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Modification of Ethyl Benzene Production Unit Based on Conceptual Design and Pinch Analysis

Kowsar Binande [1], Elham Jabarzare [2], Younes Ghalavand [3*]

[1, 2, 3] Department of Chemical Engineering, Faculty of Engineering, University of Isfahan, Isfahan, Iran

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Abstract: Increasing energy cost, reducing the available volume of the conventional fuel and environmental constraints with respect to the emission of the pollutants lead to energy saving as one of the most crucial objectives in the petrochemical plants. Here, both conceptual design (for reducing the fixed cost) and pinch analysis (for reducing the energy cost) of the ethyl benzene production unit are run. An attempt is made to propose a process for ethyl benzene production with only one alkylation reactor instead of two (available in the conventional process). Comparison between the proposed process (integrated reactors) and the conventional process (with two alkylation reactors), reveals an18GJ/h decrease in energy consumption and about 15% in equipment cost. Pinch analysis is run for both the processes and it is found that the energy consumption by this proposed process and the conventional process are reduced from 237.5 GJ/h to 143.87 GJ/h and 255.5 GJ/h to 190.9 GJ/h, respectively. The results indicate that energy consumption in this proposed process is lower than the conventional process before and after pinch analysis.

keywords: Ethyl Benzene, Pinch Analysis, Energy Minimization, Simulation, Conceptual Design

1. Introduction

Ethyl benzene (EB) is one of the important petrochemical materials consumed mainly in producing styrene. Ethyl benzene is consumed in producing stoophene, ethylene benzene, acetate cellulose, and as a solvent in some industries (Gerzeliev, Khadzhiev, & Sakharova, 2011). The most frequently applied process for producing ethyl benzene is its alkylation, which has been and is being studied in different areas, like energy optimization, improving operating conditions (Ebrahimi, Sharak, Mousavi, Aghazadeh, & Soltani, 2011), exergy Analysis (Jahromi & Beheshti, 2017), catalyst structure (Corma, Martinez-Soria, & Schnoeveld, 2000) and equipment rearrangement (Maleki, Behroozsarand, & Ghasemzadeh, 2018).

The focus of much research is on energy integration and different approaches like the mathematical programming models, the pinch technology-based graphical methods, techno-economic analysis, and conceptual design.

Techno-economic study is a tool for estimating performance, emissions and cost of a plant before it is built. When the modification is performed based on techno-economic study, the plant is built with low energy consumption or low operating cost (Frey & Zhu, 2012). One of the methods applied in decreasing the fixed capital cost is a conceptual design, which is a set of disciplines that contribute to the identification of the optimal design. In chemical engineering, the objective is to evaluate the best design variables and operating conditions that would increase the profit (Barzaghi, Conte, Sepiacci, & Manca, 2016).

Mathematical models and pinch analysis, based on graphical methods are regarded as the major means for energy integration have been and are being assessed. Pinch analysis is essentially proposed for complicated systems in determining the amount of water, energy, emissions, etc. (Luo et al., 2018). Pinch analysis is considered as a reliable means for enhancing energy efficiencies and minimizing heating and cooling utility requirement according to the first law of thermodynamics (Linnhoff & Engineers, 1994). One of the other

* **Corresponding Author.**
Authors' Email Address: K. Binande (kr.binande@gmail.com), [2] **E. Jabarzare** (eli92jabarzare@gmail.com),
[3] **Y. Ghalavand** (y.ghalavand@eng.ui.ac.ir)

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advantageous applications of pinch analysis is determining the type of the needed utilities.

Liu et al. proposed a methodology for heat exchanger network (HEN) integration, in which the cooling water variables including supply temperature, flow rate, and target temperatures were enhanced. Consequently, by applying this method in a case study, the total annual operating costs were reduced 4.5%compared to the conventional process(Liu, Ma, Feng, & Wang, 2018). Kralj applied pinch analysis for integrating heat in formal in and methanol processes, where, the graphical utilities in a case study led to a saving of 335,080 USD/year in operating cost (Kovac Kralj, 2012).

Yang et al. introduced a HEN super-structure based on a stage-like approach for heat integration, where, the results lead to 24% savings in energy consumption (Yang, Wang, Sun, & Zhang, 2016). Gadalla applied a graphical method energy performance in the existing networks based on retrofit approach, where, the exchanger in the pinch, pinching matches, incorrect arrangement of fuel consumption and network pinch are determined through this method; by applying this method in a case study 17% savings is yield in energy demand and fuel consumption (Gadalla, 2015). Ghannadzadeh and Sadeqzadeh presented a method for energy integration enhancement in a chlorine-caustic soda process based on major sources for thermal energy losses indicating that the total energy demand is reduced from 12.99MW to 0.4MW (Ghannadzadeh & Sadeqzadeh, 2017). The energy integration enhancement was applied by Azadi et al. on the methanol production unit, where an annual savings up to 6.1e6 USD/year (Azadi, Tahouni, & Panjeshahi, 2016).

