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Research Article

Integrated Process Design for n-Octane Production Enhancing Yield and Energy Saving via Recycle, Heat Integration, and Purge-gas Utilization

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Abstract

n-octane is an essential hydrocarbon in fuels and petrochemicals, yet conventional production suffers from high energy demand and material losses. This study develops an integrated process design combining recycle systems, heat integration, and purge-gas utilization for n-octane production. Results show that recycle integration raises yield from 92.81% to 97.46%, heat integration achieves 36.38% energy savings, and purge-gas valorization sustains high yield (97.41%) while delivering the greatest energy reduction (62.30%). The findings demonstrate that synergistic process intensification enhances efficiency and sustainability, offering a transferable framework for hydrocarbon production optimization.

Keywords: n-Octane; Yield; Energy Saving; Heat Integration; Purge-gas Utilization

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1. Introduction

n-octane, C_8H_{18}, is a critical hydrocarbon in the petrochemical industry, widely recognized as a reference fuel component due to its high stability and favorable combustion properties. The increasing global demand for high quality fuels and petrochemical intermediates has intensified research efforts aimed at improving production efficiency while simultaneously reducing energy consumption. However, conventional n-octane production processes often suffer from incomplete conversion, high energy requirements, and significant hydrocarbon losses through purge streams, which collectively limit yield and increase operational costs [1].

To address these limitations, process intensification strategies have been widely investigated. Recycle systems are essential for minimizing reactant losses by reintroducing unconverted feedstock into the reactor, thereby enhancing overall conversion. Heat integration enables efficient utilization of process heat by coupling exothermic and endothermic operations, significantly reducing external energy demand [2]. In addition, purge gas utilization represents an innovative approach to recover valuable hydrocarbons from waste streams, transforming potential losses into additional product yield [3]. Recent studies on naphtha recycle isomerization units have demonstrated that such modifications significantly improve octane number while simultaneously reducing energy consumption [4].

The integration of recycle systems, heat integration, and purge-gas utilization represents a holistic pathway to optimize n-octane production. While previous studies have examined these strategies individually, there is a lack of systematic evaluation of their combined and synergistic effects within a single production framework. The implementation of a thermo-economic approach in hydrocarbon production is critical for minimizing carbon emissions, while

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simultaneously optimizing operational efficiency [5]. Process intensification strategies, particularly the integration of recycle systems with energy-saving approaches, are essential for maximizing conversion and reducing operational costs [6]. To the best of our knowledge, this study is the first to comprehensively investigate the simultaneous integration of recycle systems, heat integration, and purge-gas utilization in n-octane production. By addressing this gap, the present work provides novel insights into process optimization that enhance both economic performance and environmental sustainability.

2. Methods

2.1. Process Simulators Used for Evaluation

Process simulators are sophisticated computational tools developed to represent chemical and physical phenomena within industrial process systems. These tools function by solving systems of mathematical and thermodynamic equations that govern mass and energy balances, phase behavior, and transport mechanisms. As a result, process simulators can model a wide range of unit operations, including reactors, distillation columns, heat exchangers, pumps, and compressors, as well as entire process flowsheets for the purposes of design and optimization [7].

Process simulation has become an essential element in contemporary process engineering, supporting the transition toward digitally driven and model-based analysis. Through virtual representation of process configurations, engineers, researchers, and decision-makers can evaluate, test, and optimize complex systems prior to physical realization. This capability contributes to reduced development time and cost, improved process understanding, and minimized operational uncertainty. Among the various process simulation platforms currently available, Aspen HYSYS is one of the most extensively applied tools. Developed by Aspen Technology Inc., Aspen HYSYS is a steady-state and dynamic simulator that provides comprehensive modeling features for fluid flow, heat and mass transfer, chemical reactions, separation units, and energy integration. Its reliable thermodynamic models and industrially validated unit-operation libraries enable accurate and realistic process evaluation [8].

