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Reactor Rearrangement of an Industrial Ethylbenzene Production Unit

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Abstract: In this paper, an industrial ethylbenzene production unit and two new reactor arrangements have been simulated and the results were compared. In most petrochemical plants, ethylene as ethylbenzene production feed is produced at steam thermal cracking units. Almost ethylene is produced excess in these plants because of changing feed rate, feed type and or shut down of any other user unit of ethylene. So finding a new application for consuming excess ethylene in these plants without designing new units is important. In this study, two new reactor arrangements have been proposed. In the first scenario, the 3rd bed of transalkylator plays alkylator role instead of transalkylator and in the second scenario, all three beds were used as a parallel reactor with current alkylator reactors. The results show that ethylbenzene productivity rises 22% and 20% in scenarios 1 and 2, respectively, compared to a commercial industrial unit. Finally, one of the effective parameters in ethylbenzene unit is the ratio of ethylene to benzene in the feed of all beds of reactors, so it was selected as decision variable and ethylbenzene productivity as the objective function of an optimization problem. All cases were optimized and results show 43% ethylbenzene productivity improvement in an optimized version of scenario2 in compared other scenarios.

keywords: Ethylbenzene; Optimization;Alkylation; New arrangement; Productivity

1. Introduction

Ethylbenzene (EB) is one of the significant petrochemical components. This product is the primary feed of styrene production units which is an industrial monomer (Welch, Fallon, & Gelbke, 2000). Several methods can be used for producing EB. For example catalytic alkylation of benzene (BZ) with ethylene. The other method separation from mixed xylenes by isomer separation and catalytic isomerization, or from 1, 3-butadiene in a two-step process where the butadiene is converted to vinyl-cyclohexane which is then dehydrogenated. Industrially, EB produced by alkylation of benzene and ethylene.

Generally, the benzene alkylation process consists of the following three steps (Ganji and et al., 2004):

Alkylation step, in which benzene reacts with ethylene.

Transalkylation step, in which polyethylbenzenes in presence of benzene are converted to ethylbenzene on a reverse alkylation process.

Separation step, in which unreacted benzene, polyethylbenzenes, and other components are separated from each other and EB, is produced with high purity.

EB was first produced on a commercial scale in the 1930s by BASF company in Germany and by the Dow Chemical Company in the United States (Al-Mohsen, Bader Ali, Al-Faraj, Al-Ajmi, & Ali, 2007). Because EB production process is a catalytic process, the catalyst used in the industry is the zeolite MCM-22. The process is typically worked at a temperature of 150 to 5400C. But, the catalyst provides sufficient activity for the reaction to occur at temperatures below 370 0C. Liquid phase operation is preferred, giving a lower yield of polyethylene products. The use of the selected catalyst also results in a reduction of the xylene impurity level to values below 500 $\times 10^{-3}$ kg/m^3 (500 ppm) in the product (Chu, Landis, & Le, 1994). Also, earlier processes

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were based on liquid phase alkylation using an aluminum chloride catalyst but this route required disposal of aluminum chloride waste (Speight, 2017). Last technology for producing EB has been developed by Dow Chemical and Snamprogetti Company. This company has been developed a process for producing ethylbenzene/styrene from ethane and benzene in pilot scale("http://www.icis.com/resources/news/2007/11/02/9075695/ethylbenzene-eb-production-and-manufacturing-process," 2015). The process combines the dehydrogenation of ethane and EB in one unit and integrates the processes for preparing ethylene, ethylbenzene, and styrene. This process is claimed to have lower costs than the conventional route to styrene, largely stemming from the low cost of ethane in relation to ethylene.

Many researchers have been studied modeling and simulation of EB process unit (Huber & Stubbs, 2017; Husson et al., 2013; Koshkin, Ignatova, Ivashkina, & Dolganova, 2016; Li et al., 2011), kinetics of benzene alkylation of benzene (Atanda, Al-Yassir, & Al-Khattaf, 2011; Meng, Hu, Li, & Huang, 2016; Ye et al., 2017; Yuan et al., 2016), and catalyst synthesis of benzene alkylation (Gushchin et al., 2017; Kolesnikov et al., 2016; Y. Liu, Zou, Jiang, Gao, & Chen, 2017). Of all the work done, only a limited number focused on the EB process, improvement, optimization, and modification of industrial EB units. Ebrahimi and et al. (Ebrahimi, Sharak, Mousavi, Aghazadeh, & Soltani, 2011) simulated an industrial EB production unit and compared the results against five-day experimental data. Shenglin Liu and et al. (S. Liu et al., 2009) designed a novel industrial process was designed for the highly selective production of EB. It was comprised of a reactor vessel, vapor phase ethylene feed stream, benzene, and transalkylation feed stream. Yoon and et al. (2007) studied heat integration analysis of an industrial ethylbenzene plant using pinch analysis Ganji and et al. (2004) Modelled and Simulated of benzene alkylation process reactors for production of ethylbenzene. In Table 1, a summary of recent researches on the EB process (alkylation of BZ and ethylene) has been shown. Several researchers have been published papers in the field of EB reactor catalysts. Akhtar and et al. studied transalkylation of 1, 3, 5-triethylbenzene (TEB) with EB over ZSM-5 zeolite using a riser simulator reactor with respect to optimizing diethylbenzene (DEB) yield. Rodríguez et al. (2008) studied the transalkylation of DEB with benzene to produce EB in order to establish the effect of the reaction conditions, pressure, temperature and contact time, as well as the influence of media reaction phase, supercritical or subcritical on catalysts performance were studied. Wong and et al. (2013) worked on benzene alkylation with ethane into EB over a PtH-MFI bifunctional catalyst at six different temperatures between 290 and 490 °C was thoroughly studied.