Simulation of Western Desert Gas Complex (WDGC) was implemented by HYSYS simulation software to modify HEN. According to the pinch design method, the HEN was developed for obtaining the cooling energy and minimum heating energy requirement. According to the results, hot and cold utilities saving was 42% and 21% in the WDGC process, respectively (El-Temtamy, Hamid, Gabr, & Sayed, 2010).

Heat and power integration were made for common methane reforming in a hydrogen production unit. For this purpose, a minimum utility cost problem was defined and solved for the related heat exchange network. The results indicated a 36% reduction in utility costs(Posada & Manousiouthakis, 2005).

Yoon analyzed a HEN in an ethyl benzene plant by applying pinch analysis based on the retrofit method. After HEN analysis, a heat exchanger was added, and the operating conditions were changed leading to an annual energy cost decrease by 5.6%(Yoon, Lee, & Park, 2007). Hussain et al. designed a new column by applying a side reactor for producing the ethylbenzene, where the side reactors count, reactor volume, reactor side-return tray, column trays count and the column pressure were optimized, with a total annual cost reduction. Through this optimization, energy consumption was reduced to12.9%, and after heat integration, energy consumption was reduced to 53% (Hussain, Minh, & Lee, 2017). Ebrahimi et al. simulated an ethyl benzene production unit and optimized benzene selectivity, benzene recycle ratio and energy consumption. In this process, the two double-bed alkylation reactors were made four, with a single bed. It was observed that the consumption of the energy for the heat exchangers and reboilers were decreased to 59 and 60% in comparison with conventional operating conditions (Ebrahimi et al., 2011).

The focus of the available studies is on optimization and energy minimization just by HEN modification or changing the operating conditions. In this study, an attempt is made to reduce the ethylbenzene production unit's fixed capital cost by applying the conceptual design method in comparison with the conventional process. Conceptual design may decrease operating cost because the process equipment is rearranged therein. After the conceptual design, the retrofit pinch analysis is run for the conventional and this proposed processes by applying commercial simulation software. The obtained results can be contributive in minimizing ethyl benzene energy cost or other similar processes operating cost.

2. Simulation and Result

Ethylbenzene is an aromatic compound consumed in the petrochemical industry, in producing styrene monomer in specific. Styrene monomer is a major raw material in ABS, PS, ASA, etc. production (Sahoo, 2011; Yoon et al., 2007). Ethylbenzene can be produced by alkylation of benzene in the atmospheric pressure at 500 ^{o}C. The alkylation by-products are the di-ethylbenzene and tree-ethylbenzene (ingeneral PEB). In this process, 500 ^{o}C is high; therefore, the alkylation reaction must occur in a catalytic bed at lower temperatures. The main reactions in the catalytic process are tabulated in Table 1 (Ebrahimi et al., 2011).

Table 1. The main reactions in ethyl benzene process

Benzene + Ethylene → Ethyl Benzene	(1)
Ethyl Benzene + Ethylene → Poly Ethyl Benzene	(2)
Di-Ethyl Benzene + Ethylene → Poly Ethyl Benzene	(3)
Poly Ethyl Benzene + Benzene → 2 Ethyl Benzene	(4)

The conventional process for producing ethyl benzene is shown in Figure1 (Ebrahimi et al., 2011), where, three fixed bed reactors are applied for alkylation and transalkylation. The fresh benzene stream is fed into the alkylation reactor at 200°C and 35bar a pressure with the recycled benzenes. In the reactors, the most wanted reaction (reaction1) and unwanted reactions (reactions 2 and 3) occur. These two reactors are arranged series based on benzene stream, and fresh ethylene separately fed into each reactor. The outlet stream from these condreactor (R-102) contains 35.20% ethylbenzene, 13.31% polyethylbenzene and 51.49% benzene, is fed into the light removal column (T-101) at 37 bara pressure. The outlet stream from the top of the T-101 with 99.99% benzene is recycled to the R-101, and side stream from the second tray enters to the transalkylation reactor (R-103). Topurify the ethyl benzene, the bottom stream discharged from T-101 with 82.01% ethylbenzene, 0.1% benzene and 17.89% polyethyl benzene, is fed into the second column (T-102). To achieve optimal operating conditions, polyethyl benzene production must below, that is, discharged from the bottom of T-102, and enters into the transalkylation reactor (R-103), where the polyethyl benzene react, and ethyl benzene is produced (reaction4). This product is obtained from the top of the T-102 at 99.1% purity.

