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Research Article

Enhancing Energy Efficiency of Hydrodealkylation (HDA) Toluene for Benzene Production through Optimizing Utility Tool (Pinch Analysis)

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Abstract

Benzene is one of the chemicals widely used in domestic and industrial products. There have been many extensive studies conducted on hydrodealkylation processes to produce benzene from toluene to achieve the optimum result. Aspen hysys V.11 used to simulate hydrodealkylation process. In this study, this work aims to optimize energy efficiency and manage the heat generated by the highly exothermic hydrodealkylation reaction by adjusting the utility type of the heater and cooler. The results of the analysis and calculations, the utility modifications in the heat exchanger network system have proven to have a positive impact on energy efficiency and overall performance. With high energy efficiency, the system is able to reduce reliance on auxiliary utilities while improving the sustainability of the production process. This approach is not only beneficial from an operational perspective but also contributes significantly to cost savings and reduced environmental impact, making it a very viable solution to implement.

Keywords: Benzene; Hydrodealkylation; Utilities; Pinch Analysis; Optimization Energy

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1. Introduction

Benzene is one of the chemicals widely used in domestic and industrial products. For example, gasoline used in automobile, contains as high as 5% benzene to maintain optimal octane levels and properties [1]. Based on the literature, Benzene can be produced from toluene using the hydrodealkylation method. The reactions are shown below [2]:

$$C_7H_8 + H_2 \rightarrow C_6H_6 + CH_4 \quad \Delta H = -50 \text{ kJ/mole} \quad (1)$$
$$2C_6H_6 \leftrightarrow C_{12}H_{10} + H_2 \quad \Delta H = 81 \text{ kJ/mole} \quad (2)$$

In this process toluene is hydrodealkylated in a homogeneous and non-catalytic gas beds, benzene and methane are produced as products. Then in another reaction (equilibrium), benzene loses hydrogen and turns into diphenyl. Benzene is the main product while hydrogen and diphenyl are by-products [3]. There have been extensive studies conducted on hydrodealkylation processes, with specific goals objectives including steady-state design, controllability, and effectiveness of conceptual systems, control structure selection, and controller design. For example, adopting a different approach than relying on conventional pinch analysis methods, focuses on developing the best heat exchange network design for the HDA process [4]. Another recent studies on the hydrodealkylation of toluene include considered control reconfiguration for optimizing HDA plant process that methodology is based on the self-optimizing control by regulating the liquid flow of the separator outlet, the mole fraction of the

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toluene mixer outlet, and the heat of the benzene column reboiler [5], use membrane reactors (MRs) for hydrodealkylation of toluene in modeling point of view, two-dimensional CFD model has been developed which the conversion realized is increased [6] and then investigate the energy efficiency of the conventional toluene disproportionation process with pinch technology and develop a new double flash retrofit [7].

The aim of this study is to improve the energy efficiency of the HDA process in the production of benzene by approaching the selection of equipment and design related systems for heating and cooling utilities (type of the heater and cooler) with pinch analysis using Aspen Hysis V11.

2. Methods

2.1 Process Simulator

Process simulators in these study is using ASPEN HYSYS and ASPEN Energy Analyzer. It selected for simulating the processes because of its high popularity among researchers and the open access of the automation server because it allowing all objects to be accessible by external connections [8]. Aspen HYSYS commonly used for conceptual design, control, optimization, and process monitoring at various project stages [9]. This interactive and extensible program supports steady-state and dynamic plant models, operational improvement, and business planning while allowing easy manipulation of process variables and unit operation topology [10].

2.2 Basic Process Flow Diagram (PFD)

Figure 1 shows process flow diagram for HDA Toluene process. Gas of hydrogen and liquid of toluene are combined in mixer with gas and liquid recycle streams, which has smaller amount of methane gas. Then, entering heat exchanger and continues into the furnace, to reach the required reactor inlet temperature. The reactor is adiabatic and must be run with an excess of hydrogen to prevent coking, this effluent is quenched with liquid from the separator system. Reactor outflow is fed into the phase separator, gas stream from the overhead of the contains hydrogen plus methane and can be recycled back to the reactor via a compressor. Part of the liquid from the separator serves as the reactor quench stream and directed to separate benzene and diphenyl [11].