Despite the availability of several alternative simulators, such as Aspen Plus, UniSim, CHEMCAD, PRO/II, and DWSIM, Aspen HYSYS was selected in this study based on two key considerations. First, it is widely used in academic and industrial research, ensuring consistency with established methodologies. Second, the software offers accessible automation server functionality, allowing enhanced interoperability, customization, and linkage with external analytical or optimization tools, which supports more comprehensive process evaluation [9]. In the simulation of n-octane production, the Peng–Robinson (PR) property package was employed to optimize the process, as it is well suited for representing the thermodynamic behavior of nonpolar hydrocarbon systems under the operating conditions considered.

2.2. Description of Process

n-Octane (C_8H_{18}) is a linear alkane that belongs to the homologous series of straight-chain paraffins and is widely recognized for its importance in fuel characterization and petrochemical applications. Under atmospheric conditions, n-octane is a colorless, highly flammable aliphatic hydrocarbon. It is primarily obtained through fractional distillation during petroleum refining and is subsequently utilized as a feedstock in the manufacture of various chemicals, including solvents and cleaning agents. In addition, n-octane and its branched isomers constitute fundamental components of fuels and lubricating oils. Although typically present in fuels at relatively low concentrations, n-octane has a measurable influence on fuel thermodynamic properties and must therefore be considered for accurate mixture characterization [10].

High-purity n-octane is commonly produced via catalytic hydrocracking of long-chain paraffins contained in vacuum gas oil or heavy naphtha, followed by fractionation. The process is carried out in the presence of hydrogen over bifunctional catalysts consisting of metallic sites (e.g., Ni-Mo or Pt) supported on acidic carriers, which enable hydrogenation–dehydrogenation and carbon–carbon bond cleavage reactions under elevated temperature and pressure. The reaction mechanism involves initial dehydrogenation on metal sites to form olefin intermediates, which subsequently migrate to acidic zeolite sites and undergo protonation and molecular rearrangement [11]. These steps ultimately lead to the formation of n-octane, along with possible side reactions such as over-cracking and isomerization, depending on catalyst properties and operating conditions. Subsequent rearrangement and chain-growth or coupling reactions can yield n-octane as a product. The reaction pathway can be represented as:

$$2C_2H_4 + C_4H_{10} \rightarrow C_8H_{18} \tag{1}$$

The standard reaction enthalpy at 298 K was calculated using Hess's law:

$$\Delta H^\circ_{298} = \Sigma n \Delta H^\circ_f\,(\text{products}) - \Sigma n \Delta H^\circ_f\,(\text{reactants})$$

The standard enthalpies of formation at 298 K [12]): $\Delta H^{\circ}_{f\,298}$ C_2H_4 = +52.5 kJ/mol; $\Delta H^{\circ}_{f\,298}$ C_4H_{10} = -134.2 kJ/mol; $\Delta H^{\circ}_{f\,298}$ C_8H_{18} = -208.8 kJ/mol. Substitution of these values yields a standard reaction enthalpy $\Delta H^{\circ}_{f,298} = -179.6$ kJ/mol, indicating that the reaction is exothermic. The release of heat during the reaction highlights the importance of effective heat management to maintain optimal reactor temperature and prevent excessive energy losses.

The feed stream containing ethylene and i-butane with trace impurities is preheated and mixed with a recycle stream before entering an isothermal reactor operating at 98% conversion for n-octane formation. Most n-octane is withdrawn from the reactor bottom, while the vapor effluent is sent to a distillation column for further product recovery. Unreacted components from the column overhead are compressed, recycled to the reactor, and used to preheat the fresh feed, with simulation conducted following the onion model by prioritizing the reactor before downstream units [13].

In addition to conventional petroleum-based routes, recent research has explored alkylation-based pathways for n-octane production using renewable or alternative feedstocks. Mid-chain fatty acids such as valeric acid can be converted into n-octane with improved selectivity, typically using an aqueous mixture of valeric acid and sodium hydroxide. In this process, 1-butanol may form as a side product and subsequently react with valeric acid to produce butyl valerate [14]. Advances in catalyst development show that zeolite catalysts can be tailored to enhance n-octane selectivity, while ionic liquid catalysts offer recyclability and reduced environmental impact. Furthermore, the implementation of microreactor technology and process intensification strategies has been reported to improve product yield and catalyst stability [15].