To reduce energy consumption and capital cost (less equipment), a new process is designed based on conceptual study and presented in figure 2.

Unlike the conventional process, only one alkylation reactor (R-201) is considered in this proposed process which is in series with the transalkylation reactor (R-202). Both reactors are considered as a plug flow type. The fresh benzene and ethylene feed enter R-201, and the exothermic alkylation reaction is implemented in the liquid phase (reaction1). The unwanted reactions (reactions 2 and 3) occur and polyethyl benzene is produced. Then the outlet stream from R-201 is fed into the transalkylation reactor (R-202) with the recycle benzene and recycles poly ethyl benzene streams. The polyethyl benzene to ethyl benzene conversion occurs (reaction 4) in R-202. The outlet stream from R-202 with 45.54% ethyl benzene, 32.84% benzene and 21.63% poly ethyl benzene is fed into the first distillation column (T-201) for unreacted benzene separation. The stream discharged from the bottom of T-201 contains 67.76% ethylbenzene, 32.22% polyethylbenzene and 0.01% benzene is fed into the second column (T-202) for ethyl benzene purification. The outlet stream from the top of the T-202 with 99.1% ethylbenzene is obtained as the main product. The bottom stream from the T-202 is recycled to R-202. In both processes, the ethylbenzene product is 99.1% purity.

By changing the conventional process according to Figure 2, the process equipment cost is reduced by about 15% in comparison with the conventional process computed through Aspen I carus software.

