

Enhancing Energy Efficiency of Cumene Production Through Reactor Output Recycling Modification in a Heat Exchanger

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Abstract

Cumene production generally involves irreversible and exothermic reactions that leads to an increase in product temperature and needs to be cooled for further processes. The high temperature of reactor product can be utilized as a heat transfer fluid in heat exchanger. This modification process is essential for improving energy efficiency by recycling the reactor output with high temperature as a heat transfer fluid, so that the implementation of replacing the heater with a heat exchanger can be carried out for the process of increasing the initial feed temperature. In an effort to enhance energy efficiency in the cumene production process, simulations were conducted using HYSYS and the comparison of energy efficiency for both basic and modified processes can be evidenced by comparing the total amount of energy required during the process. The results shows that the total amount of energy required for the modified process is 39,814,003.7 kJ/h, while for the basic process is 40,588,937.4 kJ/h, with a difference of 774,933.7299 kJ/h. Since the total amount of energy required in the modified process is smaller than the basic process, then the modification process will increase the energy efficiency of cumene production.

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Keywords: Cumene; Process modification; Energy efficiency; Reactor output; Heat exchanger

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1. Introduction

Currently, many raw materials or supporting materials in the domestic chemical industry still rely on imports from abroad, and one of them is cumene, which is a primary raw material for the production of phenol and acetone. Phenol and its derivatives find applications in the production of polycarbonate and epoxy resins, detergents, nylon, bakelite, herbicides, and more. The majority of cumene is typically manufactured

through the alkylation of benzene (C₆) with propylene (C₃) using an acid catalyst [1]. The manufacturing process of cumene has received significant attention in recent years, and efforts have been invested in developing alternative catalyst systems to optimize cumene production [2]. The global demand for cumene is expected to reach USD 17.63 billion by 2025, as cumene is one of the five chemical reagents produced on a large scale globally due to its widespread distribution, along with ethylene, propylene, benzene, and ethylbenzene [3]. The increasing production of cumene is attributed to its versatile nature.

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Cumene, also known as cum ole or isopropylbenzene, is a colorless liquid. It is an aromatic hydrocarbon compound utilized in the chemical industry, particularly in the production of phenol and acetone through an oxidation process [4]. Cumene serves as an intermediate product with a crucial role in the production of various industrial products, including bisphenol-A, polycarbonate, epoxy resins, nylon 6, and others [5].

The production of cumene involves the Friedel-Crafts alkylation of benzene with

propylene, an irreversible and exothermic reaction (Figure 1). Alkylomatic compounds also used in the chemical and petrochemical industries as raw materials for the commercial production of ketones, aldehydes, acids, polymer materials, synthetic surfactants, fuel additives, etc. Ethylbenzene and isopropylbenzene (cumene) are of the most practical importance as the raw materials for the manufacture of styrene [6]. The reactions take place in a gas-phase reactor at high temperature and pressure, resulting in the formation of cumene and an undesired side product, p-diisopropylbenzene (PIDB). The mixture then enters the separator unit to remove impurities in the form of propane, and unreacted benzene is removed through a distillation process. In the final stage, p-diisopropylbenzene is separated from cumene using another distillation column [7]. Design optimization in the cumene process includes intensification and topological changes aimed at achieving lower capital and energy costs.

In recent years, there has been much interest in improving process efficiency by making process modifications, including in the cumene production process. Fleigel *et al.* [9] proposed the concept of process modification in cumene production by using a purge column with the purpose of reducing material loss during the process as can be seen in Figure 2 and Figure 3. However, in this research, the process

