has increased in tandem to support integrated downstream operations [2]. Market projections estimate that the global cumene sector will reach USD 17.63 billion by 2025, driven by sustained industrial and polymer-grade phenolics consumption [3]. These trends have intensified research interest in developing more efficient cumene manufacturing routes that enhance product quality, operational efficiency, and resource utilization.

Industrial cumene is predominantly produced through the Friedel–Crafts alkylation of

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benzene with propylene, an irreversible and exothermic reaction typically conducted in vapor-phase packed bed reactors employing solid acid catalysts. While the primary pathway yields cumene, secondary alkylation produces p-diisopropylbenzene (PDIB), an undesired by-product that increases separation load and depresses overall selectivity. Because this side reaction exhibits a higher activation energy, rigorous control of reactor temperature, benzene-to-propylene ratio, and catalyst microenvironment is essential to maintain selectivity [4]. Excess benzene is commonly applied to suppress PDIB formation; however, this strategy elevates recycle requirements and downstream distillation energy consumption [5].

Recent advances in process systems engineering have emphasized the significant role of reactor configuration, heat-integration strategies, and recycle optimization in improving cumene plant performance. Integrated alkylation–transalkylation schemes have demonstrated substantial improvements in conversion and reductions in by-product formation through optimized reactor staging and catalyst distribution [6]. Complementary studies in process control highlight that temperature-profile management, hotspot mitigation, and uniform flow distribution critically influence product purity, catalyst life, and operational reliability [7]. These insights underscore the need for reactor-level optimization in tandem with catalyst and flowsheet improvements.

Energy efficiency has likewise become a central design consideration in modern cumene facilities. Heat-integration analyses show that recovering exothermic heat from the alkylation reactor and repurposing it for feed preheating or utility reduction can substantially decrease external energy requirements and improve overall plant sustainability [8]. In addition, optimization frameworks employing advanced reactor models and predictive analytics have enhanced the accuracy of yield and selectivity forecasting, enabling more robust process control and improved operational stability [9]. Building on these developments, the present study investigates reactor-level modifications and heat-integration schemes aimed at enhancing cumene purity, conversion, and net energy efficiency. By incorporating plug-flow reactor (PFR) operation, strategic recycle loops, and comprehensive heat-recovery configurations, this work seeks to contribute to the development of a more sustainable, selective, and economically competitive cumene production process.

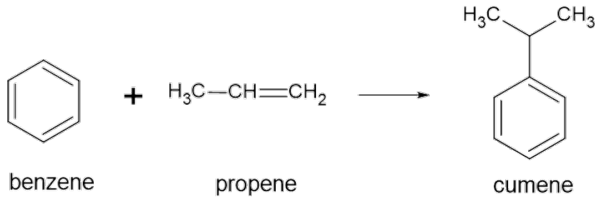

Figure 1. Main reaction scheme [11].

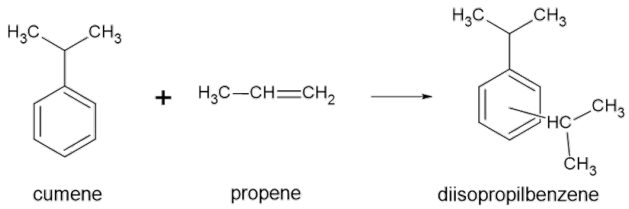

Figure 2. Side reaction scheme [11].

2. Methods

2.1. Cumene Production

Cumene is produced via the Friedel–Crafts alkylation of benzene with propylene, an irreversible and exothermic reaction conducted industrially in high-temperature, high-pressure gas-phase packed-bed reactors employing solid acid catalysts [2]. The primary pathway yields cumene (isopropylbenzene) through direct alkylation of benzene with propylene, with optimal operation typically occurring near 350 °C to balance conversion and selectivity [10] (see Figure 1 [11]).

Under these thermodynamic and catalytic conditions, sequential secondary alkylation can also take place, wherein cumene reacts further with propylene to form p-diisopropylbenzene (PDIB), an undesirable by-product that reduces selectivity and increases downstream separation demand (Figure 2 [11]). The overall reaction network can be represented as follows [10]:

$$C_6H_6 + C_3H_6 \rightarrow C_9H_{12} \text{ (main reaction)}$$
$$\Delta H^0{}_{298K} = -94.69 \text{ kJ/mol} \quad (1)$$
$$C_9H_{12} + C_3H_6 \rightarrow C_{12}H_{18} \text{ (side reaction)}$$
$$\Delta H^0{}_{298K} = -52.1 \text{ kJ/mol} \quad (2)$$

The conceptual design of the cumene production process was first introduced by Turton *et al.* and has subsequently been refined by various researchers to improve both economic viability and process sustainability [12]. In the conventional flowsheet, a preheated benzene–propylene mixture is fed into a pressurized packed-bed reactor to facilitate efficient vapor-phase alkylation. Typical industrial operating conditions involve reactor inlet temperatures near 350 °C, bounded by catalyst thermal stability and hot-spot suppression, and pressures of up to 25 bar to ensure complete vapor-phase operation and avoid condensation within the reactor system [13].