2.3 Reaction Mechanism

In the process of making benzene, toluene undergoes hydrodealkylation within a uniform and gaseous non-catalytic medium, resulting in the production of benzene and methane as primary products. Additionally, through an equilibrium reaction, benzene can lose hydrogen and transform into diphenyl. The main product obtained is benzene, while hydrogen and diphenyl (biphenyl) are generated as by-products. The reaction and their corresponding rate laws are provided below [2]:

$$C_7H_{8\,(g)} + H_{2\,(g)} \rightarrow C_6H_{6\,(g)} + CH_{4\,(g)} \quad \Delta H = -50 \text{ kJ/kmol} \tag{3}$$

and side reaction:

$$2C_6H_{6\,(g)} \leftrightarrow C_{12}H_{10\,(g)} + H_{2\,(g)} \quad \Delta H = 81 \text{ kJ/mol} \tag{4}$$

2.4 Operating Conditions

2.4.1 Temperature

The experiment of hydrodealkylation of toluene involves varying the temperature at the reactor inlet within the range of 1100 to 1400 °F. In this study inlet temperature of reactor is to be set at 1200 °F (649 °C) because the hydrodealkylation of toluene process operates within a temperature range of 500–660 °C (932–

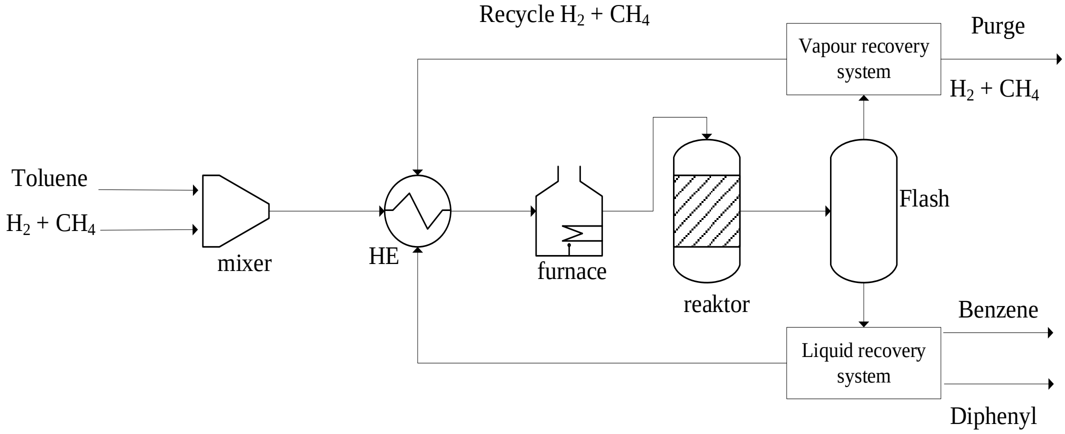

Figure 1. Simplified process flow diagram of HDA toluene to produce benzene

1220 °F), then an outlet temperature of 1263 °F (684 °C) was obtained [4].

2.4.2 Reactor pressure

The initial feed-in reaction is carried out with the reaction pressure at 569 psia (38.7181 atm). Then the pressure of stream enter the reactor at 494 psia (33.6 atm). The pressure is chosen because the hydrodealkylation process can run at a pressure of 20-60 bar (2909.07-870.23 psia) [4].

2.5 Modification Strategy for Heat Transfer Unit

Process modification of Hydrodealkylation (HDA) Toluene to product benzene related with heat transfer processes that utilize a wide variety of heating and cooling utilities. The type of heating and cooling utilities used in a process has a significant influence on various aspects of system performance, such as operating costs, heating and cooling network performance, and overall energy efficiency. The selection design and optimization of the right type of utilities can reduce energy consumption [12] and thus reduce production costs, improve network performance stability, and have the potential to minimize energy losses and increase heat transfer effectiveness and energy savings [13]. This is done to create a more environmentally friendly and sustainable system.

In the references [2], there was benzene production through toluene hydroalkylation with several heat exchangers with stream specifications as shown in Figure 2. E-100 is a process exchanger that uses hot fluid, 5_To_7 and cooling fluid 1_To_3. E-101 is a heater type heat exchanger that uses very high temperature hot fluid and cooling fluid 1_To_3. Then, for the utility that used in basic process before modification is shown in Figure 3.