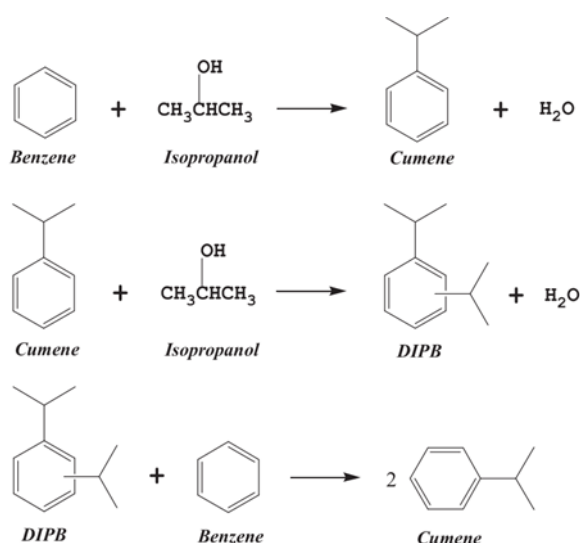


Figure 1. Reaction scheme of benzene isopropylation to cumene [8]

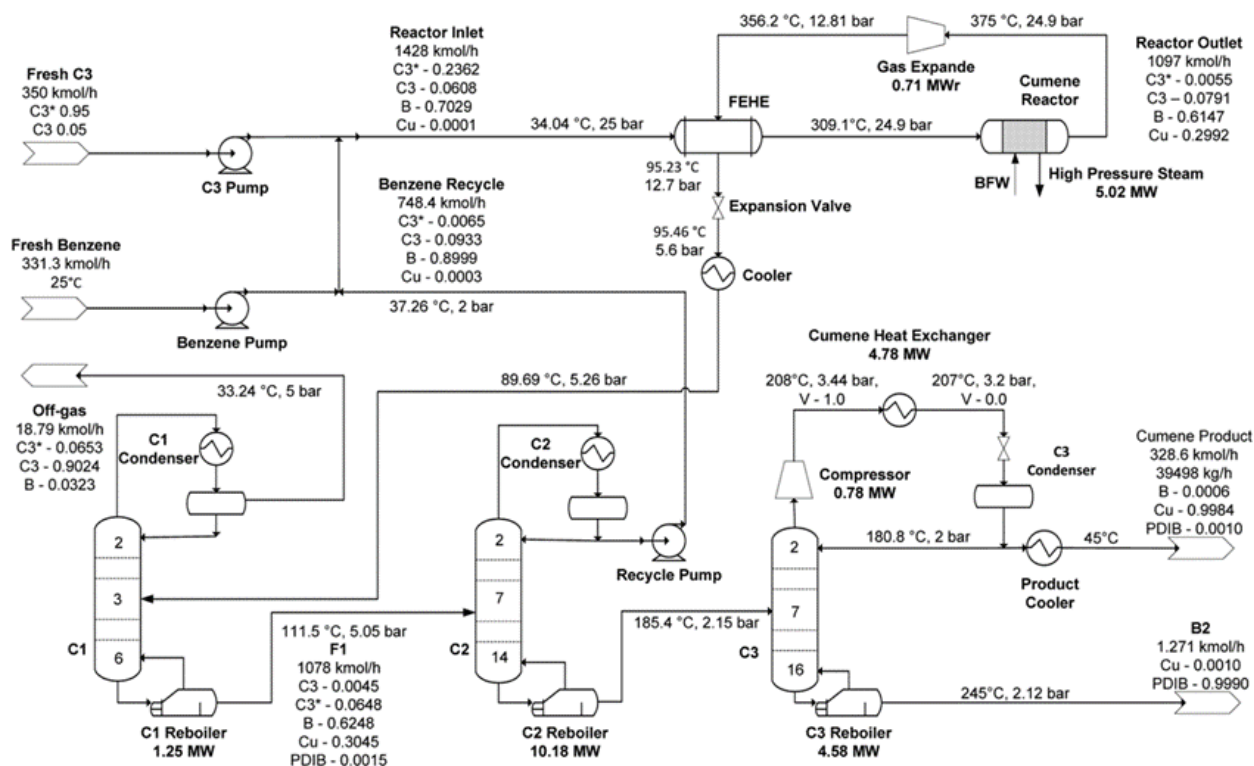


Figure 2. Cumene process modification using purge column [9]