As indicated by the reaction kinetics (Table 1 [12]), the activation energy of the secondary alkylation pathway is significantly higher than that of the primary alkylation reaction. Consequently, lower reactor temperatures thermodynamically favor cumene formation while simultaneously reducing the overall reaction rate. Selectivity toward cumene can also be enhanced by maintaining low concentrations of cumene and propylene within the reactor, thereby limiting secondary reactions. This is most commonly achieved through the use of excess benzene, which inevitably increases recycle load and elevates downstream separation energy requirements [14].

Benzene is deliberately selected as the excess reactant, whereas propylene is employed as the limiting reactant. Operating with benzene in excess not only promotes selectivity toward cumene but also provides an effective heat-sink medium to absorb the substantial heat released from the highly exothermic alkylation reaction. This thermal buffering effect helps stabilize reactor temperature profiles and mitigates the risk of undesired propylene polymerization, which can otherwise lead to the formation of heavier linear hydrocarbons and catalyst deactivation [15]. The production process model for cumene via the alkylation of benzene with propylene was developed using Aspen HYSYS V11. The components included in the simulation were benzene, propylene, cumene, diisopropylbenzene, oxygen, nitrogen, methane, and water. The Peng–Robinson fluid package was employed for the thermodynamic calculations.

2.2. Thermodynamic and Kinetic Review

Data $\Delta H^0_{f\,298K}$ of each component to determine ΔH_r at 298 K can be seen in Table 2. [16] The value of $\Delta H^0_{r\,298K}$ for the reaction of alkylation of benzene with propylene is obtained by:

$$\Delta H^0_{r\,298K} = \sum \Delta H^0_{f\,298K\,product} - \sum \Delta H^0_{f\,298K\,reactant} \quad (3)$$
$$\Delta H^0_{r\,298K} = \Delta H^0_{f\,298K\,C_9H_{12}} - (\Delta H^0_{f\,298K\,C_6H_6} + \Delta H^0_{f\,298K\,C_3H_8})$$
$$\Delta H^0_{r\,298K} = -94.69\ \text{kJ/mol}$$

Table 1. Kinetic characteristics of the primary and secondary reactions in cumene and PDIB synthesis. [12].

Kinetic parameter	Main reaction	Side reaction
Pre-exponential factor, A (kmol/m^3.s)	2.8×10^7	2.32×10^9
Activation energy, E_a (kJ/mol)	104.174	146.742

Based on the calculation, obtained $\Delta H^0_{r\,298K} = -94.69$ kJ/mol with negative value that indicates the reaction is exothermic. Data $\Delta G^0_{f\,298K}$ of each component to determine ΔG_r at 298K can be seen in Table 3. [16] The value of $\Delta G^0_{r\,298K}$ for the reaction of alkylation of benzene with propylene is obtained by:

$$\Delta G^0_{r\,298K} = \sum \Delta G^0_{f\,298K\,product} - \sum \Delta G^0_{f\,298K\,reactant} \quad (4)$$
$$\Delta G^0_{r\,298K} = \Delta G^0_{f\,298K\,C_9H_{12}} - (\Delta G^0_{f\,298K\,C_6H_6} + \Delta G^0_{f\,298K\,C_3H_8})$$
$$\Delta G^0_{r\,298K} = -55.3\ \text{kJ/mol}$$

Based on the calculation, obtained $\Delta G^0_{r\,298K} = 59.6$ kJ/mol with positive value that indicates the reaction is spontaneous.

The value of equilibrium constant (K) at 298 K can be calculated by:

$$\ln K_{298} = \frac{-\Delta G^0_{r\,298K}}{RT} \quad (5)$$
$$\ln K_{298} = \frac{-\left(-55300 \frac{J}{mol}\right)}{8.314 \frac{J}{mol.K} \times 298\ K}$$
$$K_{298} = 4.938 \times 10^{-11}$$

For the reaction temperature 350 ℃ or 623.15 K, the equilibrium constant (K) can be calculated by:

$$\ln \frac{K_{623.15}}{K_{298}} = \frac{\Delta H^0_{r\,298K}}{R} \times \left(\frac{1}{T} - \frac{1}{T_{ref}}\right) \quad (6)$$
$$\ln \frac{K_{623.15}}{4.938 \times 10^{-11}} = \frac{-94690 \frac{J}{mol}}{8.314 \frac{J}{mol.K}} \times \left(\frac{1}{623.15\ K} - \frac{1}{298\ K}\right)$$
$$K_{623.15} = 9.847 \times 10^{-10}$$

Based on the calculation, the equilibrium constant value of the reaction operates at 350 ℃ ($K_{623.15}$) = 9.847×10^{-10}, so the reaction is irreversible.