2.3. Method to Enhance Yield and Energy Saving n-Octane Production

Addressing the dual challenge of hydrocarbon production efficiency and sustainability requires the implementation of integrated strategies that enhance overall process performance. The efficiency of n-octane production can be substantially improved through the combined application of recycle systems, heat integration, and the productive utilization of purge gas. Gas fractions that would otherwise be vented are directed to a separator, enabling the recovery of valuable light hydrocarbons such as ethylene and butane, which are subsequently recycled into the feed stream. To measure the effectiveness of this recovery process, the production yield is calculated based on the mass flow rates, as defined in Equation (1):

$$\text{Yield} = \left(\frac{\dot{m}_{\text{total product}}}{\dot{m}_{\text{feed}}}\right) \times 100\% \qquad (1)$$

A controlled portion of the gas is allocated as purge to prevent the accumulation of inert species; however, this stream is simultaneously harnessed as an auxiliary energy source, thereby improving resource efficiency. This integrated approach has been shown to reduce net energy consumption while enhancing exergy efficiency in hydrocarbon separation processes [16]. Moreover, heat integration between the recycle stream and distillation units significantly decreases the energy demand of these inherently energy-intensive operations [17]. The impact of these improvements is quantified by the % energy saving, which compares the reduction from the current load to the target load, as shown in Equation (2):

$$\%\ \text{Energy saving} = \left(\frac{\text{Current Load} - \text{Target Load}}{\text{Current Load}}\right) \times 100\% \qquad (2)$$

Taken together, the simultaneous application of recycle, heat recovery, and purge-gas utilization not only increases n-octane yield but also achieves substantial energy savings, underscoring its potential as a sustainable process intensification strategy in hydrocarbon production.

3. Results and Discussion

3.1. Comparison Between Basic and Modified Process

Simulation results of n-octane production, as illustrated in Figures 1-5, highlight the differences between the base process and the

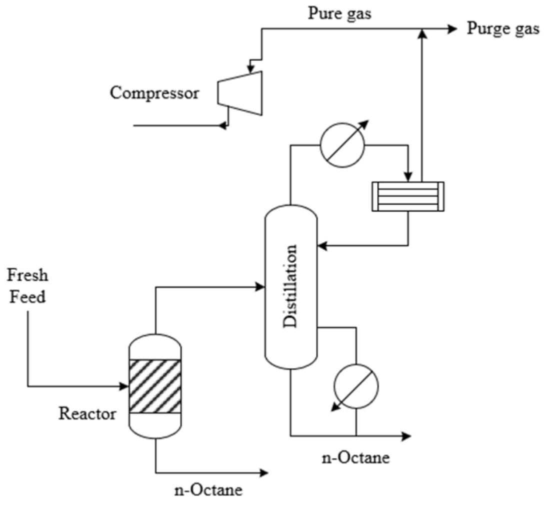

Figure 1. Basic Process Flow Diagram of n-Octane production.

modified configuration. In the base process (Figure 1), fresh feed is introduced into the reactor to generate a product mixture, which is subsequently directed to the distillation column. n-octane is recovered as the bottom fraction, while lighter hydrocarbons exit through the overhead stream. A small portion of the overhead stream is purged to prevent the accumulation of inert compounds, whereas the remaining fraction is compressed. This initial configuration was deliberately designed in a simplified manner, without incorporating recycle streams or heat integration, which results in a high energy demand for both heating and cooling operations. Based on simulations conducted using Aspen HYSYS with a feed rate of 1,174 kg/h, the process can produce n-octane at 1,089.59 kg/h. This corresponds to a yield of 92.81%; however, no energy savings (0% energy reduction) are achieved due to the absence of heat integration.