modification is carried out with replacing the heater with a heat exchanger by utilizing the reactor output product as a heat transfer fluid, as well as replacing the separation unit by using one regular gas-liquid separator in the form of a knock-out drum and two distillation columns as shown in Figures 4 and 6, instead of using three distillation columns as in common. The knock-out drum functions is only to separate the gas phase from the liquid phase, then the liquid phase flow will enter the first distillation column for the benzene separation process. The benzene produced as the top product is recycled to be re-mixed with pure benzene in the mixer. While the bottom product will be flowed into the pump to increase the pressure and then entered into the second distillation column for the separation process of cumene and PDIB. Therefore, the cumene yield reached up to 99.84 % as can be seen on the Table S1 (Supporting Information). However, this research is more focused on improving energy efficiency of the cumene production process by the innovation in recycling

reactor output in heat exchangers using the reactor output as a heat transfer fluid in the heat exchanger so it can replace the heater which requires additional energy. As a result, this modification does not require the use of an additional heater for the process of heating the initial feed. This research aims to examine the extent of the potential for energy reduction in cumene production through modification of reactor output recycling in the heat exchanger process to achieve optimal energy efficiency which is simulated using Aspen HYSYS.

2. Methods

In order to improve energy efficiency in cumene production process, the thermodynamic pinch points analysis is used as a benchmark for optimizing and enhancing heat transfer in the system so that energy efficiency can be maximized [10]. For example, by applying the high temperature of reactor product that can be utilized as a heat transfer fluid in heat exchanger. So, the innovation may be proposed by replacing