Reaction kinetics were incorporated in the simulation to properly describe the behavior of the plug flow reactor (PFR). The reaction rate constant was calculated using the Arrhenius equation. The values of A and E_a used in this study are summarized in (Table 1 [12]). At the

Table 3. $\Delta G°_{f\,298K}$ data for each component [16].

Component	$\Delta G^0_{f\,298K}$
C_6H_6	129.8
C_3H_6	62.6
C_9H_{12}	137.1
$C_{12}H_{18}$	147.8

Table 2. $\Delta H°_{f\,298K}$ data for each component [16].

Component	$\Delta H^0_{f\,298K}$
C_6H_6	82.9
C_3H_6	19.7
C_9H_{12}	7.91
$C_{12}H_{18}$	-77.6

reactor operating temperature of T = 623.15 K, the reaction rate constant was determined as follows:

$$k = A\, e^{\frac{-E_a}{RT}} \quad (6)$$

$$k = 2.8 \times 10^7 \frac{kmol}{m^3.s} \exp\left(\frac{-104174 \frac{J}{mol}}{8.314 \frac{J}{mol.K} \times 623.15K}\right)$$

$$k = 5.183 \times 10^{-2} \frac{kmol}{m^3.s}$$

The calculated reaction rate constant was subsequently applied in the plug flow reactor (PFR) simulation to ensure consistency between the kinetic model and the reactor performance analysis.

2.3. Energy Optimization Method

Energy efficiency enhancement in the production of cumene from benzene and propene was evaluated through rigorous process simulation using Aspen HYSYS. The conversion of benzene and propene to cumene proceeds via a Friedel–Crafts alkylation mechanism, which is strongly exothermic [17]. In the simulation framework, the reaction was modeled under isothermal conditions at 350 °C within a plug flow reactor (PFR), allowing the exothermic heat release to be quantified and incorporated into the overall heat-integration strategy. The thermal energy generated by the reactor was subsequently recovered and repurposed to support upstream heating requirements, thereby reducing the dependence on external utilities [18].

In the proposed heat-integration scheme, the recovered reactor energy is supplied to heater E-100, increasing the feed temperature from 160 °C to 273.9 °C prior to entering the fired heater. Under the baseline (pre-modification) configuration, this heating duty was met entirely through high-pressure steam at 254.8 °C and 42.37 bar. Additionally, the reactor effluent exiting at 350 °C is cooled to 90 °C in a downstream cooler. This cooling step liberates approximately 3.048×10^7 kJ/h of thermal energy, which is subsequently recovered and reused to power the pumping system responsible for increasing the feed pressure from 1 bar to 31.5 bar. This approach minimizes both furnace duty and steam demand, strengthening the overall thermal integration of the process.

The energy performance of the modified flowsheet was assessed using the net energy (NE) metric, defined as:

$$NE = EP - EC \quad (8)$$

where *NE* represents the net energy of the system (kJ/h), *EP* denotes the total energy produced internally (kJ/h), and *EC* corresponds to the total external energy consumed (kJ/h) [19]. A comparative evaluation was then performed between the modified and baseline cumene production schemes to quantify the improvement in net energy efficiency resulting from the integration of reactor-derived heat and recovered cooler duty.

2.4 Conversion Optimization Method

Conversion in the plug-flow reactor (PFR) can be further enhanced by incorporating a recycle stream into the cumene production flowsheet. In the modified configuration, the vapor-phase effluent leaving the knock-out drum is returned and mixed with the fresh benzene feed. This recycle loop is required because the overhead vapor still contains a significant quantity of unreacted benzene, while the remaining components consist primarily of propane impurities. Given that benzene is the key reactant and a high-value aromatic feedstock, purging this stream would lead to unnecessary raw-material losses; thus, a separation unit and recycle loop are introduced to recover and reuse benzene efficiently [20]. Implementing this recycle strategy increases overall conversion, minimizes reactant waste, and improves process sustainability.

Simulation results show that the separated benzene stream retains a mass flow rate of 45.4974 kg/h. Since this stream remains benzene-rich and is fully in the vapor phase, it cannot be directly blended with the liquid fresh benzene feed. Therefore, it is routed to a secondary mixer before entering the reactor. Returning this benzene-rich vapor stream to the PFR has been shown to substantially enhance overall conversion, as the recovered reactant reduces the requirement for additional fresh benzene input. Furthermore, during downstream fractionation, the higher benzene conversion achieved through recycling directly increases the cumene flowrate in the product stream, thereby improving overall yield and reducing separation burden.