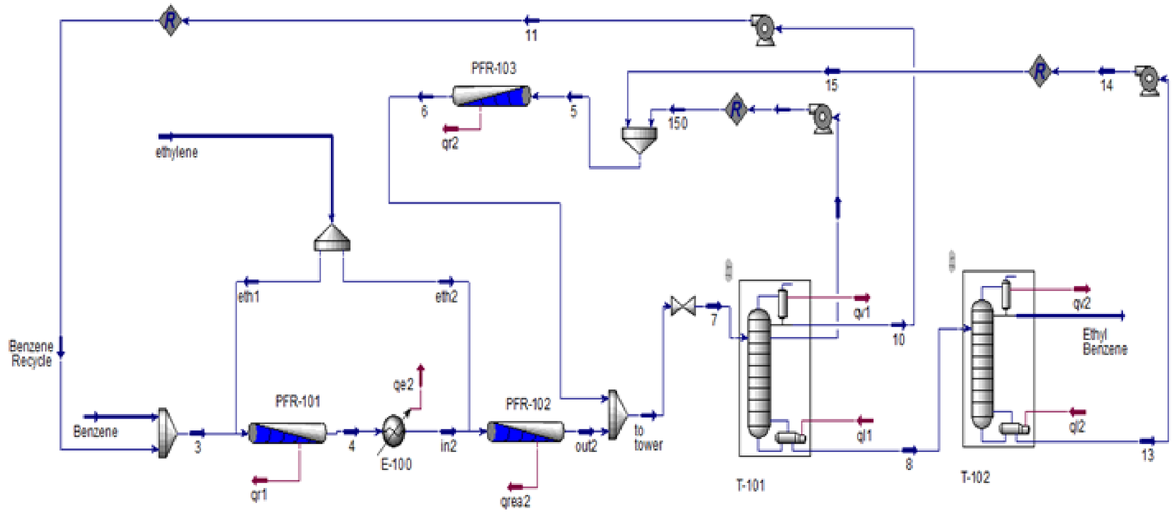

Figure 1. Scheme of the conventionalprocess

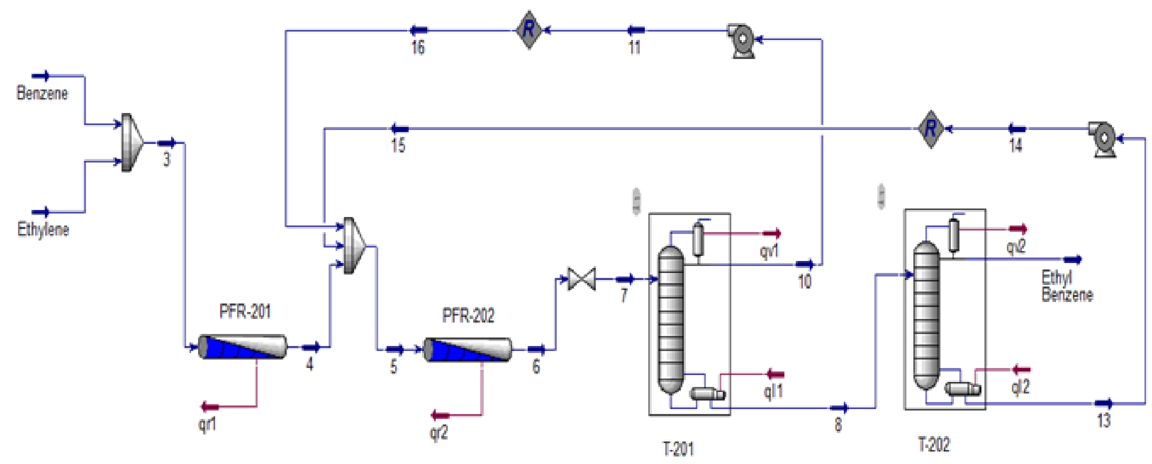

Figure 2. Scheme of proposed process

2.1. Simulation Procedure

The conventional and proposed processes are being assessed in this study. Both are simulated based on 99.1% ethyl benzene purity and 74220 kg/h productivity.

The applied kinetics for reactions 1 and 2 in these simulations are expressed in Equations 1 and 2 (Han Ng, Sharma, & Rangaiah, 2016).

$$r_1=1.528\times10^6\times\exp(-\frac{7.113\times10^4}{RT})C_{Et}C_{BZ} \qquad (kmol/m^3.s) \qquad (1)$$

$$r_2=2.778\times10^7\exp(-\frac{8.368\times10^4}{RT})C_{EB}C_{Et} \qquad (kmol/m^3.s) \qquad (2)$$

In the transalkylation reactor, reaction 4 occurs according to the kinetics expressed in Equation 3 (Han Ng et al., 2016).

$$r_3=1000\times\exp(-\frac{6.276\times10^4}{RT})C_{DEB}C_{BZ} \qquad (kmol/m^3.s) \qquad (3)$$

In this simulation, the distillation columns trays are considered equilibrium and the reactors are considered plug flow type.

2.2. Pinch Analysis

The main route in this investigation consists of several stages:

- Design a new process based on a conceptual study to decrease fixed capital costs.
- Simulation of both new and conventional processes and determination amount of utility consumption.
- Assessing maximum energy saving according to composite curves for both processes.
- Design HEN for both processes based on pinch analysis.
- Comparing the results for both processes, before and after pinch analysis.

Pinch analysis is run after simulation for both processes and the amount of current energy consumption and minimum energy consumption are obtained followed by determining the maximum energy saving for each process based on composite curves.

To perform pinch analysis, hot streams, cold streams and, utility streams should be identified in the simulation software. The process flows that should be cooled are defined as hot flows and vice versa. When heat transfer between process streams is not feasible or sufficient, heating or cooling is made by utility streams like cooling water, hot oil, air and LP, MP and HP steam. Supply, target, heat capacity and enthalpy for process streams are extracted where the output and input temperatures are required. These data should be extracted from simulation software, applied to determine the process streams energy for both conventional and this proposed process. A minimum temperature approach (ΔT_{min}) is selected and the composite curves are drawn. The composite curves consist of temperature-enthalpy (T-U) plots, applied to set energy targets. The curves of hot and cold composite derived from the summations of the product flow rate and specific heat are drawn together (Sunasar & Makadia, 2018; Tibasiima & Okullo, 2017; Yoon et al., 2007).

When portions of two curves in the composite curve overlap, the energies required for heating and cooling of process streams are provided with no need for utility streams, thus that maximum energy recovers. The minimum energy consumption can be practically achieved by running the pinch analysis, and the diagram of the HEN drawn (Sunasar & Makadia, 2018; Tibasiima & Okullo, 2017).

The conventional and proposed processes are simulated, and some information like the input and output stream's temperature of the heat exchangers and heat loads are extracted from the simulation software. The stream's data for the pinch analysis are tabulated in Tables 2 and 3.

The current energy consumption for the conventional process is 255.5 GJ/h including 91.29 GJ/h heating utilities and 164.2 GJ/h cooling utilities. The current energy consumption for this proposed process is 237.5 GJ/h including 84.85GJ/h heating utilities and 152.6 GJ/h cooling utilities. It is observed that this proposed process consumes lower energy in comparison with the conventional process.

The HENs for the conventional and this proposed processes before pinch analysis are shown in Figures 3 and 4, respectively.