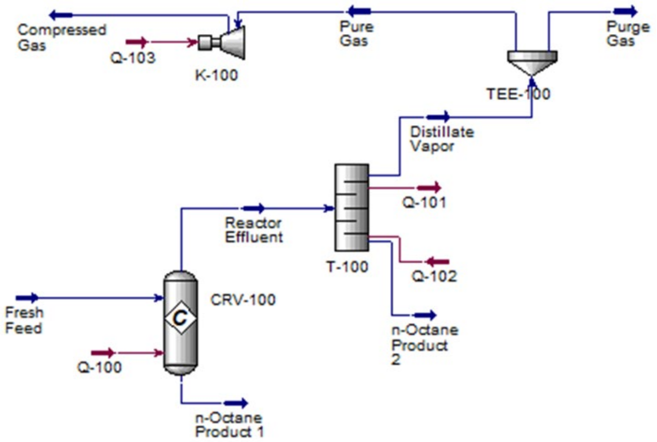

Figure 2. Process simulation of basic process of n-Octane production using Aspen HYSYS.

In contrast, the modified configurations illustrated in Figures 3-5 implement process intensification strategies through the incorporation of recycle subsystems and advanced energy integration. In this design, the overhead stream from the distillation column is separated in TEE-100, where most of the stream is compressed (K-100), cooled (E-100), and subsequently returned to the feed mixer (MIX-100) to maximize reactant utilization. System efficiency is further enhanced by internal heat integration and a waste-to-energy mechanism, in which the purge-gas stream is

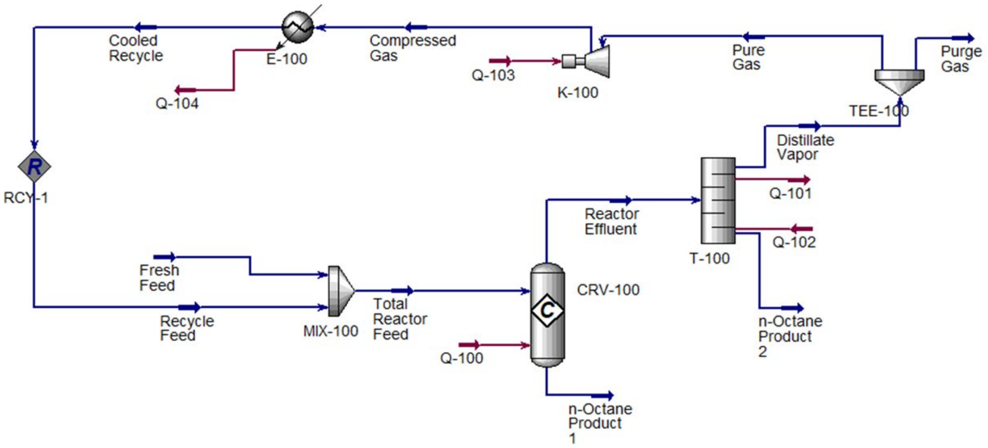

Figure 3. Process simulation of modified process 1 (with recycle) of n-Octane production using Aspen HYSYS.