The enhancement in cumene conversion between the unmodified and modified processes is quantified using the following expression:

$$Cumene\ conversion = \left(\frac{reacted\ benzene}{unreacted\ benzene}\right) \times 100\% \quad (9)$$

3. Results and Discussion

3.1. Comparison Between Basic and Modified Processes

The simulations of both the baseline and modified cumene production processes developed using Aspen HYSYS are presented in Figures 3–

6. Figure 3 illustrates the simulation flowsheet of the baseline configuration, while its corresponding process flow diagram (PFD) is shown in Figure 5. In this conventional scheme, feed preheating is achieved using a heat exchanger supplied with high-pressure steam. In contrast, the modified process is depicted in Figure 4, with its PFD shown in Figure 6. In this enhanced configuration, the steam-based heat exchanger is replaced with a heater that recovers energy from the plug-flow reactor (PFR), the thermal energy released in the cooler is utilized to drive the pump, and the vapor stream exiting the knock-out drum is recycled back to the mixer.

The principal distinctions between the two configurations arise from improvements in energy integration and material utilization. In the modified process, the heat released during cooling of the reactor effluent is recovered and applied to the pump duty, while the exothermic energy generated in the PFR is repurposed to preheat the reactant mixture prior to entering the furnace. Furthermore, the benzene-rich vapor stream obtained from vapor–liquid separation is reintegrated into the feed system, thereby enhancing overall conversion and reducing fresh reactant consumption.

By contrast, in the baseline process, the heat liberated from both the PFR and the cooler is not

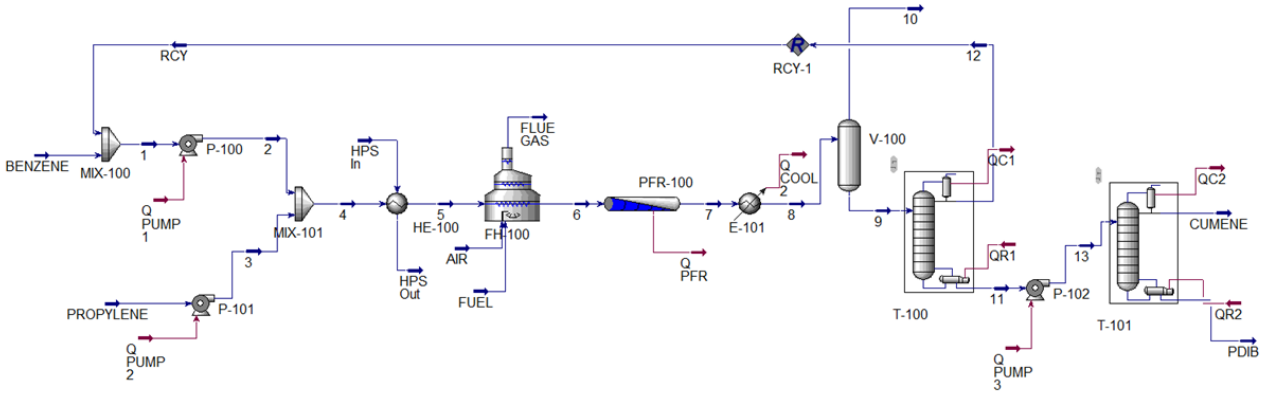

Figure 3. Simulation using Aspen HYSYS of basic (unmodified) process.

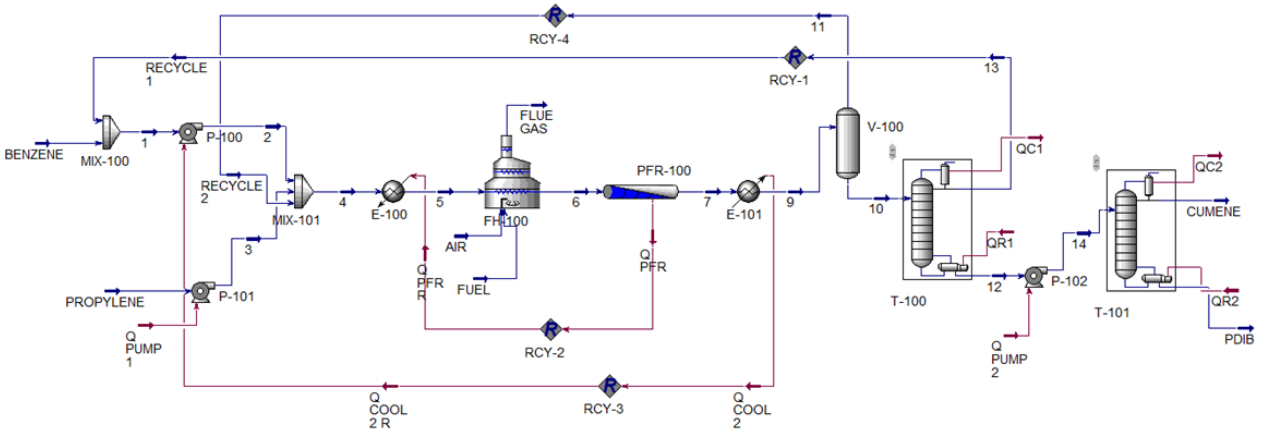

Figure 4. Simulation using Aspen HYSYS of modified process.