In this study, three reactor arrangements for EB production have been considered:

1- Conventional and industrial route.

2- New proposed arrangement with 3rd bed transalkylator as alkylator.

3- New proposed arrangement with all beds of transalkylator as alkylator.

The simulation results were compared against operational data. The effects of arrangement changing on the production of EB were investigated. Finally, we also optimized the productivity of EB with considering that the EB selectivity and reactor inlet temperatures were kept constant. Only the decision variable in this optimization process was the ratio of ethylene to benzene in the inlet of reactor beds. Comparison of productivity of all scenarios at the optimal condition and real unit data showed the advantage of new proposed arrangements.

Table 1. Data sources used in simulation

Scope	Reference
Thermodynamic Analysis of Benzene Alkylation with Ethylene	(Khlebnikova, et al., 2015)
MCM-49 zeolite catalyst	(Gao, et al., 2015)
MCM-56 zeolite catalyst	(Zhang, et al., 2012)
Extractive distillation processes	(Jongmans, et al., 2012)
A novel catalyst for alkylation of benzene	(Faghihian and Mohammadi, 2012)
kinetic study of benzene alkylation	(Lukyanov and Vazhnova, 2008)
Coke burning behavior of a catalyst of ZSM-5/ZSM-11	(Song, et al., 2006)

2. Process Description

Hydrocarbon feed of the EB process are fresh benzene, recycled benzene, and ethylene. The fresh benzene and recycled benzene are mixed and preheated and fed to packed bed columns for dehumidification, which goes to the alkylator and the transalkylator reactors. At the top of the light removal column, light compounds such as methane and hydrogen are purged or sent to flare. Fresh benzene after heating and mixing with ethylene enters the first reactor (R-101) as alkylator. Ethylene is completely converted in this reactor. The outlet from the first reactor warms up the feed of the second reactor while cooling down and after mixing with ethylene enters the second reactor (R-102). In the alkylation process, unfavorable excess alkylation is also occurring and produces polyethylbenzenes (PEB). Selectivity is about 90% to EB and about 6% to PEB. Because the price of ethylene is higher than that of benzene and excess alkylation is reduced under excess benzene, the amount of the benzene feed is more than the amount required stoichiometric. Feed molar ratio of benzene to ethylene is about 6. The outlet from the second reactor is then sent to benzene tower in the separation unit. The benzene column recovers the unreacted benzene, which goes to the light removal column for purification. The bottom flow of the benzene column goes to the EB column purifying EB (Yoon, Lee, & Park, 2007). The top flow of the column has EB product and the bottom flow goes to the PEB column. The PEB column separates the PEB and other heavy compounds and the PEB goes to the transalkylator via PEB storage tanks. The reaction between polyethylbenzenes with BZ (Transalkylation) will be carried out in Transalkylation reactor (R-103). The feed to this reactor is a mixture of benzene stream taken from benzene tower and recycled PEB stream. This feed is first heated by reactor outlet stream and furnace before entering the reactor. The transalkylator produces EB by Transalkylation of PEB. Flux oil, the bottom product of the PEB column, is used as an energy source of heaters (Yoon et al., 2007). The outlet stream of the transalkylator reactor is then sent to benzene tower in the separation unit. In this industrial case, the target process adopts liquid phase alkylation process licensed by ABB Lummus which produces EB by alkylation of benzene and ethylene on the zeolite catalyst. Fig.1 shows a simplified process flow diagram of the EB production process. The process has two alkylators (R-101 & R-102), one transalkylator (R-103), and four columns (T-201 to T-204) for purification (UOP, 1991).

2.1. Ethylbenzene Production

The chemical reactions that take place in the EB unit reactors (R-101, R-102, and R-103) are described in this section. The reactions fall into two categories; those occurring in the two alkylation reactors (R-101 and R-102) and those occurring in the transalkylation reactor (R-103).

2.1.1. Alkylation Reactions

The alkylation reaction involves the combination of ethylene with benzene to form EB as shown in Equation (1). This reaction is activated by the zeolite catalysts. More than one molecule of ethylene can be bind to each benzene molecule, as can be seen in Equation (2). The acid function of the zeolite donates a proton to an ethylene molecule to form a highly reactive carbonium ion. This carbonium ion then produces an electron bond with the benzene molecule, releasing the proton for further reaction. Proton donors in decreasing strength are inorganic acids, Lewis acids, Bronsted acids, and zeolite catalysts(Yoon et al., 2007).

$$\mathrm{Et} + \mathrm{BZ} \leftrightarrow \mathrm{EB} \quad \Delta H_{298} = -1.054 \times 10^5 \frac{\mathrm{J}}{\mathrm{mol}} \tag{1}$$

$$\mathrm{EB} + \mathrm{Et} \leftrightarrow \mathrm{DEB} \quad \Delta H_{298} = -1.044 \times 10^5 \frac{\mathrm{J}}{\mathrm{mol}} \tag{2}$$