The heating utilities used are very high temperature, while the cooling utilities are cooling water, HP steam generation, and air. Henceforth, the modification strategy used in this study is to improve energy efficiency by changing the heating and cooling utilities in the process, heating utilities used are fired heat (1000) and LP steam while the cooling utilities are cooling water and LP steam generation, as shown in Figure 4.

2.6 Pinch Analysis using Aspen Energy Analyzer

Pinch analysis is a systematic approach used in process design to minimize energy consumption in production. The goal is to create the most efficient Heat Exchanger possible, while optimizing energy use [4]. The use of pinch technology to optimize the integration of SMR-PSA heat during the hydrogen production process; total energy consumption decreased by 60.5% compared to hydrogen production in conventional production [14]. By calculating the energy consumption in each process plant, businesses can lower the cost of products for customers and increase revenue. To analyze the process, the heat load (enthalpy), supply temperature, and desired temperature are required from each process stream. To balance the

Name		Inlet T [C]	Outlet T [C]	MCp [kJ/C-h]	Enthalpy [kJ/h]	Segm.	HTC [kJ/h-m2-C]	Flowrate [kg/h]	Effective Cp [kJ/kg-C]	DT Cont. [C]
5_To_7		664.0	37.8	---	9.378e+007		----	4.268e+004	----	Global
1_To_3		51.1	648.9	---	8.784e+007		----	4.069e+004	----	Global
Q-101@Main		683.9	683.4	8.569e+004	4.284e+004		720.00	----	----	Global
New										

Figure 2. Data stream heat exchanger basic process before modification

Utility		Cost Index [Cost/s]	Load [kJ/h]	% of Target
Cooling Water		1.427e-003	2.418e+007	6616
HP Steam Generation		-2.963e-005	4.284e+004	3.344
Very High Temperature		4.509e-002	1.824e+007	INF
Air		0.0000	0.0000	0.0000

Figure 3. Utilities used before modification

Utility		Cost Index [Cost/s]	Load [kJ/h]	% of Target
LP Steam Generation		-2.249e-005	4.284e+004	100.0
Cooling Water		5.535e-003	9.378e+007	100.0
Fired Heat (1000)		0.1037	8.784e+007	100.0
LP Steam		0.0000	0.0000	0.0000

Figure 4. Utilities used after modification

minimal utility requirement with the area of the HEN, the minimal approach temperature ($\Delta T_{\min}$) has been adjusted. A decrease in $\Delta T_{\min}$ reduces utility costs, but requires more surface area on the heat exchanger for the temperature difference between process streams to be maintained [4].

3. Results and Discussion

3.1 Basic Process Flow Diagram and Simulation

In simulation with Aspen HYSYS software, SRK model equation choosed due to its established reliability for accuracy predicting phase behavior and properties such as vapor-liquid equilibrium and applicability to the toluene hydrodealkylation process. Effective heat management is crucial to prevent overheating, maintain ideal reaction rates, and ensure the stability and durability of catalysts when applicable.

The Basic Process Flow Diagram is taken from reference [2], as shown in Figure 5 with the temperature and pressure specified for each flow. To simplify the calculation, a panel heater (E-101) is used here instead of a furnace. Then, the type of reactor used is a conversion reactor because it is known that the conversion of toluene in the reactor is 75%, and the 2 mole percent of benzene remaining after the first reaction is converted to biphenyl (also called diphenyl). To optimize energy efficiency and manage the heat generated by the highly exothermic hydrodealkylation reaction, adjusting the reactor inlet temperature within the range of 1100–1400 °F [2]. While this adjustment does not affect the molar flow rate or conversion (which remains at 75% for toluene), it directly impacts the reactor outlet temperature and the energy required by utilities such as heat exchangers. Therefore, obtained in the basic process [2] or before modification, the energy stream for heat flow has the values listed in Table 1.

3.2 Modification of Simulation Process based on Heat Integration

A modification of the process simulation performed using Aspen HYSYS V11 to model the overall system performance, as shown in Figure 6. Modifications were made by adding several operating units starting from cooler E-102, separator V-100, tee-100, pump P-100, and mixer MIX-101. Also Recycle RCY-100 to recycle flow 10 and adjust ADJ-1 with variable control flow ratio TEE-100 and target variable temperature flow 5 to 1227.02 °F. This modification is aimed at reusing the vapor product from the CRV-100 reactor so that it can be reused as a heater in E-100.