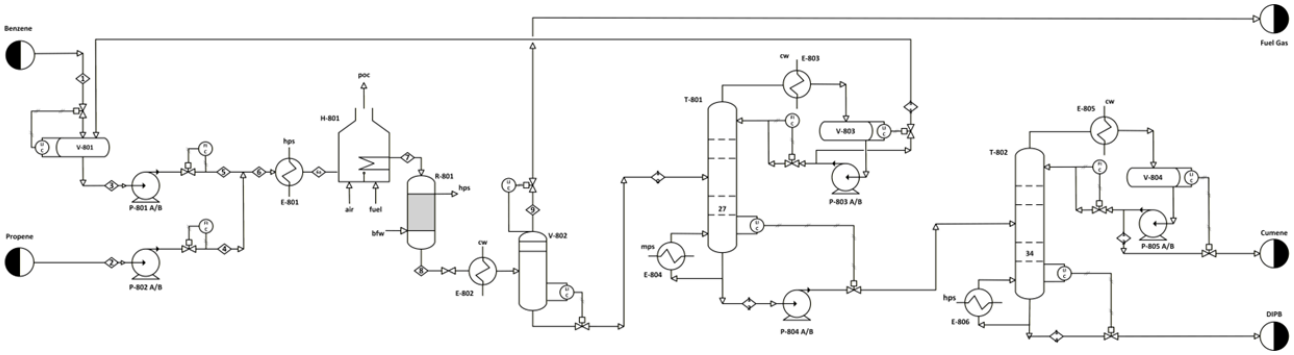

Figure 5. Process flow diagram of basic (unmodified) process.

recovered and is instead rejected to the surroundings, resulting in significant energy losses. Moreover, the vapor stream from the knock-out drum is discarded rather than reused, leading to unnecessary loss of unreacted benzene. In the modified configuration, this previously wasted energy is effectively harnessed for pumping and feed preheating, with the recovered cooler energy replacing the original steam-based heat exchanger required to heat the primary feed stream.

3.2. Mass and Energy Balance Results

In the modified process configuration, the effluent from the PFR-100 reactor exits the unit at a molar flow rate of 440.5 kmol/h, with component mole fractions of 0.0801 benzene, 0.0069 1,4-iP-BZ, 0.2769 cumene, 0.0020 propene, and 0.6342 propane. This stream is then sent to separator V-100, which splits it into a top product (stream 10) and a bottom product (stream 9). The top product flows at 323 kmol/h and contains 0.0763 benzene, 0.0004 1,4-iP-BZ, 0.0723 cumene, 0.0026 propene, and 0.8484 propane. Because this stream still carries a significant number of unreacted components, it is recycled back to the reactor for further conversion. The bottom product (stream 9) has a molar flow of 117.5 kmol/h and is enriched in cumene, with a mole fraction of 0.8393. The remaining components include 0.0905 benzene, 0.0249 1,4-iP-BZ, 0.0001 propene, and 0.0452 propane. This cumene-rich stream is subsequently purified through two distillation columns, T-100 and T-101.

In column T-100, the top product (stream 12) has a flow rate of 13.12 kmol/h and consists of 0.5938 benzene, 0.0011 propene, and 0.4050 propane. Because this stream still contains a high concentration of unreacted benzene, it is returned to the system as recycle. The bottom product (stream 11) flows at 104.4 kmol/h and contains 0.0272 benzene, 0.0280 1,4-iP-BZ, and 0.9448 cumene. This stream is then fed to the second distillation column, T-101, for further purification. In column T-101, the top product (cumene stream) has a molar flow of 101.4 kmol/h with a composition of 0.9720 cumene and 0.0280 benzene. The bottom product (1,4-iP-BZ stream) flows at 2.921 kmol/h and contains 0.9999 1,4-iP-BZ with only trace amounts of cumene. Overall, the separation sequence produces a final cumene product stream with a mass flow rate of 11,851.4291 kg/h.

As shown in Figure 4, the plug-flow reactor (PFR-100) releases approximately 1.022×10^7 kJ/h of thermal energy. This recovered heat is redirected to the feed preheater (E-100), increasing the inlet feed temperature from 160 °C to 273.9 °C before entering the furnace (FH-100). Downstream of the reactor, the effluent stream, initially at 350 °C, is cooled to 90 °C using cooler E-101. This cooling step discharges an additional 3.048×10^7 kJ/h of energy, which is subsequently recycled and utilized to supply the mechanical energy requirement of pump P-100, enabling the feed pressure to be elevated from 1 bar to 31.5 bar.