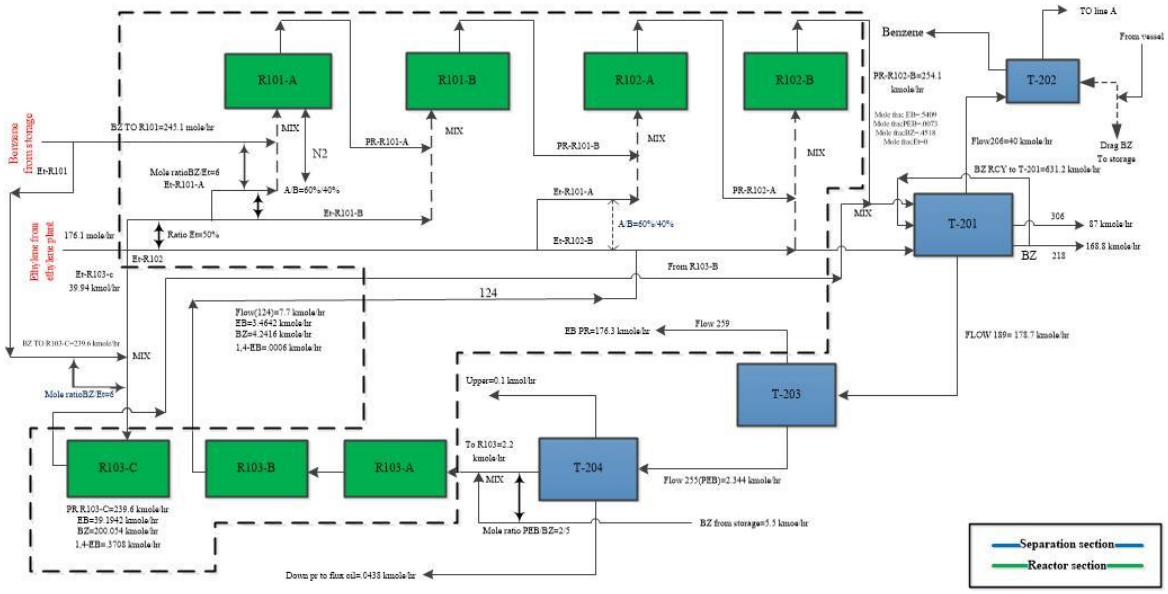


Figure 1. Block flow diagram of ethylbenzene unit

2.1.2. Transalkylation

In the transalkylation reactor, the PEB produced in the alkylation reactions is converted back to an equilibrium mixture with a higher concentration of EB. The Transalkylation reactions involve the transfer of ethyl groups from phenyl ring to another. For example, one benzene molecule reacts with a DEB molecule to produce two molecules of EB. Typical Transalkylation reactions are shown in Equation (3) and Equation (4). The equilibrium composition as a function of the phenyl-to-ethyl ratio is again illustrated in Fig.2. The reaction conditions are again chosen to result in the best equilibrium(UOP, 1991).

$$DEB + Et \rightarrow 2EB \quad \Delta H_{298} = -1.09 \times 10^3 \frac{J}{mol} \qquad (3)$$

$$TEB + Et \leftrightarrow 3EB \Delta H_{298} = -5.45 \times 10^3 \frac{J}{mol} \qquad (4)$$

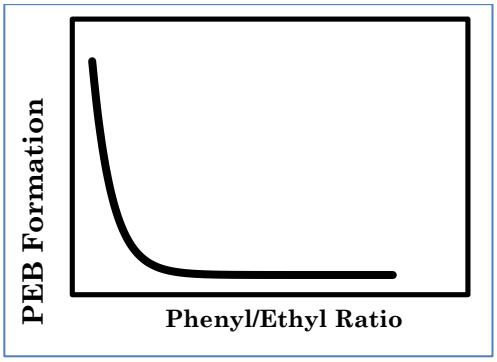


Figure 2. Distribution of PEB at various Phenyl/Ethyl Ratio [Operating Manual of EB Unit, UOP. 1991]

Regarding litterateur's data presented in Table 1, all the rate of alkylation and trasalkylation reactions of EB unit are shown in Table 2.

2.1.3. Side Reactions

Impurities which enter the reactor either with the benzene or ethylene charge may react to form compounds which contaminate the EB product and/or waste feedback to form byproducts that are listed below:

Propylene (C_3H_6); Acetylene (C_2H_2); Toluene (C_7H_8).

The side reactions are illustrated in Equation(5) to Equation(7)(UOP, 1991).

$$Popylene + benzene \rightarrow Cumene \qquad (5)$$

$$Acetylene + 2Benzene \rightarrow 1.1\ DPE + 1.2\ DPE \qquad (6)$$

$$Toluene + Ethylene \rightarrow Ethyltoluene \qquad (7)$$

After the reaction stage, the alkylator and transalkylator effluent streams are fractionated into recycle benzene, product EB; recycle PEB, and byproduct flux oil using three distillation columns in series. A fourth column, the Drag Benzene Column is used to remove small amounts of non-condensable, light non-aromatic compounds, and water from the benzene. In this study, all these reactions have been used.