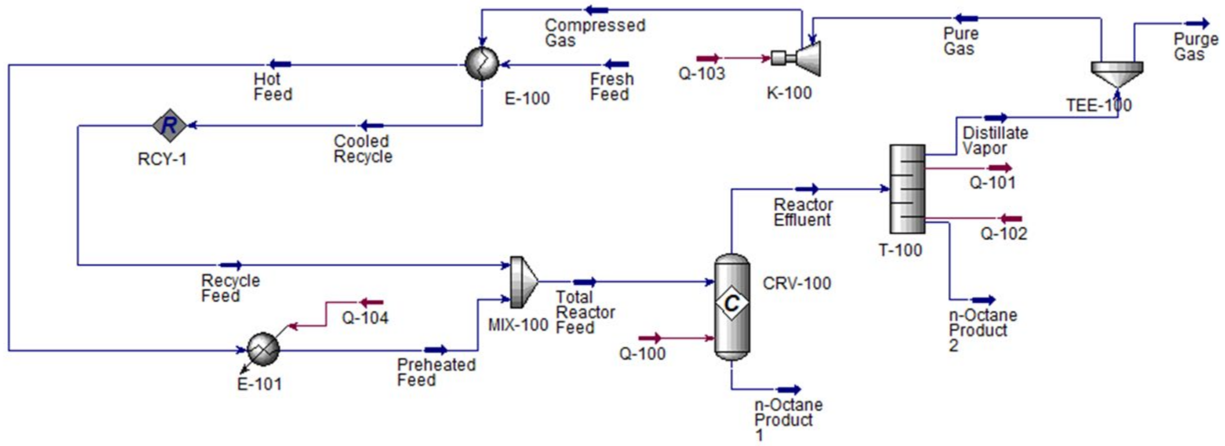

Figure 4. Process simulation of modified process 2 (with recycle and Heat Integration) of n-Octane production using Aspen HYSYS.

combusted in a conversion reactor and the generated heat is recovered via E-102 as Q-Recovered. The simultaneous application of these mechanisms increases the overall conversion of raw materials, reduces external utility demand, and delivers substantial operational cost savings compared with the base design.

3.2. Process Modification via Recycle System

This study presents a simulation of n-octane production from ethylene and i-butane using Aspen HYSYS, applying a process intensification strategy through recycle integration. In the proposed configuration, the overhead vapor stream from the distillation column is directed to a flow splitter (TEE-100). A small fraction of this stream is purged to prevent the accumulation of inert components (e.g., nitrogen), which could otherwise reduce reactor efficiency. The main fraction is recycled back into the system via a recycle loop.

The recycle stream is compressed using a compressor (K-100) to match the operating pressure of the fresh feed. Subsequently, thermal conditioning is performed in a heat exchanger (E-100) to ensure thermodynamic compatibility before mixing with the fresh feed stream. Process performance was comprehensively evaluated by examining the total liquid product yield relative to the feed. The process yield was calculated according to Equation (1).

Simulation results with a feed mass flow rate of 1,174 kg/h demonstrate that the integrated configuration successfully recovers products from both the reactor (CRV-100) and the separation unit (T-100), achieving a total production rate of 1,144.13 kg/h. Thus, the yield obtained from this configuration is 97.46%.

3.3. Process Modification via recycle and heat integration

This study investigates the simulation of n-octane production from ethylene and i-butane using Aspen HYSYS, implementing process intensification strategies that combine a recycle loop and heat integration. The modifications aim to maximize reactant conversion while minimizing external energy demand. In the integrated process configuration, the distillate vapor stream from the distillation column (T-100) is directed to a splitter unit (TEE-100). A minor fraction is withdrawn as purge gas to prevent the accumulation of inert components (e.g., nitrogen), whereas the main fraction is recycled back into the system. The recycle stream is compressed using a compressor (K-100) to achieve operating pressure compatibility with the reactor.

To enhance thermal efficiency, heat integration is applied through the heat exchanger (E-100). The fresh feed, entering at 30 °C and 165.5 °C, undergoes pre-heating in E-100 by utilizing the sensible heat of the compressed recycle stream. This mechanism enables waste heat recovery of 6,217 kJ/h, directly reducing the thermal load on the utility heater (E-101) prior to the feed entering the conversion reactor (CRV-100) at the operating temperature of 93 °C.

Process performance was evaluated based on two key parameters: product yield and energy efficiency. From a mass balance perspective, the implementation of the recycle system significantly improves raw material utilization. With a feed mass flow rate of 1,174 kg/h, the integrated configuration achieves a total product output of 1,143.9 kg/h. Thus, the yield obtained from this configuration is 97.44%.

Furthermore, the activated energy analysis confirms the effectiveness of thermal integration.