It is possible to apply a composite curve for obtaining the highest energy recovery, provided for both processes based on ΔT_{min}=10°C in Figures 5 and 6. The diagram shape depends on the minimum temperature driving Force (ΔT_{min}) in heat exchangers and by varying in ΔT_{min}a change is observed in heat exchangers areas.

The cold and hot composite curves overlap in Figure 5 and 6, indicates the amount of 88.78 GJ/h and 93.6 GJ/h of possible energy that can be recovered in both the conventional and this proposed processes, respectively, which is reaching the target level of 166.7 GJ/h and 143.9 GJ/h, respectively.

Table 2. Heating and cooling summary for the conventional process

Heat Exchanger	Type	Base Duty (GJ/h)	Hot Inlet Temp.[°C]	Hot Outlet Temp.[°C]	Cold Inlet Temp.[°C]	Cold Outlet Temp.[°C]
qrea2@Main_Exchanger	Cooler	32.3	250.0	249.5	174.0	175.0
qr1@Main_Exchanger	Cooler	9.128	266.0	265.5	249.0	250.0
E-100@Main	Cooler	2.961	266.0	256.0	174.0	175.0
Condenser@COL1	Cooler	75.03	117.6	117.6	30.0	35.0
Condenser@COL2	Cooler	44.81	179.2	178.7	124.0	125.0
Reboiler@COL1	Heater	47.51	250.0	249.0	194.6	197.2
Reboiler@COL2	Heater	43.78	280.0	250.0	237.2	240.9

Table 3. Heating and cooling summary for the proposed process

Heat Exchanger	Type	Base Duty [GJ/h]	Hot Inlet Temp.[°C]	Hot Outlet Temp.[°C]	Cold Inlet Temp.[°C]	Cold Outlet Temp.[°C]
qr1@Main_Exchanger	Cooler	46.8	266.0	265.5	249.0	250.0
Condenser@COL1	Cooler	57.3	117.8	117.7	30.0	35.0
Condenser@COL2	Cooler	48.47	179.4	178.8	124.0	125.0
Reboiler@COL1	Heater	36.24	3000	2999	199.6	203.2
Reboiler@COL2	Heater	48.6	3000	2999	244.5	245.0