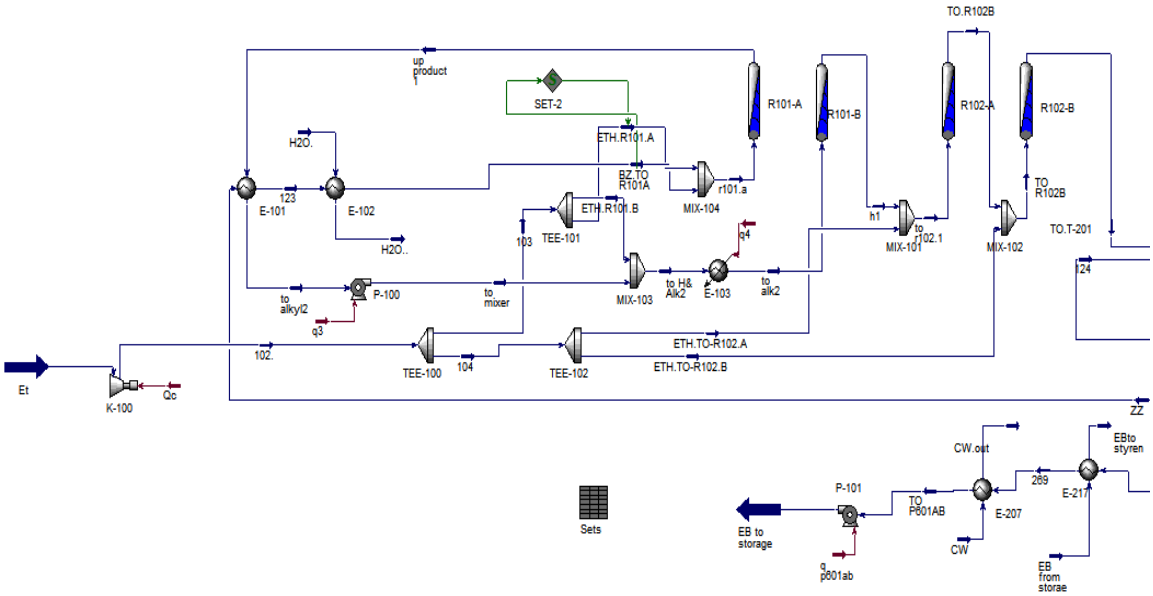
3. Results and Discussion

3.1. Simulation Procedure

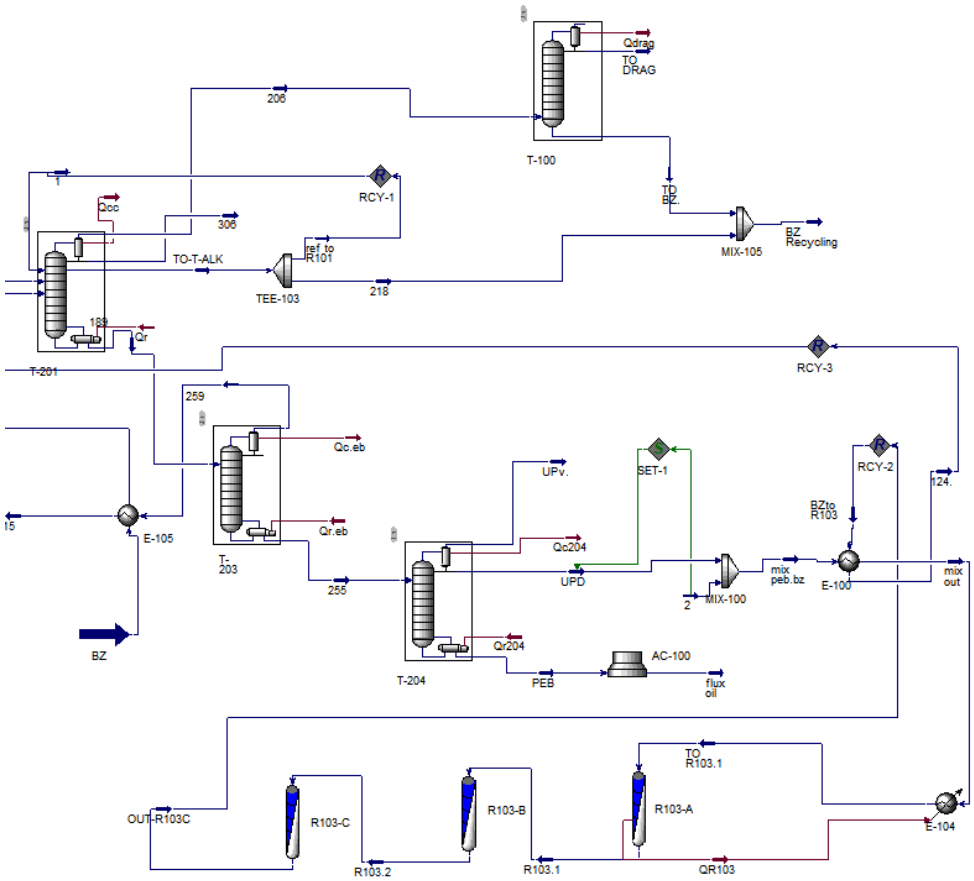
In this study, for comparison between the operating conditions of industrial EB unit, proposed new reactor arrangement and optimized operating condition of two scenarios, all EB units in various structures were simulated using Aspen HYSYS process simulator Simulation environment of EB unit in Aspen HYSYS simulatorV.7.3 is shown in Fig.3.

Table 2. Rate of alkylation and transalkylation reactions (Ebrahimi, et al., 2011)

Reaction No.	Rate equation	Unit
1	$r_1 = \frac{k_r . C_{Et}}{1 + k_{EB} C_{EB}}$, $k_r = 0.69 * 10^6 \exp\left(\frac{-6.434 * 10^4}{RT}\right)$	$\frac{\text{Kmol Bz}}{\text{kg. cat. hr}}$
2	$r_2 = 2.08 * 10^2 \exp\left(\frac{-4.7030 * 10^{-2}}{RT}\right) C_{EB}$	$\frac{\text{Kmol Bz}}{\text{kg. cat. hr}}$
3	$r_3 = 2.378 * 10^2 \exp\left(\frac{-6.128 * 10^4}{RT}\right) C_{DEB} C_{BZ}^{1.0218} \div (1 + 3 * 10^{-7} C_{BZ})$	$\frac{\text{Kmol Bz}}{\text{kg. cat. hr}}$
4	$r_4 = 2.434 * 10^2 \exp\left(\frac{-5.5077 * 10^4}{RT}\right) C_{TEB} C_{BZ}^{-1.0503} \div (1 + 1.76 * 10^{-5} C_{BZ})$	$\frac{\text{Kmol Bz}}{\text{kg. cat. hr}}$



(a)



(b)

Figure 3. Simulation environment of EB unit in Aspen HYSYS simulator (a & b)

For all cases input data of feed (temperature, pressure, and composition) except flow rate of feeds, reactors, and columns size are similar. Table 3 shows all data and specification of the EB unit, equipment.