From the simulation data of process modification, it is found that after modification, the heat flow value of CRV-100 reactor changes to 4.061E4 (after modification) with exothermic reaction. Based on Table 2, before modification, the heat flow value was 6.596E7 Btu/h and after modification, the heat flow of the CRV-100 reactor has decreased to 4.061E4 Btu/h. This reduction

Table 1. Energy stream of reactor CRV-100 before modification

Energy Streams	
	Q (Btu/h)
Heat Flow	6.597E7

Table 2. Comparison energy stream of reactor CRV-100.

Energy Streams		
Heat Flow	Before	After
Q (Btu/h)	6.597E7	4.061E4

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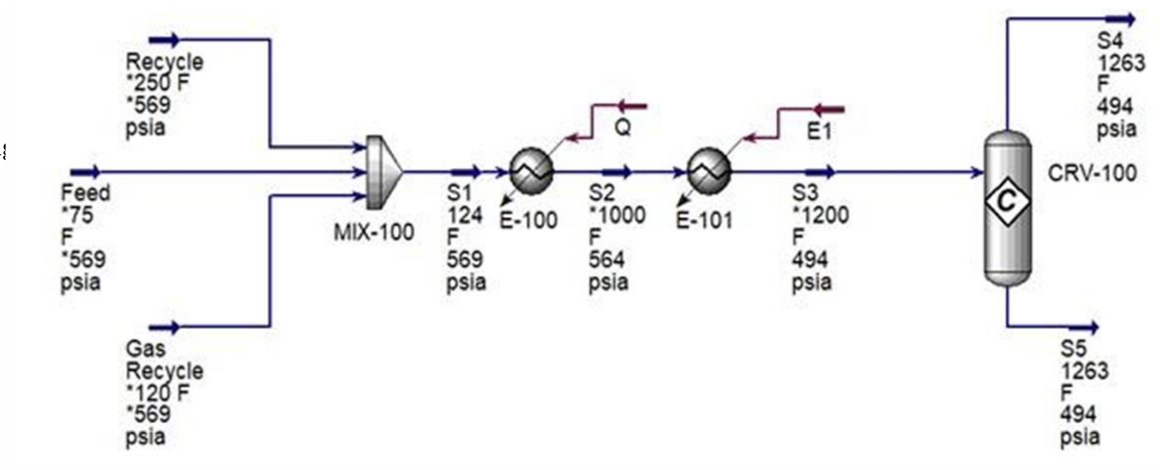

Figure 5. Process Flow Diagram (PFD) before modifications [2]

shows that the system has significantly reduced energy consumption and become more efficient than the basic process.

3.3 Modification of Simulation Process based on Pinch Analysis

Pinch analysis is used to get optimal Maximum Energy Recovery (MER), raising total energy utility, and design the Heat Exchanger Network (HEN) [17]. The analysis includes composite curves, shifted composite curves, and grand composite curves are supported by stream population algorithms to get a pinch point [19]. The simulation of production benzene with HAD process was analyzed using Aspen Energy Analyzer to analyze pinch, evaluate heat integration and modify the utilities and heat exchanger network design used.

The composite curve (Figure 7) is used to determine the energy target, which represents the heating and cooling consumption needs during the heat exchanger design process [20]. This curve is created by plotting temperature against enthalpy to identify the Maximum Energy Recovery (MER) as the utility target for heat recovery, utilizing $\Delta T_{\min}$ as a key parameter [21].

The Grand composite curve (Figure 8) is designed to determine hot and cold utility targets and illustrates the difference between heat flow and cold flow [22]. By using the heat exchanger network design as shown in Figure 9 and the operating conditions, the data as shown in Figure 10 are obtained.

The effect of the modification can be seen by comparing the results of the basic process network heat exchanger design and the modified and most optimal operating conditions as in Table 3.