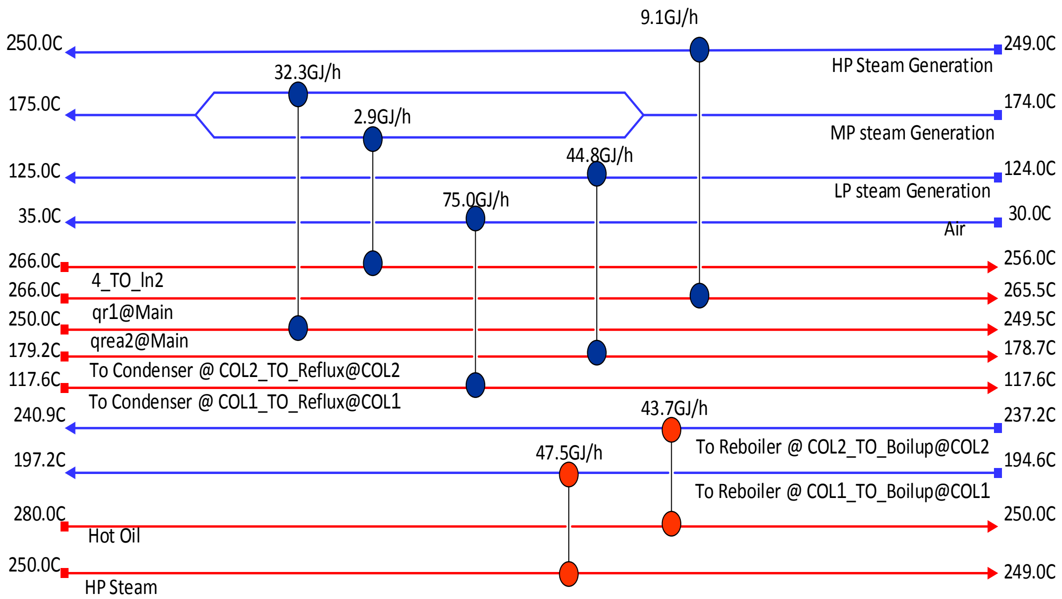

Figure 3. Grid diagram of heat exchanger network for conventional process

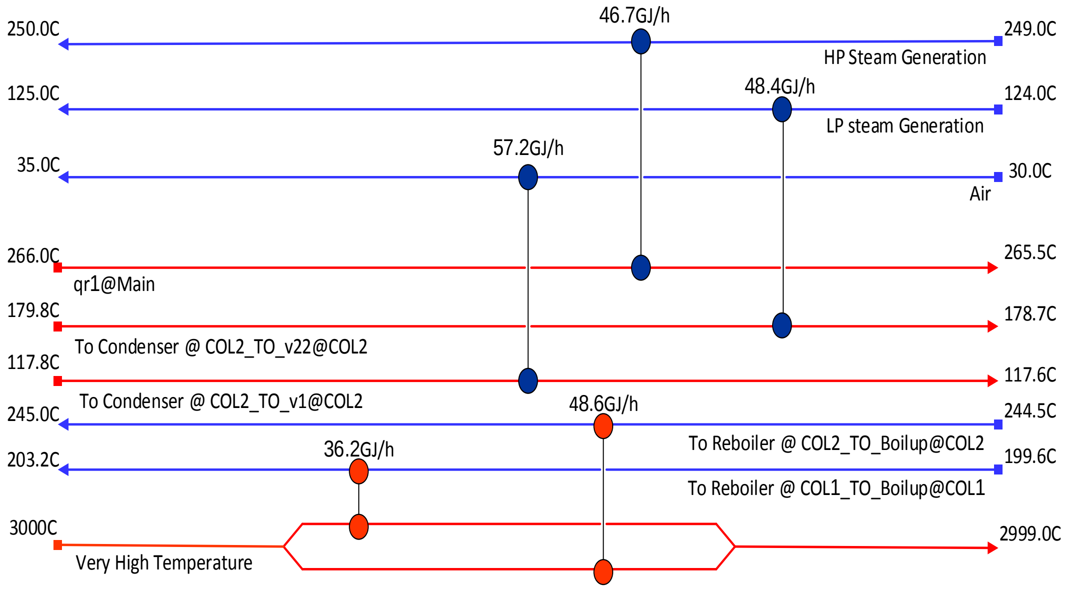

Figure 4. Grid diagram of heat exchanger network for the proposed process

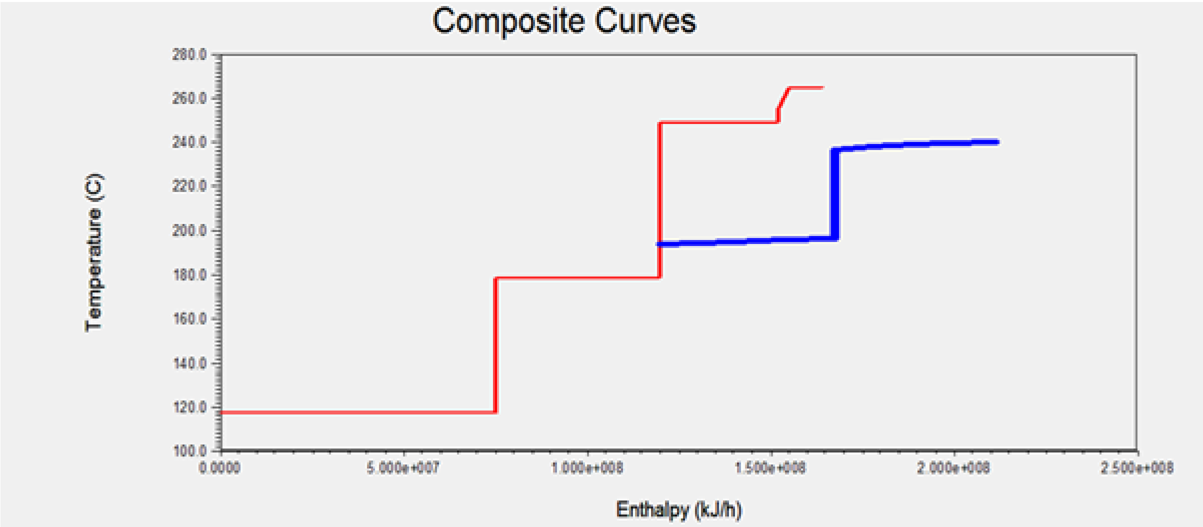

Figure 5. Composite Curve for Conventional Process

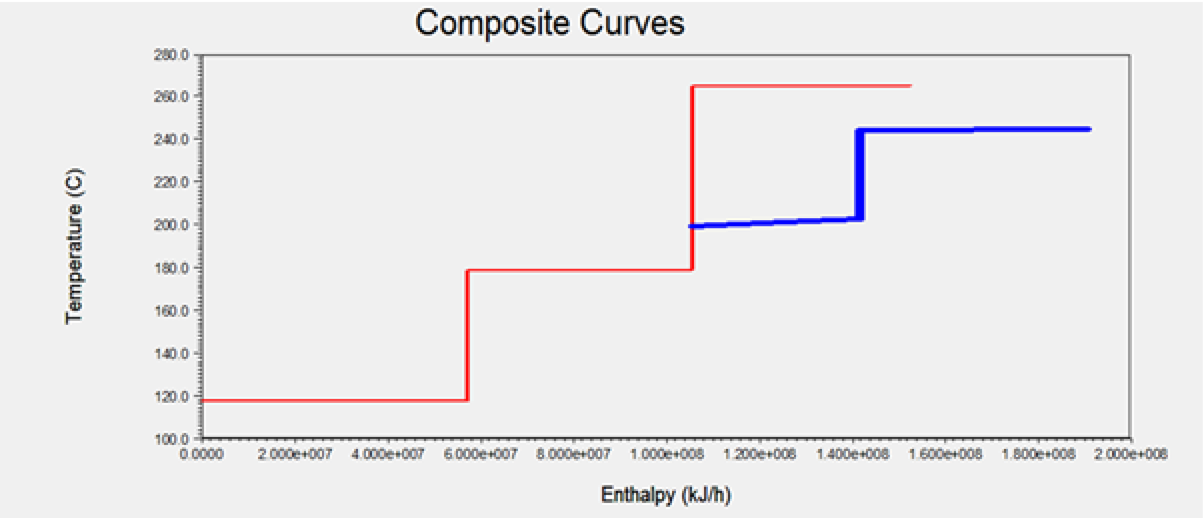

Figure 6. Composite Curve for Proposed Process

The amount of the current and target energy required for heating and cooling in both processes are tabulated in Tables 4 and 5.

By running pinch analysis, the total energy consumption of the conventional process reaches 190.9GJ/h with 59GJ/h heating utilities and 131.9GJ/h cooling utilities. The final heat exchanger arrangement is designed according to figure 7 based on pinch analysis. By comparing of Figure 3 with Figure 7, it is revealed that a heat exchanger (highlighted in dash-line oval) in Figure 7 is added to recover energy between two hot and cold process flows.

The same procedure is run for proposed process and the findings indicate the total consumption of energy is reduced to 143.87GJ/h while the heating and cooling utilities are 38.08 GJ/h and 105.8 GJ/h, respectively. The HEN for this proposed process is shown in Figure 8, whereas observed a new heat exchanger (highlighted in dash-line oval) in Figure 8 is added to recover the process stream's energy similar to the conventional process.

Table 4. Current and target energy consumption for conventional process

	Current [GJ/h]	Target [GJ/h]
HP Steam	47.51	43.37
Hot Oil	43.78	3.539
Total Hot Utilities	**91.29**	**46.91**
Air	75.03	75.03
LP Steam Generation	44.81	44.81
MP Steam Generation	35.26	0
HP Steam Generation	9.128	0
Total Cold Utilities	**164.2**	**119.8**

Table 5. Current and target energy consumption for proposed process

	Current [GJ/h]	Target [GJ/h]
Very High Temperature	84.85	0
HP Steam	0	36.11
Hot Oil	0	1.937
Total Hot Utilities	**84.85**	**38.05**
Air	57.3	57.3
LP Steam Generation	48.47	48.47
HP Steam Generation	46.8	0
Total Cold Utilities	**152.6**	**105.8**