Table 3. All data and specification of EB unit equipments

Reactors specifications			
Reactor Tag. name	**R-101**	**R-102**	**R-103**
Number of Beds	2	2	3
Bed Height (m)	5.15	5.15	5.58
Internal Diameter (m)	1.1	1.1	1.5
Beds Distance (m)	0.51	0.51	0.71
Weight of Catalyst ineach Bed (kg)	4370	4370	6042

Separation columns specifications				
Column Tag. name	**T-201**	**T-202**	**T-203**	**T-204**
No. of Trays	47	Packed	53	18
Tray type	Valve tray	Pull ring	Sieve tray	Sieve tray

Pure Ethylene feed data	
Temperature (^{0}C)	191
Pressure (Pa)	38×10^5
Pure Benzene feed data	
(Makeup)	
Temperature (^{0}C)	72
Pressure (Pa)	38×10^5

3.2. Simulation of Industrial EB Unit

Conventional industrial Block Flow Diagram (BFD) of EB reactor section has been shown in Fig. 4. This BFD is compatible with EB unit of Tabriz Petrochemical Company (TPC). According to this figure, first mixture of ethylene and benzene with the ratio of (1/6) entered to the 1st bed of R-101. The outlet of this bed after mixing with fresh ethylene is conducted to the 2nd bed of R-101. The outlet stream of R-101 has no ethylene because the ethylene conversion is 100% in this reactor. The unreacted benzene, EB, and PEB mixture after mixing with fresh ethylene are flown to the 1st bed of R-102. Similar to R-101, outlet of the 1st bed of R-102 after mixing fresh ethylene is entered to the 2nd bed of this reactor. It is noted that the ratio of ethylene to benzene is controlled at the input of the 1st bed of R-101,

but this ratio is not adjusted in R-102. But, the split ratios between ethylene to the 1st bed of R-101 to 2rd bed of R-101 and 1st bed of R-102 to 2rd bed of R-102 are considered. Normally, these ratios are (0.6:0.4). Another important ratio in this section is the split ratio of ethylene between R-101 and R-102. The value of this ratio is (0.5:0.5).

Output product of R-102 is sent to the fractionation section. Fractionation section consists of four distillation columns. Finally, EB as the main product is sent to the styrene unit and PEB as a byproduct is sent to R-103. In this reactor by occurring Transalkylation reactions, PEB with unreacted benzene is reacted and is produced impure EB. The output of this reactor is mixed with an output of R-102. This conventional industrial EB unit has been simulated in Aspen HYSYS software. All indicated streams data has been tabulated in Table 4.

If we focus on the results of the EB simulation unit, five highlight points could be seen:

1- The mole fraction of ethylene in the outlet of R-101 is zero. So, ethylene conversion in this reactor is 100%

2- The mole fraction of ethylene in the outlet of R-102 is zero too. So, ethylene conversion in this reactor is 100%

3- The mole composition of PEB in the inlet of R-103 is 8%.

4- The mole composition of PEB in the outlet of R-103 is zero. Therefore, all PB in R-103 was converted to EB.

5- The mole composition of BZ in the outlet of R-103 is not zero (1431 kg/hr.). Therefore, unreacted BZ has remained in the outlet of R-103.

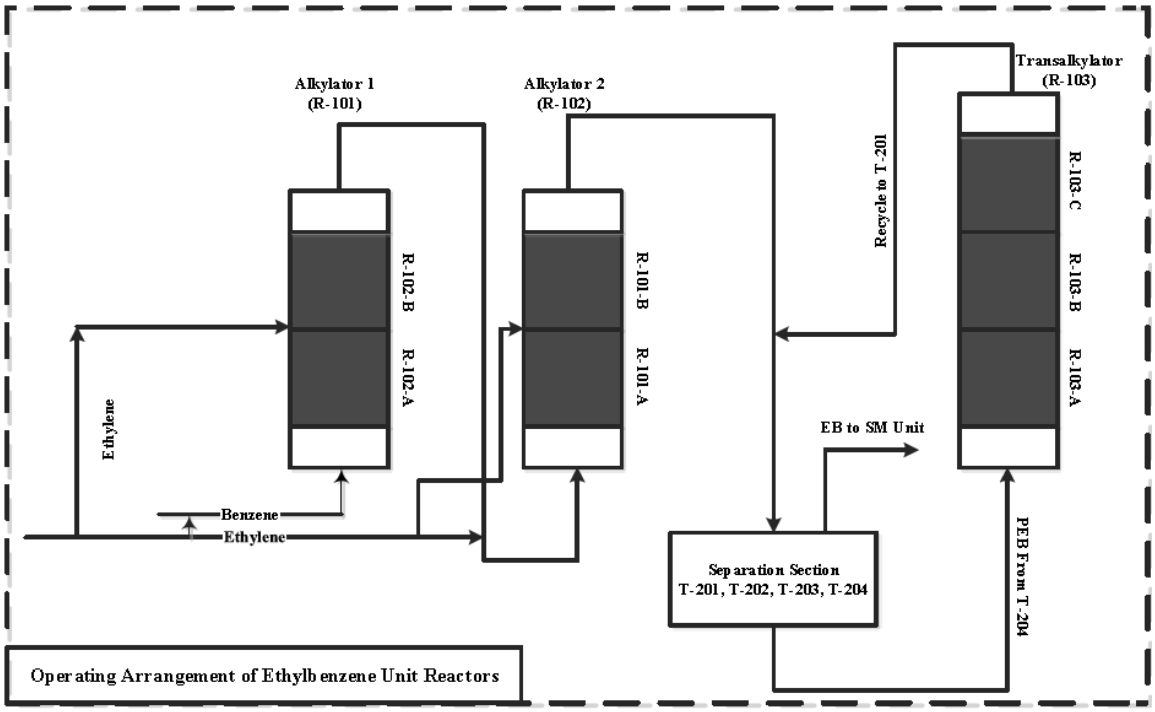


Figure 4. BFD of conventional reactor arrangement of EB unit

Table 5 shows detailed results of three bed of R-103. According to this Table, mole percent of PEB has been decreased from 8% to 0.9% value in the 1st bed of R-103. Also, this value has been decreased to 0.2%, that is very low value and we can ignore it. So, it is concluded that two bed is enough for converting PEB to EB and BZ product and the 3rd bed is inert in most times. This result has been observed and proved in industrial operation when bed catalysts of R-103 should be regenerated or changed. Experimental results showed that catalysts of 3rd bed were approximately fresh. Therefore, this bed can be used for other applications. In this study two applications have been proposed:

1- 3rd bed of R-103 is used as same as R-101 and R-102 (Scenario 1).

2- All three beds of R-103 were used as same as R-101 and R-102 (Scenario 2).

3.3. Simulation of Proposed Reactor Rearrangement of EB Unit (Scenario 1)

BFD of the new proposed arrangement of EB reactor section has been shown in Fig.5. In this arrangement, two streams from the main ethylene and benzene lines are separated and conducted to the 3rd bed of R-103. As mentioned in the previous section, remained unreacted BZ reacts with this injected ethylene and cause increasing EB production. Results of this rearrangement have been illustrated in Table 6.

Table 4. Simulation results for conventional industrial EB unit

Stream Name/Properties	BZ to 1rd bed of R-101	Et to 1rd bed of R-101	Et to 2rd bed of R-101	Et to 1rd bed of R-102	Outlet of R-101	Et to 2rd bed of R-102	Outlet of R-102	Inlet of R-103	Outlet of R-103
T (^0C)	219	191	191	191	270	191	333	225	275
P (Pa)	38×10^5	38×10^5	38×10^5	38×10^5	37.90×10^5	38×10^5	34.9×10^5	38×10^5	35×10^5
M.F. (kg/hr)	19079	1142	761	1142	20982	761	22886	1800	1800
Composition (mole %)									
Ethylene	0	100	100	100	0.0	100	0	0	0
Benzene	100	0	0	0	72.6	0	45	92	84.1
H_2O	0	0	0	0	0.0	0	0	0	0
Nitrogen	0	0	0	0	0.0	0	0	0	0
E-Benzene	0	0	0	0	27.0	0	54	1	15.9
124-E-BZ	0	0	0	0	0.0	0	0	0	0
14-EBenzene	0	0	0	0	0.4	0	1	8	0

Table 5. Simulation detailed results of R-103 for conventional industrial EB unit

Stream Name/Properties	Input of R-103	Output of 1rd bed of R-103	Output of 2rd bed of R-103	Output of 3rd bed of R-103
T (^0C)	225	279	277	275
P (Pa)	38×10^5	37×10^5	36×10^5	35×10^5
M.F. (kg/hr)	1800	1800	1800	1800
Composition (mole %)				
Ethylene	0	0.0	0.0	0.0
Benzene	92	85.0	84.2	**84.1**
H_2O	0	0.0	0.0	0.0
Nitrogen	0	0.0	0.0	0.0
E-Benzene	1	14.1	15.6	15.9
124-E-BZ	0	0.0	0.0	0.0
14-EBenzene	**8**	**0.9**	**0.2**	**0.0**