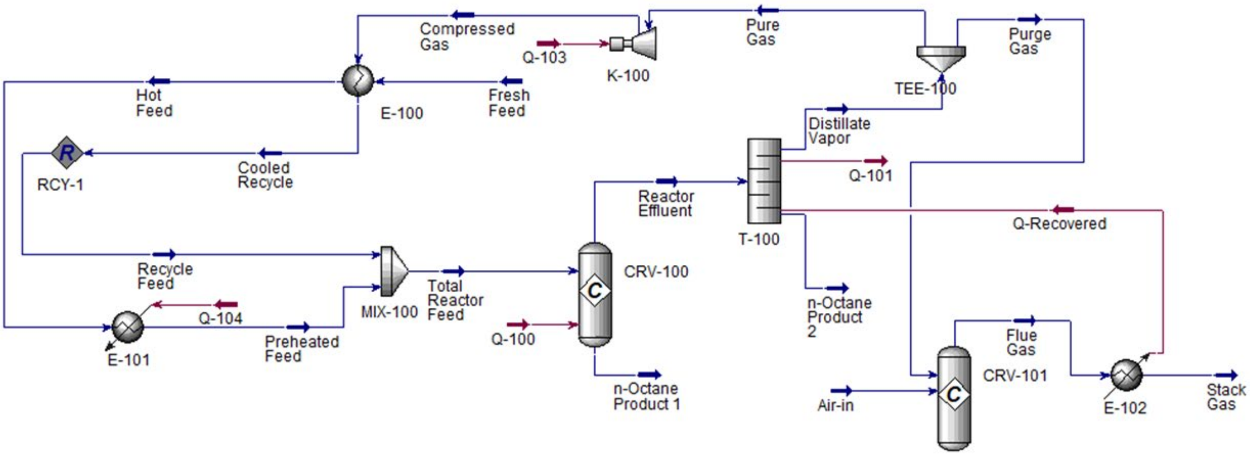

Figure 5. Process simulation of modified process 3 (with recycle, heat integration, and purge gas utilization) of n-Octane production using Aspen HYSYS.

The coupling of hot and cold process streams through the heat exchanger (E-100) successfully reduced the total thermal utility demand (Current Load) from 2.958×10^5 kJ/h to a target external load (Target Load) of 1.882×10^5 kJ/h. The percentage of energy savings was calculated according to Equation (2).

Accordingly, the integrated configuration demonstrates an energy saving potential of 36.38%, corresponding to a reduction in utility demand of 1.076×10^5 kJ/h. These findings substantiate that the combined application of heat integration and material recycling constitutes a pivotal approach for enhancing process efficiency and optimizing operational expenditures in industrial plant systems.

3.4. Process Modification via Recycle, Heat Integration and Purge Gas Utilization

The final stage of the modified process strategy focuses on the implementation of a Waste-to-Energy scheme to validate the potential utilization of the purge-gas stream as an internal energy source. In the base configuration, the purge stream from the splitter unit (TEE-100), which contains residual light hydrocarbons such as ethylene and i-butane along with a minor fraction of n-octane, is typically released into the environment or combusted in a flare system. This study proposes a reconfiguration of the purge stream toward a thermal oxidation unit (CRV-101), thereby enabling its conversion into usable energy within the process boundary.

This intensification mechanism operates by combusting the purge-gas stream with excess air to ensure complete oxidation. The sensible heat generated from this exothermic reaction ($Q_{\text{Recovered}}$) is subsequently recovered through the heat exchanger unit (E-102). The recovered thermal energy is then reintegrated into the system to supply the heating duty of the distillation column reboiler (T-100), thereby substituting a substantial portion of the external low-pressure steam utility requirement. This approach effectively transforms the purge stream from a waste material into a valuable energy asset, achieving valorization within the process boundary.

Thermal efficiency analysis conducted using the activated energy analysis feature within the Aspen HYSYS simulation environment demonstrates the significant impact of this integration on the plant's overall energy balance. Prior to the implementation of the Waste-to-Energy scheme, the total thermal utility demand (Current Load) was recorded at 2.958 × 10^5 kJ/h. Following the combustion of the purge-gas stream, the target requirement for external energy (Target Load) was drastically reduced to 1.115 × 10^5 kJ/h. The simulation results confirm that this scheme successfully decreases the external utility burden by 62.30%, corresponding to an energy saving of 1.843 × 10^5 kJ/h.