Through this integrated heat-recovery approach, the system substantially decreases its dependence on external heating utilities, reduces furnace duty, and improves thermal utilization across the process. These modifications demonstrate the effectiveness of energy recycling and waste-heat recovery in enhancing the overall sustainability, efficiency, and operational economy of the cumene production pathway.

3.3. Recovery and Utilization of System-Released Energy

Before entering the reactor, the feed mixture of propene and benzene must be conditioned to satisfy the reactor's temperature and pressure requirements. Utilities are employed to elevate the feed temperature to 350 °C, the operating temperature of the PFR-100 reactor. The reactor effluent is subsequently cooled from 350 °C to 90 °C using cooler E-101. In the base (unmodified) process (Figure 3), feed preheating is carried out in heat exchanger HE-100 using high-pressure steam at 42.37 bar and 254.8 °C. Generating

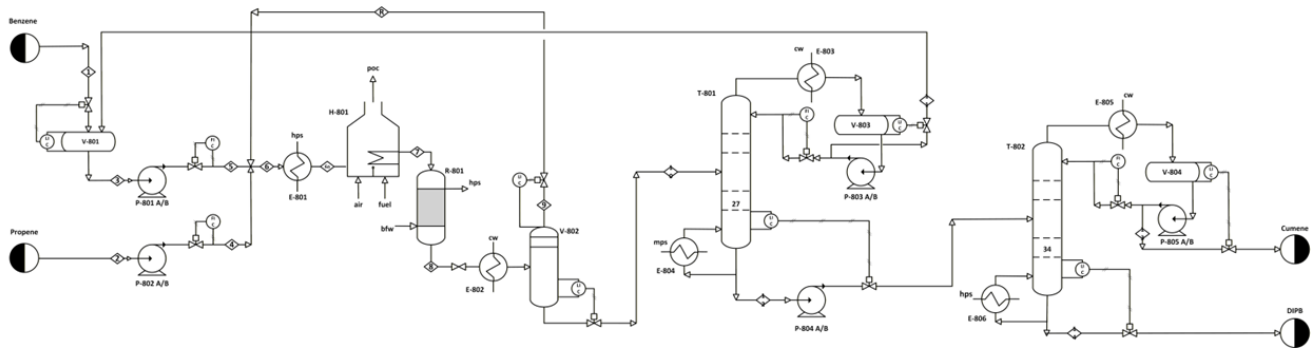

Figure 6. Process flow diagram of modified process.

steam at these conditions requires substantial energy input. Under this configuration, HE-100 increases the feed temperature from 26.49 °C to 214 °C prior to its final heating in the furnace, while pump P-100 relies entirely on external utilities to raise the feed pressure.

Within the PFR-100 reactor, the alkylation of benzene with propene proceeds isothermally at 350 °C. As the reaction is exothermic, a significant quantity of heat is released and may be recovered for other process operations. In the modified configuration (Figure 4), the thermal energy liberated by the reactor, amounting to 1.065×10^7 kJ/h, is recycled and utilized as the heat source for heater E-100. This recovered energy increases the feed temperature from 160.1 °C to 273.9 °C before entering the furnace for final temperature adjustment. Additionally, in the modified system, the heat released during effluent cooling in cooler E-101 is recovered and used to supply the mechanical energy required by pump P-100, which previously relied on external power.

Overall, this modified configuration demonstrates superior energy integration, providing more efficient feed preheating, reducing reliance on external utilities, and improving the overall thermal efficiency of the cumene production process compared to the base case.

3.4. Net Energy Efficiency and Surplus in Exothermic Reactor Systems

The total net energy for both the basic and modified processes is presented in Table 4. In the basic process, the value of E_p is 28,053,436.01 kJ/h, obtained from the heat generated by the reactor since the reaction is exothermic. However, the value of E_c is 31,173,118.59 kJ/h, as energy is required to operate the pumps in the process. In contrast, the modified process has an E_p value of 28,053,642.06 kJ/h, derived from the heat generated by the reactor as well as the energy recovered from the E-101 cooler used to cool the stream. The E_c value is 30,108,756.85 kJ/h, of which approximately 21,294,605.8 kJ/h is recycled energy. It can be concluded that the net energy (NE) in the basic process is 3,119,682.58 kJ/h, while in the modified process it is 2,055,114.79 kJ/h. Around 21,294,605.8 kJ/h of the energy is produced by the reactor and cooler is then allocated to power the pumps.

Net energy values approaching zero represent energy neutrality, which is favorable for self-sufficiency and sustainability [21]. To maximize energy output, the energy produced by the reactor's exothermic reaction and the energy recovered from cooling the stream are reallocated to power the pumps. Consequently, the energy required to operate the pumps is significantly reduced, thereby lowering the net energy.