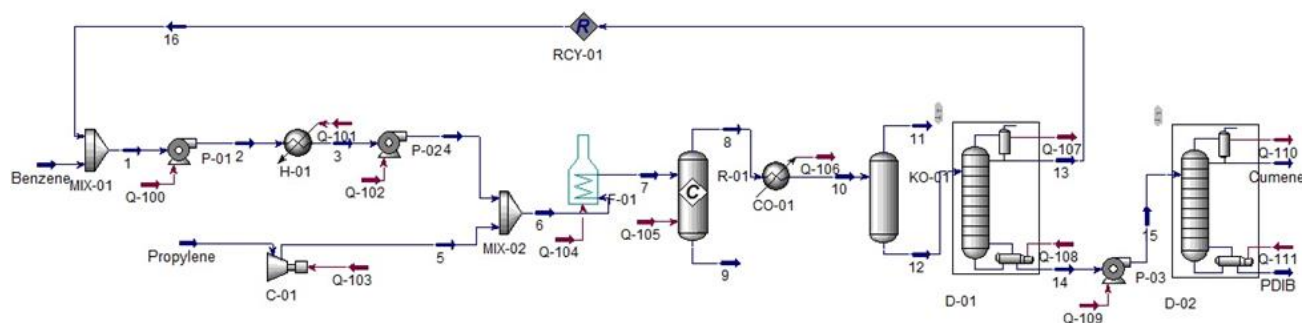


Figure 3. Simulation using Aspen HYSYS of basic process

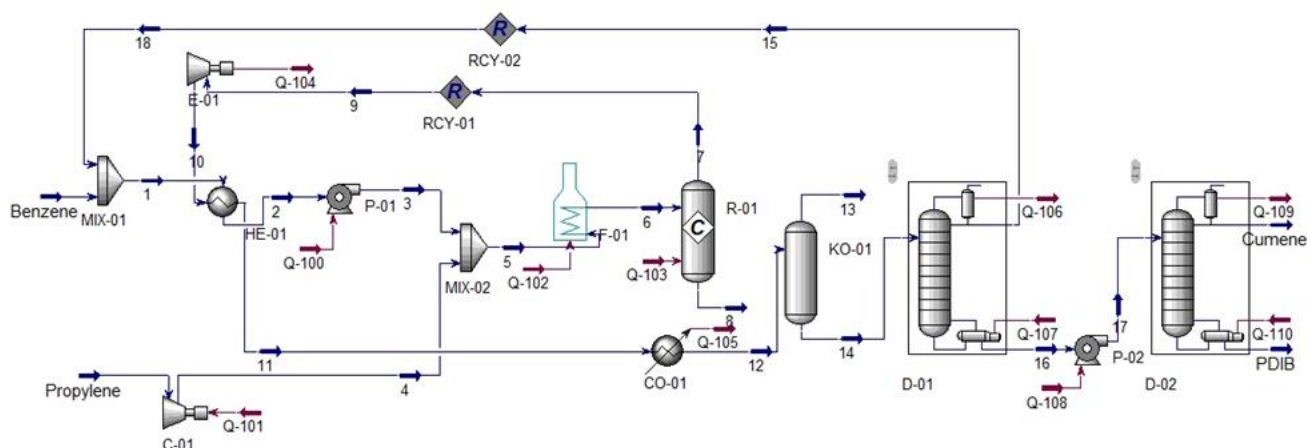


Figure 4. Simulation using Aspen HYSYS of modified process

the heater with a heat exchanger. The reactor output in the form of vapor is recycled into the heat exchanger. This vapor has a temperature of 370 °C and a pressure of 25 atm. However, before entering the heat exchanger, the vapor pressure is reduced using an expander, producing vapor with a temperature of 315.8 °C and a pressure of 1.6 atm. The generated vapor flows into the heat exchanger is used to heat the feed, thus increasing the initial feed temperature. The modification process to improve the energy efficiency is simulated using Aspen HYSYS and the comparison of energy efficiency between the basic and modified process can be evidenced by comparing the total amount of energy required during the process. If the total amount of energy required is less, then the overall production process becomes more efficient.

3. Result and Discussion

3.1 Difference Between Basic and Modified Process

The simulation of the cumene production for basic and modified process using Aspen HYSYS is as follows. Figure 3 and Figure 5 shows the simulation using HYSYS and the process flow diagram of basic process. Whereas for the modified process, the simulation using HYSYS is shown by Figure 4 and the process flow diagram is shown by Figure 6. In the basic process, there is

only one recycle process, i.e. from the top of the distillation column (D-01) which is recycled to be re-mixed with pure benzene feed in the mixer (MIX-01). In addition, due to the absence of a stream that can be used as a heat transfer fluid to heat the output of the mixer (MIX-01), the heater is chosen to be used in heating the feed by using additional energy. However, in the modified process, there are two recycle processes, i.e. from the top product of the reactor output (R-01) and from the top product of the distillation column (D-01). The top product of the reactor output (R-01) is recycled and utilized as a heat transfer fluid in the heat exchanger (HE-01) to heat the feed that coming out of the mixer (MIX-01).

3.2 Reactor Output Recycle as a Heat Transfer Fluid

The cumene production process requires a series of thermal procedure to heat and cool the compound. Since the cumene production is classified as an exothermic reaction, there is heat generated that can be used for other processes so that it is not be wasted [11]. One example is the heat generated from the reactor output product (R-01) in the form of fluidized gas during its operation. This heat can be utilized as a heat transfer fluid in a heat exchanger. In the basic process, the reactor output product (R-01) is directly fed into the cooler (C-01) to be cooled and then enter the separation stage without any utilization of the heat generated. While in the modified process, the reactor output product (R-01) is recycled to be put into the heat exchanger