Exchanger operation & capital cost depends on several factors, such as heat exchanger area, number of heat exchanger, number of shells, materials of construction, equipment type, pressure rating, etc. [16]. Based on the modifications made, the operating cost and total cost values can be minimized by 0.04488 cost/s

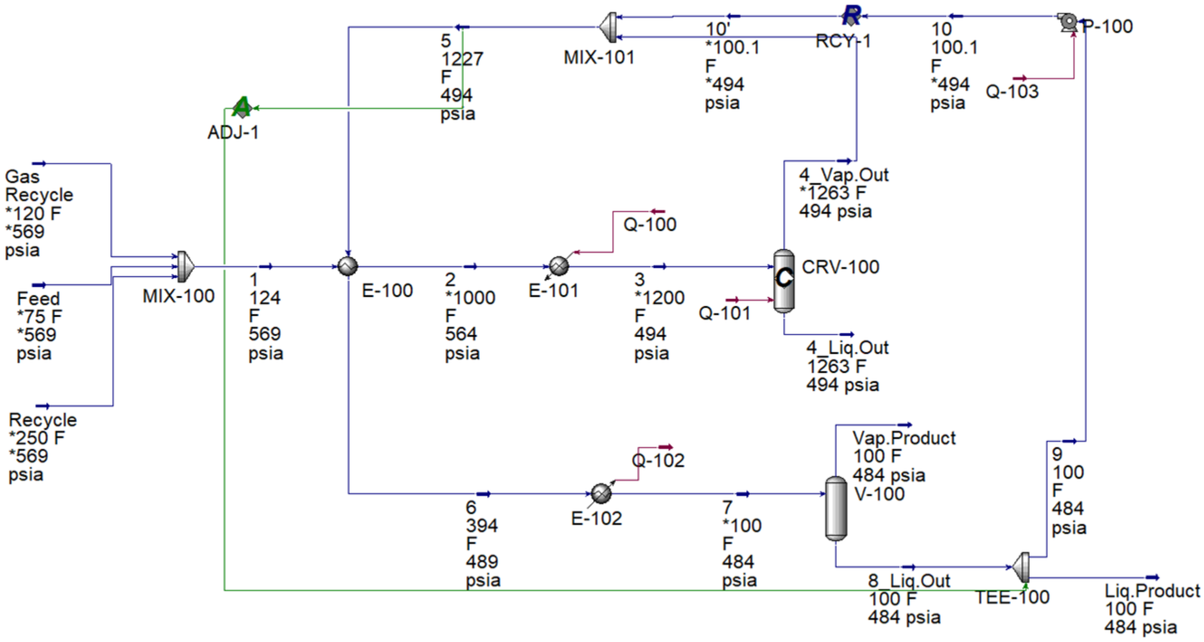

Figure 6. Process Flow Diagram (PFD) of the modified process

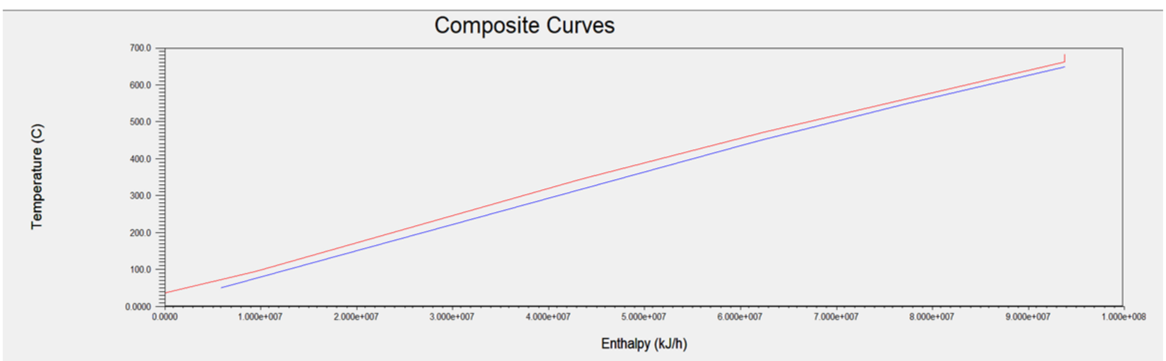

Figure 7. Composite curve

and 0.02633 cost/s lower than before modification. In addition, the value of heating target and cooling target achieved is reduced by 1.72E7 and 1.7196E7. However, as a result of the efforts to reduce the operating conditions, the number of units and shells were impacted. The results show that the number of units increased by 2 units and 37 more shells compared to before the modification. Increasing the number of units and shells in heat exchanger systems occurs to distribute the heat transfer load more evenly, reducing energy losses due to large temperature differences between hot and cold fluids [15]. By increasing the heat transfer area, the energy losses that occur can be minimized, although this increases the complexity of the design with the increase in units and shells.