3.5 Cumene Conversion Enhancement Due to Process Modification

The implementation of a vapor-phase recycle stream significantly increases the overall conversion of benzene to cumene in the modified production scheme. In the basic configuration, the benzene conversion is limited by the once-through operation of the plug flow reactor, where unreacted benzene in the reactor effluent is discharged and therefore not available for further reaction. In contrast, the modified process routes the vapor-phase benzene recovered in the knock-out drum back to the reactor feed. This recycled benzene stream maintains a high benzene-to-propylene molar ratio entering the reactor, which suppresses secondary alkylation and increases the effective utilization of the limiting reactant, propylene.

From Table 5, when compared to the unmodified system, the performance improvement becomes evident. Initially, the system operated with a propylene conversion of 94.53% and a main-reaction extent of 99.25 kmol/h, accompanied by a very small secondary

Table 4. Total Net Energy for unmodified and modified process.

Parameter	Unmodified Process	Modified Process
Energy Consumed	31,173,118.59 kJ/h	30,108,756,85 kJ/h
Energy Produced	28,053,436,01 kJ/h	28,053,642,06 kJ/h
Accumulation	3,119,682.58 kJ/h	2,055,114.79 kJ/h

Table 5. Comparison of reaction performance between the unmodified and modified cumene production processes.

Process Parameter	Unmodified Process	Modified Process
Propylene Conversion (%)	94.53%	96.42%
Main Reaction Extent (Rxn-1)	99.25 kmol/h	102 kmol/h
Side Reaction Extent (Rxn-2)	5.746 kmol/h	2.925 kmol/h

reaction extent of 5.746 kmol/h. After modification, simulation data reveal that the extent of the main alkylation reaction (Rxn-1) increases to 102 kmol/h, corresponding to a higher effective conversion of 96.42%. Meanwhile, the secondary reaction (Rxn-2) decreases to 2.925 kmol/h, indicating a reduction in the formation of by-products. This trend is consistent with the compositional shift observed between Sample 6 and Sample 7: propene decreases from 0.4602 to 0.0000 (full conversion), cumene increases sharply from 0.0000 to 0.7594, and the by-product 14-iP-BZ rises only moderately to 0.0467. These changes confirm that the recycle loop intensifies the main alkylation pathway while suppressing excess transalkylation.

The improvement is further supported by the change in reactor outlet composition. With recycle, the benzene mole fraction decreases markedly, while the cumene mole fraction increases from 0.0420 to 0.2768 between reactor stages, demonstrating a more complete consumption of benzene across the reactor length. Overall, the recycle loop enables unreacted benzene to re-enter the reactor rather than being purged, leading to higher material efficiency, reduced fresh benzene demand, and a significant increase in cumene yield.

4. Conclusion

The modification of the cumene production process was conducted to improve energy efficiency and reaction performance. The results indicate that the integration of reactor-level modification, heat recovery, and vapor-phase benzene recycle significantly enhances process efficiency, as evidenced by a reduction in net energy consumption from 3.12×10^6 kJ/h to 2.06×10^6 kJ/h through internal heat recovery of approximately 21.29×10^6 kJ/h. In addition, the modified process achieves higher reaction performance, with propylene conversion increasing from 94.53% to 96.42%, the main reaction extent rising from 99.25 to 102 kmol/h, and the side reaction extent decreasing from 5.746 to 2.925 kmol/h. These results demonstrate that the modified configuration is more efficient than the unmodified process and fulfills the study objectives, implying that combined heat integration and recycle optimization can effectively reduce energy demand, improve raw material utilization, and enhance the sustainability of industrial cumene production processes.

CRedit Author Statement

Author Contributions: D.A. Alghiffary: Conceptualization, Methodology, Investigation, Software, Visualization, Writing, Review & Editing, Supervision. A.M. Gempa: Conceptualization, Methodology, Visualization, Writing, Review & Editing, Project Administration, Validation. N.A.A. Nugroho: Conceptualization, Methodology, Formal Analysis, Resources, Validation, Writing. J.R. Syahid: Conceptualization, Methodology, Investigation, Resources, Data Curation, Writing. O.G. Rajendra: Conceptualization, Methodology, Investigation, Resources, Data Curation, Writing. All authors have read and agreed to the published version of the manuscript.