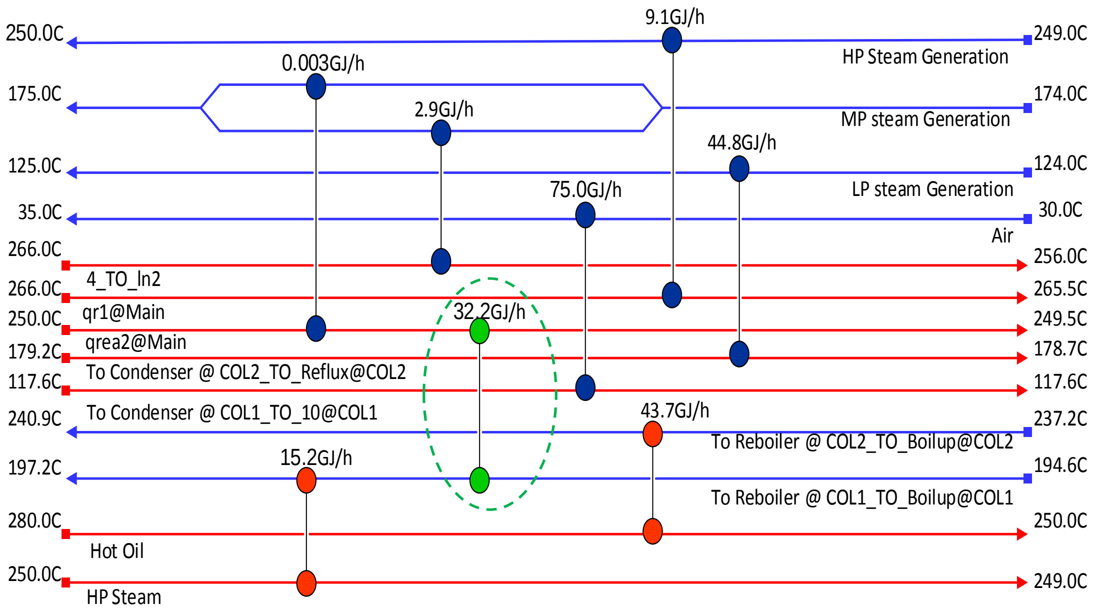

Figure 7. Grid diagram of heat exchanger network for the conventional process after pinch

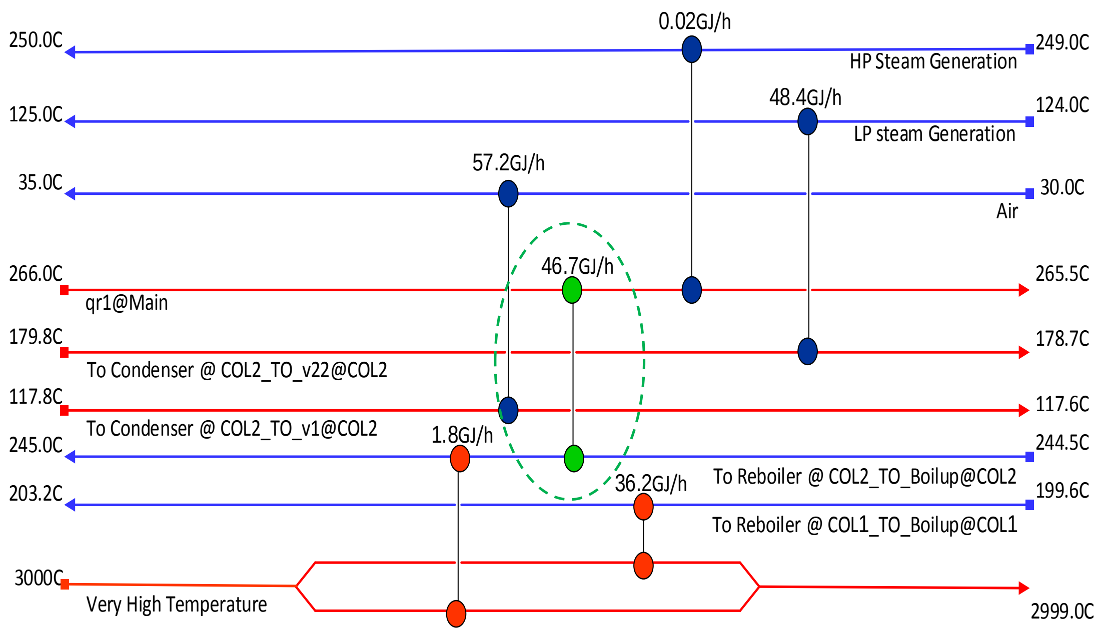

Figure 8. Grid diagram of heat exchanger network for the proposed process after pinch

3. Conclusion

A new process for ethyl benzene production was proposed and the arrangement of equipment was chosen to reduce both the utility consumption and equipment cost without any change in productivity and purity. This process was compared with the conventional process where energy consumption of this proposed process and the conventional process was obtained 237.5 GJ/h and 255.5 GJ/h, respectively. As observed, the proposed process is more energy-efficient than the conventional process without applying pinch technology.

To achieve higher energy recovery and lower energy consumption in both processes, HEN is improved by running pinch analysis, where the total energy consumption is reduced from 255.5 to 190.9GJ/hand from 237.5 to 143.87 GJ/h for the conventional and this process, with saving of 64.4 GJ/hand 93.63 GJ/h, respectively. The results indicate that the energy consumption of the proposed process is always lower than that of the conventional process (even before and after pinch analysis).

To improve this process, it is recommended to optimize the process operating conditions by applying an optimization algorithm (like DE, Genetic, ACO or other appropriate algorithms). Optimization of operating conditions can be highly contributive in operating costs.

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