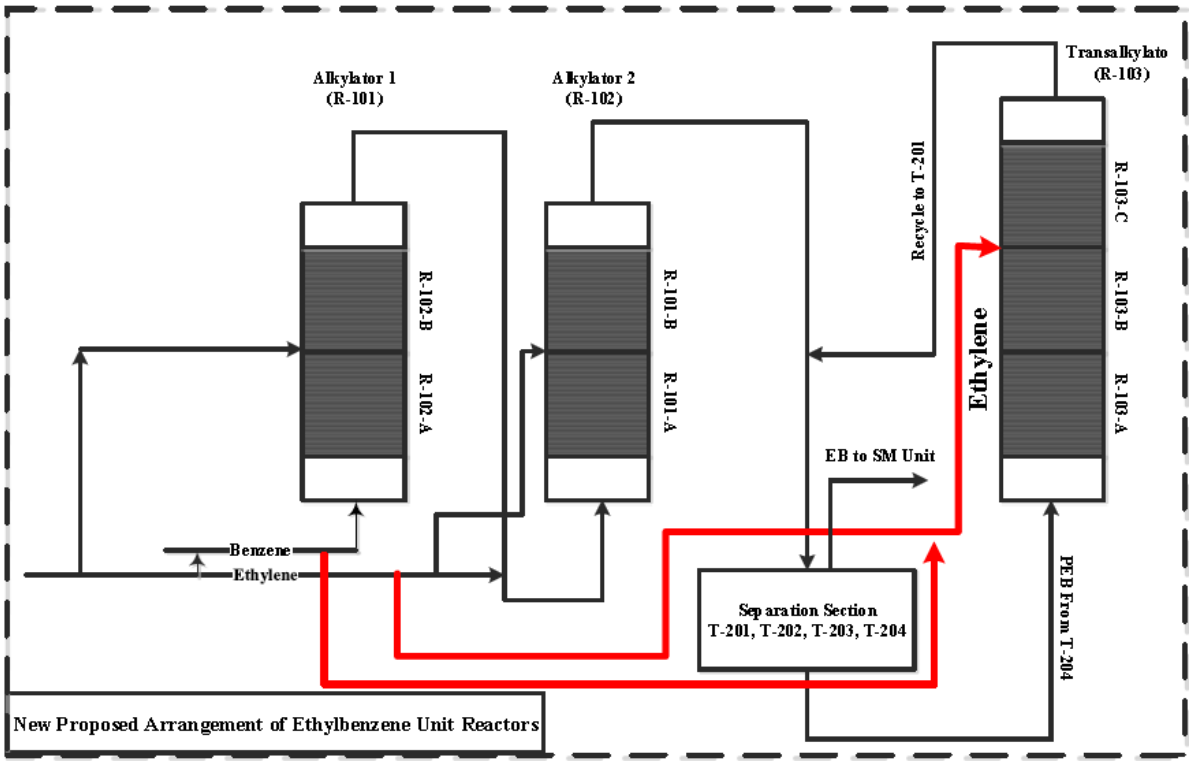


Figure 4. BFD of reactor arrangement for scenario 1 of EB unit

Table 6. Detailed simulation results of R-103 for scenario 1

Stream Name/Properties	Input of BZ to 3rd bed of R-103	Input of Et to 3rd bed of R-103	Output of 3rd bed of R-103 in new rearrangement
Temperature (^{0}C)	219	191	278
Pressure (Pa)	38×10^5	38×10^5	37×10^5
Mass flow (kg/hr)	18745	1122	19867
Composition (mole %)			
Ethylene	0	100	0.0
Benzene	100	0	83.5
H_2O	0	0	0.0
Nitrogen	0	0	0.0
E-Benzene	**0**	**0**	**16.4**
124-E-BZ	0	0	0.0
14-EBenzene	0	0	0.2

According to Table 5, 16.4% of mole fraction of output of 3rd bed of R-103 in the new arrangement will be EB. The mass flow of EB will be 4167 kg/hr. It is noted that by using this new proposed arrangement of reactor beds, the overall flow of output of R-103 will be fixed because the simulation results of conventional industrial EB unit (see the last column of Table 4) showed that 3rd bed has not the main role in Transalkylation reaction performance.

3.4. Simulation of proposed reactor rearrangement of EB unit (Scenario 2)

BFD of the new proposed arrangement of EB reactor section has been shown in Fig.6. In this scenario against the previous scenario, two streams from main ethylene and benzene lines

are separated and ethylene stream is divided into three lines; one to 1st bed, another one to 2nd bed, and last one is conducted to the 3rd bed of R-103. It means that R-103 does not play the role of the transalkylator reactor and similar to reactors R-101 and R-102 play role of alkylator reactor in a parallel position with R-101 and R-102. It is noted that in the most petrochemical plants, ethylene feed is produced in steam thermal cracking units. Sometimes ethylene is produced excess in these plants because of changing feed rate, feed type and or shut down of any other user unit of ethylene. In many cases, ethylene is used as fuel in burners but this work is not acceptable because ethylene is an expensive and valuable product. Hence, the authors proposed a new arrangement of reactors to consuming excess ethylene in EB unit by using transalkylator reactors as alkylator reactor. On the other hands, maybe this question is highlighted: which process will be done on PEB streams that exit from T-204? According to Table7 (5th column), the mass flow rate of the PEB stream to R-103 is about 2200 kg/hr. This value is very lower than the output of R-103 in the new arrangement (19867 kg/hr- 3rd columns). So, it is logical this PEB stream sent to a storage tank for a limited time and after decreasing ethylene productivity, R-103 return to the previous structure as a transalkylator reactor. Table 7 indicates simulation results of scenario 2.

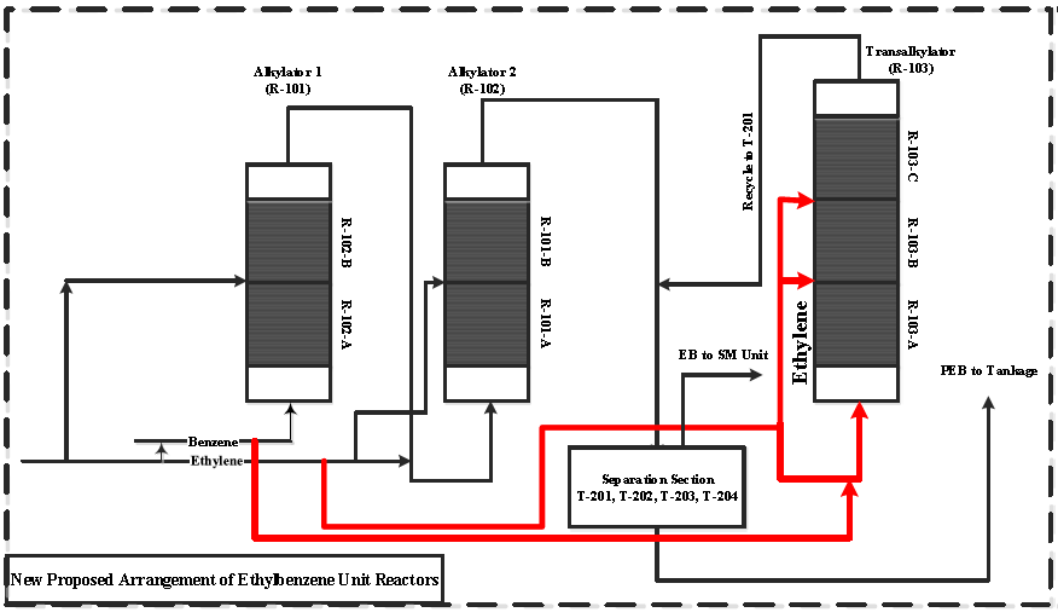


Figure 5. BFD of reactor arrangement for scenario 2 of EB unit"