From the completion of the pinch analysis that has been done, the MER (Maximum Energy Recovery) of the modified simulation results can be calculated. MER is the quantity or maximum

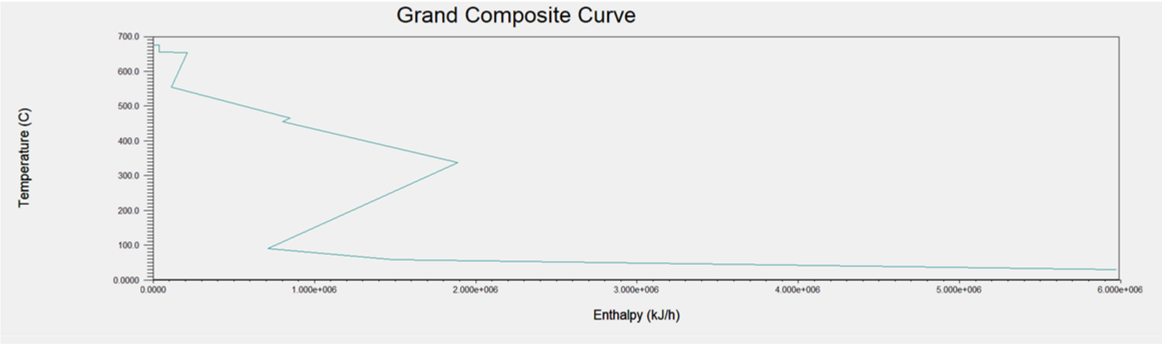

Figure 8. Grand composite curve

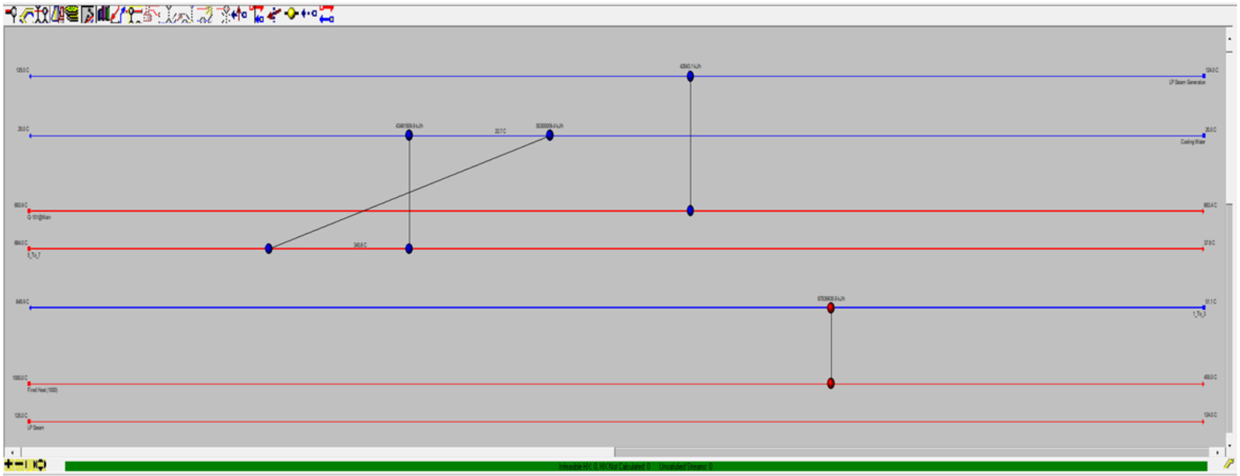

Figure 9. Heat Exchanger Network (HEN) matches after modification

Network Cost Indexes

	Cost Index	% of Target
Heating [Cost/s]	1.227e-003	INF
Cooling [Cost/s]	3.824e-004	262.8
Operating [Cost/s]	1.610e-003	464.5
Capital [Cost]	3.600e+006	128.3
Total Cost [Cost/s]	3.172e-002	138.8

Network Performance

	HEN	% of Target
Heating [kJ/h]	1.040e+006	INF
Cooling [kJ/h]	7.024e+006	117.4
Number of Units	6.000	120.0
Number of Shells	45.00	112.5
Total Area [m2]	1.353e+004	128.9