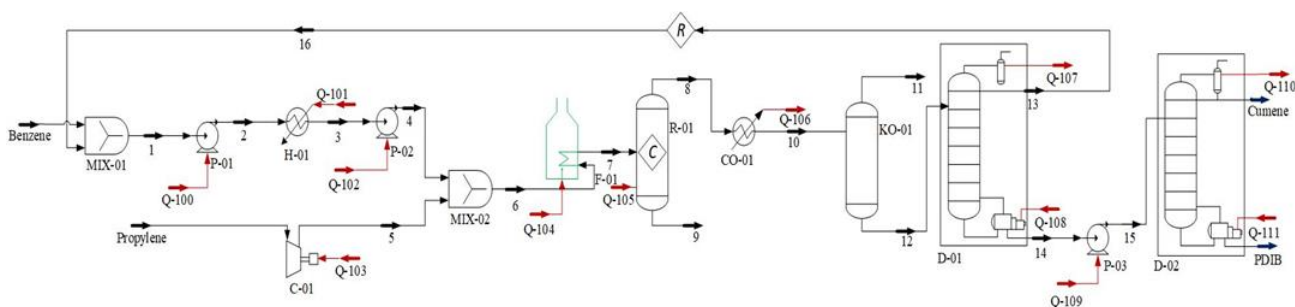


Figure 5. Process flow diagram of basic process

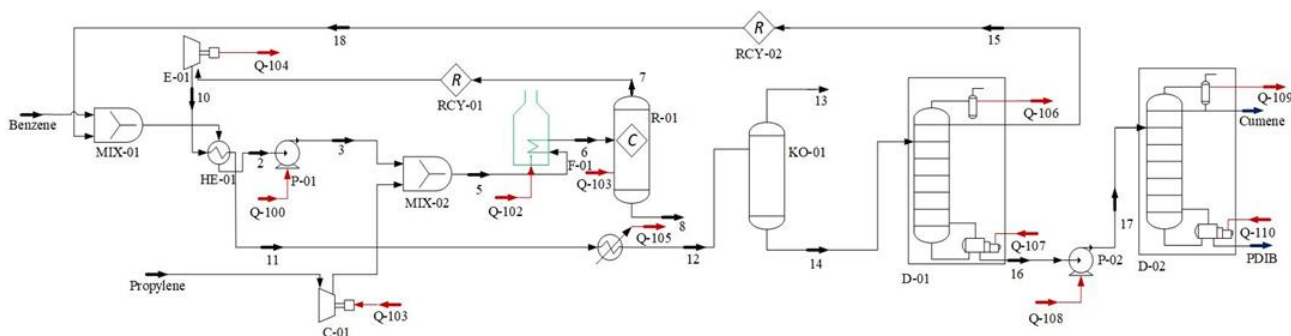


Figure 6. Process flow diagram of modified process

(HE-01) as a heat transfer fluid to heat the feed that coming out of the mixer (MIX-01). With this series of modification processes, the heat generated from the reactor output product will not be wasted. In addition, the use of a heat exchanger by utilizing the heat as a heat transfer fluid will also be more efficient in energy than using a heater that requires additional energy during the process.

3.3. Selection Between Heater and Heat Exchanger

Heat exchanger units are necessary in the cumene production process, either in the form of heat exchangers, heaters, or coolers. For example, a heater or heat exchanger is used in the process of heating the feed that coming out of the mixer (MIX-01) before entering the benzene-propylene mixer (MIX-02) and furnace (F-01). While the cooler (C-01) is used in the process of cooling the reactor output product before entering the separation stage. The selection for the use of a heater or heat exchanger is based on the presence or absence of a heat transfer fluid that can be utilized to heat the feed. If there is a heat transfer fluid, then the use of a heat exchanger is preferred over a heater. But, if there is no heat transfer fluid, then the use of a heater is selected by using additional energy. The use of heat exchangers will be more efficient in terms of energy used because it does not require additional energy during the process. In addition, the heat exchanger also has two functions because it can be used to heating and cooling the fluid that enters the heat exchanger by transferring heat between two fluids that have a difference in temperature where the two fluids are arranged separately and given a barrier in the form of a wall with the aim of preventing mixing between those two [12,13]. While the heater only has one function to increase the temperature of the fluid that enters the heater so that it requires additional energy during the process [14].