References

[1] Ecoinvent. (2024). *Cumene production, benzene alkylation, UOP process – Documentation* [Dataset documentation]. ecoQuery. https://ecoquery.ecoinvent.org/3.11/cutoff/dataset/94226/documentation

[2] Junqueira, P.G., Mangili, P.V., Santos, R.O., Santos, L.S., Prata, D.M. (2018). Economic and environmental analysis of the cumene production process using computational simulation. *Chemical Engineering and Processing: Process Intensification, 130*, 309–325. DOI: 10.1016/j.cep.2018.06.010

[3] Ahmad, F., Ahmad, N., Al-Khazaal, A.A.Z. (2024). Machine learning-assisted prediction and optimization of exergy efficiency and destruction of cumene plant under uncertainty. *Engineering, Technology & Applied Science Research, 14*(1), 12892–12899. DOI: 10.48084/etasr.6654

[4] Ayub, A., Zulkefal, M., Sethi, H. (2024). Artificial intelligence assisted investigation of quality and yield of cumene production. *Materials Proceedings, 17*(1). DOI: 10.3390/materproc2024017010

[5] Sutjahjo, F., Medri, L., Alyani, S., Budhy, C.L. (2024). Enhancing energy efficiency of cumene production through reactor output recycling modification. *Journal of Chemical Engineering Research Progress.* 1(1), 64-73. DOI: 10.9767/jcerp.20100

[6] Hazmi, H.A. (2022). Process simulation and sensitivity analysis of cumene production from an integrated alkylation and transalkylation reaction. *Journal of Chemical Process Engineering, 7*(2), 64–78. DOI: 10.33536/jcpe.v7i2.787

[7] Luyben, W.L. (2012). Principles and case studies of simultaneous design. John Wiley & Sons.

[8] Naniwadekar, M., Jadhav, S. (2017). Optimum heat integration of cumene process by heat exchanger network. *International Journal of Current Research, 7*(8), 18995–19003.

[9] Wosu, C.O., Anisa, O., Nelson, F.O. (2025). Comparative design of flow reactors for the production of 100,000 tons per year of cumene from the catalytic alkylation of propylene and benzene. *LAUTECH Journal of Engineering and Technology, 19*(1), 142–153.

[10] Ojong, O.E., Wosu, O.C., Emenike, A., Ubi, P.A. (2024). Design and simulation of 30000 tons per year of cumene plant from natural gas field. *Pure and Applied Chemistry, 96*(6), 795–805. DOI: 10.1515/pac-2023-1135

[11] Zou, Y., Jiang, H., Liu, Y., Gao, H., Xing, W., Chen, R. (2016). Highly efficient synthesis of cumene via benzene isopropylation over nano-sized beta zeolite in a submerged ceramic membrane reactor. *Separation and Purification Technology, 170*, 49–56. DOI: 10.1016/j.seppur.2016.06.031

[12] Turton, R., Shaeiwitz, J.A., Bhattacharyya, D. (2018). *Analysis, Synthesis, and Design of Chemical Processes* (5th ed.). Pearson Education.

[13] Srivastava, P., Gupta, A., Kaistha, N. (2023). Compact process for cumene manufacture: Synthesis, design and control. *Chemical Engineering Research and Design, 190*, 220–232. DOI: 10.1016/j.cherd.2022.12.026

[14] Mahmoudian, F., Moghaddam, A.H., Davachi, S.M. (2022). Genetic-based multi-objective optimization of alkylation process by a hybrid model of statistical and artificial intelligence approaches. *The Canadian Journal of Chemical Engineering, 100*(1), 90–102. DOI: 10.1002/cjce.24072

[15] Hasibuan, F.A.Y., Tarigan, K. (2024). Process simulation of cumene production via liquid phase reaction pathway. *Jurnal Rekayasa, Teknologi Proses dan Sains Kimia (REPROKIMIA), 3*(1), 7–17.

[16] Yaws, L.C. (1999). *Chemical Properties Handbook*. McGraw-Hill.

[17] Kavitha, S., Kurian, M. (2022). Friedel Craft's alkylation of benzene to cumene over doped cobalt nanoferrite catalysts. *Results in Chemistry, 4*, 100585. DOI: 10.1016/j.rechem.2022.100585

[18] Aminov, R.Z., Yurin, V.E., Bessonov, V.N. (2017). Investigation of the possibility of using residual heat reactor energy. *Journal of Physics: Conference Series, 891*(1), 012175. DOI: 10.1088/1742-6596/891/1/012175

[19] Sánchez-Luján, J., Molina-García, Á., López-Cascales, J.J. (2024). Integrated heat recovery system based on mixed ionic–electronic conducting membrane for improved solid oxide co-electrolyzer performance. *Polymers, 16*(7), 932. DOI: 10.3390/polym16070932

[20] Seider, W.D., Seader, J.D., Lewin, D.R. (2004). Product and Process Design Principles: Synthesis, Analysis, and Evaluation. Wiley.

[21] FENG, J. (2021). Research on input and output of China's energy industry from the perspective of net energy. *China Mining Magazine, 30*(10), 18–23. DOI: 10.12075/j.issn.1004-4051.2021.10.007.