Targets

	Targets	Base Case	%
Heating [kJ/h]	0.0000	1.040e+006	***
Cooling [kJ/h]	5.984e+006	7.024e+006	117.4
Area [m2]	1.04979e+04	1.35283e+04	128.87
Capital Cost Index [Cost]	2.806e+006	3.600e+006	128.3
Op. Cost Index [Cost/s]	-6.087e-004	1.610e-003	464.5
Total Cost Index [Cost/s]	2.286e-002	3.172e-002	138.8
Number of Units	4.000	6.000	150.0
Shells	40.00	---	---

Pinch Temperatures

Hot	Cold
683.9 C	673.9 C
97.2 C	87.2 C

Figure 10. Summary data heat exchanger network after modification

energy load during heating or cooling, which can be reduced after integration with pinch analysis. The MER value is the difference between the heat and cooling loads before and after the integral analysis [18]. The calculation obtained is as follows:

Total intial heating energy = 3.972E8 kW
Total intial cooling energy = 2.389E8 kW
Heating Duty = 0 kW
Cooling Duty = 5.984E6 kW

$$MER = \frac{(\text{total initial cooling energy} + \text{initial heating}) - (\text{he}}{2}$$

$$MER = \frac{(3.972E+8 + 2.389E+8) - (0 + 5.984E+6)}{2}$$

$$MER = 3.151E+8\ KW$$

$$\%\ \text{Heating Energy Recovery} = \frac{(3.972E+8+8-0)}{3.972E+8} \times 100\% = 100\%$$

$$\%\ \text{Cooling Energy Recovery} = \frac{(2.389E+8-5.984E+6)}{2.389E+8} \times 100\% = 97.495\%$$

Through the utility modifications that have been done, the analysis results show that the energy recovery from the system is quite significant. The total initial heating energy was recorded at 3.972×10^8 kW, while the total initial cooling energy was 2.389×10^8 kW. With this modification, the heating duty was successfully reduced to 0 kW, while the cooling duty was shown to be 5.984×10^6 kW. The calculation results show that the Maximum Energy Recovery (MER) achieved is 3.151×10^8 kW, which is the energy successfully recovered through system optimization. The energy recovery efficiency is also seen to be very high, with 100% heating energy recovery and 97.495% cooling energy recovery. These figures confirm that the utility modifications implemented not only improved energy efficiency but also significantly reduced the need for external utilities.

4. Conclusion

The modifications were performed to aim the lowest energy used for benzene production by Hydrodealkylation (HDA) toluene process. By modificate the unit operation in process by reprocessing the vapor from the CRV-100 reactor product to be reused as a heater in the E-100 heater, heat flow in reactor CRV-100 decreased from 6.597E7 Btu/h to 4.061E4 Btu/h. In addition, the modification of utility usage from the process was also carried out by comparing it based on pinch analysis. Modification were performed by changing the heating utilities to fired heat (1000) and LP steam, while the cooling utilities are cooling water and LP steam generation. The results after modification show maximum energy recovery (MER) 3.151E8 KW, % heating energy recovery 100%, and % cooling energy recovery 97.495%. These values confirm the effectiveness of the heating and cooling utility modifications to maximize energy efficiency and minimize the use of energy used in the process as not much energy is wasted in the process.

CRediT Author Statement

Author Contributions: Audrey Olivia Adlai Pardede: Conceptualization, Methodology, Investigation, Resources, Formal Analysis, Writing Original Draft, Writing Review and Editing, Supervision; Izzah Nabila Itsnainie: Conceptualization, Methodology, Resources, Writting Draft Preparation, Writing Review and Editing, Visualization; Sanandha Azwa Fazila : Conceptualization, Methodology, Software, Formal analysis, Writing Original Draft, Writing Review and Editing, Data Curation, Visualization, Supervision; Sinta Kamila: Conceptualization, Methodology, Investigation, Resources, Writing Original Draft, Writing Review and Editing. All authors have read and agreed to the published version of the manuscript.

Table 3. Comparison of operating conditions before and after modification

	Before Modification	After Modification
Operating Cost (cost/s)	4.649e-002	1.610e-003
Total Cost (cost/s)	5.805e-002	3.172e-002
Heating Target (kJ/h)	1.824+007	1.040e+006
Cooling target (kJ/h)	2.422e+007	7.024e+006
Number of Units	4	6
Number of Shells	8	45

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