3.4. Heater Replacement with Heat Exchanger Effect in Modified Process

In the basic process, a heater (H-01) is used in the process of heating the feed that coming out of the mixer (MIX-01) before entering the benzene-propylene mixer (MIX-02) and furnace (F-01). At the same time, the reactor (R-01) emits heat in the form of fluidized gas during the process, requiring subsequent cooling in the cooler (C-01) before proceeding to the separation stage. This thermal management approach has been identified as non-optimal, resulting in a decrease in the overall energy efficiency of the system. To address this, a process modification is proposed, which involves replacing the heater with a heat

exchanger. The incorporation of a recycling loop and replacement of the heater (H-01) with a heat exchanger (HE-01) in the modified process was motivated by the inherent inefficiencies of the conventional heating process and operational optimization to control heat losses. Heaters, which depend on external energy sources for their operation, are considered energy-intensive in heating the feed. An alternative to heaters is the application of heat exchangers, which are capable of utilizing the heat-laden gaseous fluid of the reactor output product (R-01) in the form of high-temperature and high-pressure steam. This steam, in a cascading effect, serves as a powerful way to heat the initial feed used for the mixing process. This strategic integration not only maximizes the utilization of thermal energy but also contributes to the overall sustainability and efficiency of the process [15-17].

Before proposed the process modification, the special heating function of the heater requires additional external energy. In the envisioned modification, where the heater is replaced by a heat exchanger, the hot fluid from reactor output product (R-01) can be integrated as a heat transfer fluid in a heat exchanger (HE-01) so that the heat produced will not be wasted. Operating at 370 °C and 25 atm, the high-temperature gaseous fluid undergoes a pressure drop through an expander (E-01). This strategic step is critical to prevent excessive pressure drop in the subsequent heat exchanger (HE-01), ensuring optimal performance without compromising system integrity [18]. After the pressure drop, the fluid is directed to the heat exchanger (HE-01) and then used as a heat transfer fluid to heat the feed exiting the mixer (MIX-01). This modification effectively increases the initial feed temperature, achieving the same goal as the pre-modified process but with better efficiency.

In addition to the previously stated benefits, the adoption of heat exchangers over heater in cumene production systems yields further advantages. Heat exchangers enable precise temperature control promoting a more uniform distribution of thermal energy throughout the processes. This not only enhances reaction efficiency but also minimizes the risk of thermal degradation of reactants and product [19,20].

3.5. Evidence of Energy Efficiency Improvement By Modification Process

The energy required for the basic and modified process is shown by Table 1. In the basic process, there are a total of 11 energy streams, namely Q-100 to Q-111, where Q-101 is the energy required for heater with a value of 1,274,979.72 kJ/h. While in the modified process, there are only a total of 10 energy streams, namely Q-100 to Q-

110. The reduction of total energy streams in the modified process is due to the replacement of the heater with a heat exchanger by utilizing the recycling process of the reactor output as a heat transfer fluid.

Based on the Table 1, the total amount of energy required in the modified process is 39,814,003.7 kJ/h, while for the basic process is 40,588,937.4 kJ/h. Since the total amount of energy required in the modified process is smaller than the basic process, it's safe to say that the modified process has better energy efficiency than the basic process with a difference in value of 774,933.7299 kJ/h.

4. Conclusion

The reactor output recycling modification in a heat exchanger will increase the energy efficiency that required in the production of cumene. This is evidenced by the total amount of energy required in the modified process is 39,814,003.7 kJ/h, while for the basic process is 40,588,937.4 kJ/h. With a difference in the total value of energy required for both process is by 774,933.7299 kJ/h, then it can be concluded that the modified process has better energy efficiency than the basic process by utilizing the recycling process of the reactor output as a heat transfer fluid in the heat exchanger to replace the role of the heater which requires additional energy.

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Table 1. Comparison of energy required for basic and modified processes

Energy Stream	Energy Required (kJ/h)	
	Basic Process	Modified Process
Q-100	499.892933	60,917.4143
Q-101	1,274,979.72	382,873.244
Q-102	62,388.0349	17,475,581.4
Q-103	382,873.244	-12,925,189
Q-104	16,522,576.3	1,745,036.03
Q-105	-12,923,426	13,527,766.7
Q-106	15,641,148.8	3,397,859.35
Q-107	3,401,032.43	3,084,496.13
Q-108	3,088,564.83	825.808889
Q-109	830.445276	6,530,803.1
Q-110	6,567,580.37	6,533,033.6
Q-111	6,569,889.17	-
Total	40,588,937.4	39,814,003.7

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