In addition to achieving substantial energy efficiency, production performance remains well preserved. With a feed mass flow rate of 1,174 kg/h, the modified configuration yields a total product output of 1,143.6 kg/h. This corresponds to a yield of 97.41%, thereby confirming that the integration of the Waste-to-Energy scheme represents the most effective strategy for minimizing operational costs without compromising n-octane production capacity.

3.5. Yield and Energy Analysis between Unmodified and Modified Processes

Overall, the implementation of the recycle system exerts the most significant impact on yield improvement. The basic process (without modification) demonstrates the lowest performance, with a yield of 92.81% (producing 1,089.6 kg/h from a feed of 1,174 kg/h) (Table 1). In contrast, all modified configurations exhibit a substantial increase, reaching approximately 97.4%. The first modification stage records the highest yield of 97.46% (1,144.13 kg/h), as this mechanism returns unreacted components from the distillation column to the reactor, thereby minimizing material losses [18].

From the perspective of energy conservation, substantial efficiency improvements are observed at each modification stage, consistent with process-integration principles that emphasize minimizing thermodynamic irreversibility. Both the base process and the recycle-only

Table 1. Comparison of yield performance and energy analysis of n-octane production.

Process Simulation	Feed Stream	Total Product (kg/h)	Yield (%)	Current Load (kJ/h)	Energy Saving (%)
Unmodified Process	1,174 kg/h	1,089.6	92.81	2.958×10^5	0
Modified 1 (With Recycle)	1,174 kg/h	1,144.13	97.46	2.958×10^5	0
Modified 2 (With Heat Integration)	1,174 kg/h	1,143.9	97.44	1.882×10^5	36.38
Modified 3 (With Purge Gas Utilization)	1,174 kg/h	1,143.6	97.41	1.115×10^5	62.3

configuration require a very high thermal utility load of 2.958 × 10^5 kJ/h. The application of heat integration via E-100 significantly reduces this demand to 1.882 × 10^5 kJ/h, corresponding to an energy saving of 36.38%. This reduction is achieved because heat integration enables energy recovery from high-temperature process streams to preheat cold streams, thereby decreasing reliance on external utilities. The most optimal efficiency is attained in the final stage through purge-gas utilization, where the external utility requirement drops drastically to 1.115 × 10^5 kJ/h, resulting in the maximum energy saving of 62.30% This substantial improvement validates the waste-to-energy strategy; rather than discarding purge gas with calorific value, the stream is combusted to supply heat for the distillation reboiler [19].

4. Conclusion

The study concludes that integrating recycle systems, heat integration, and purge-gas utilization is a highly effective strategy to optimize n-octane production. Compared to the base process with a yield of 92.81% and no energy savings, recycle loops raised yield to 97.46%, heat integration reduced utility demand by 36.38%, and purge-gas utilization achieved the greatest energy savings of 62.30% while sustaining a 97.41% yield. These results prove that synergistic process intensification enhances conversion efficiency, minimizes energy consumption, and supports sustainability, offering a transferable model for economically viable and environmentally responsible hydrocarbon production.

CRedit Author Statement

Author Contributions: M. B. Purasetya: Conceptualization, Methodology, Investigation, Software, Visualization, Writing, Review & Editing, Project Administration, Supervision; A. R. Yustifasari: Conceptualization, Methodology, Visualization, Software, Writing, Review & Editing, Validation; A. A. Sagita: Conceptualization, Methodology, Formal Analysis, Software, Resources, Validation, Writing, Review & Editing; A. W. Ardinta: Conceptualization, Methodology, Software, Investigation, Resources, Data Curation, Writing, Review & Editing; N. A. B. Sinaga: Methodology, Software, Investigation, Resources, Data Curation, Writing, Review & Editing. All authors have read and agreed to the published version of the manuscript.

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