Table 7. Detailed simulation results of R-103 for scenario 2

Stream Name/Properties	Input of BZ to R-103	Input of Et to R-103	Output of R-103 in new rearrangement	PEB to storage
Temperature (°C)	219	191	274	225
Pressure (Pa)	38×10^5	38×10^5	35×10^5	38×10^5
Mass flow (kg/hr)	18745	1122	19867	2200
Composition (mole %)				
Ethylene	0	100	0	0
Benzene	100	0	83	92
H_2O	0	0	0	0
Nitrogen	0	0	0	0
E-Benzene	0	0	16	1
124-E-BZ	0	0	0	0
14-EBenzene	0	0	0	8

Until now, the simulation results of the three scenarios have been reported. Summary of all cases results have been indicated in Table 8. Almost, the productivity of the main product is the most important index in selecting superior technology. As you have seen in Table 7, the conventional route has the lowest productivity between all routes. On the other hands, the new arrangement scenario 1 has the highest productivity. The productivity of scenario 1 is about 23% higher than the conventional model. It is noted that the purity of EB in all cases is acceptable. Therefore, it can be concluded that new proposed scenarios have been improved performance of EB unit with the remaining quality of products.

3.5. Optimization of all Reactor Arrangements

Several parameters affect the performance of EB units such as process pressure, reactor temperature, the residence time in the reactor, the number of column trays, feed tray number, and etc. But attention to this implies that simulation and optimization are required for an existing process. Therefore, the choice of parameters must be logical and feasible in the process. On the other hand, because the main objective is to optimize the increase in product production, therefore, the parameters containing the raw material flow or the flow intensity variables will be more important parameters. Since ethylene to benzene ratio in reactor section as an effective parameter in value of EB unit productivity has been selected for an optimization problem. As noted above, the ratio of ethylene to benzene is considered to be the only effective parameter for a variety of production process scenarios. Therefore, this optimization problem is converted to a single objective function (EB productivity) with a single decision variable (ratio of ethylene to benzene). So, this problem is sensitivity analysis problem and there is no need to use a particular optimization method. The most important innovation in the problem is to find the most productive product in the proposed new structures and in comparison with the existing industrial state.

Problem definition:

Objective Function: Maximization
EB Productivity (kg/hr.)
Decision Variable:
1<Ratio of ethylene to benzene [-] <6

In this section by changing and controlling of ethylene to benzene ratio in each section of reactors R-101, R-102, and R-103, optimized condition of EB unit will be calculated. As mentioned in the process description section, this ratio is about (1:6) in an operating state. But, in the operating state, only an inlet of the 1st bed of R-101 this ratio is adjusted. So, for optimization of all EB units, this ratio was adjusted for all beds of reactors (1st bed of R-101, the 2nd bed of R-101, the 1st bed of R-102, the 2nd bed of R-102, the 1st bed of R-103, the 2nd bed of R-103, and 3rd bed of R-103). Simulation results have been illustrated in Table 9.

Table 8. Results of all arrangements simulation

Scenario Name/Parameters	Et in (kg/hr)	BZ in (kg/hr)	EB out (kg/hr)	EB purity (%)	Et to BZ ratio	Productivity improvement (%)	Min. /Max. of productivity
Previous arrangement-Conventional scenario	3806	16247	14453	99.54	0.234	0	Min.
New arrangement-scenario 1	4948	23407	18707	99.83	0.211	22.77	Max.
New arrangement-scenario 2	4948	26950	17978	99.99	0.183	19.64	

Table 9. Results of all arrangements simulation

Scenario Name/Parameters	Et in (kg/hr)	BZ in (kg/hr)	EB out (kg/hr)	EB purity (%)	Et to BZ ratio	Productivity improvement (%)	Min. /Max. of productivity
Previous arrangement-Conventional scenario (Code#1)	3806	16247	14453	99.54	0.234	0	Min.
New Arrangement-Scenario 1(Code#2)	4948	23407	18707	99.83	0.211	22.77	
New Arrangement-Scenario 2(Code#3)	4948	26950	17978	99.99	0.183	19.64	
Optimized New Arrangement-Scenario 1 (Code#4)	5514	24461	20087	99.84	0.225	28.08	
Optimized New Arrangement-Scenario 2 (Code#5)	**7945**	**30387**	**29570**	**99.88**	**0.261**	**43.40**	**Max.**

Results showed that "Optimized New Arrangement-Scenario 2 (Code#5)" has an optimal case. The productivity of this optimized scenario is 29570 kg/hr. The productivity improvement was about 43.4% that was noticeable value. Fig.7 (A, B, C, and D) shows a comparison of all parameters between all simulated cases. Because, "Optimized New Arrangement-Scenario 2 (Code#5)" has the highest increasing productivity, therefore it seems logical rising of ethylene and benzene input mass flow7945 and 30387 kg/hr. respectively with increasing (52%) and (47%) to conventional industrial EB process.

4. Conclusion

In this work, an industrial EB production unit and two proposed arrangement of reactors have been simulated. The following conclusion could be listed below:

- In the new proposed scenario-1, EB productivity rise22%compared to the operating state.
- In the new proposed scenario-2, EB productivity rise20%compared to the operating state.
- In the new optimized proposed scenario-1, EB productivity rise28%compared to the operating state.
- In the new optimized proposed scenario-2, EB productivity rise43%compared to the operating state.
- In all cases, the purity of EB in the final product is greater than 99.5% and it is an acceptable value.

According to simulation results, in all new proposed reactor arrangements, EB productivity as the main parameter in the performance of EB unit has been increased. Between all simulated cases, "Optimized New Arrangement-Scenario 2 (Code#5)" has the highest increasing productivity, it seems logical rising of ethylene and benzene input mass flow7945 and 30387 kg/hr. respectively with increasing (52%) and (47%) to conventional industrial EB process.

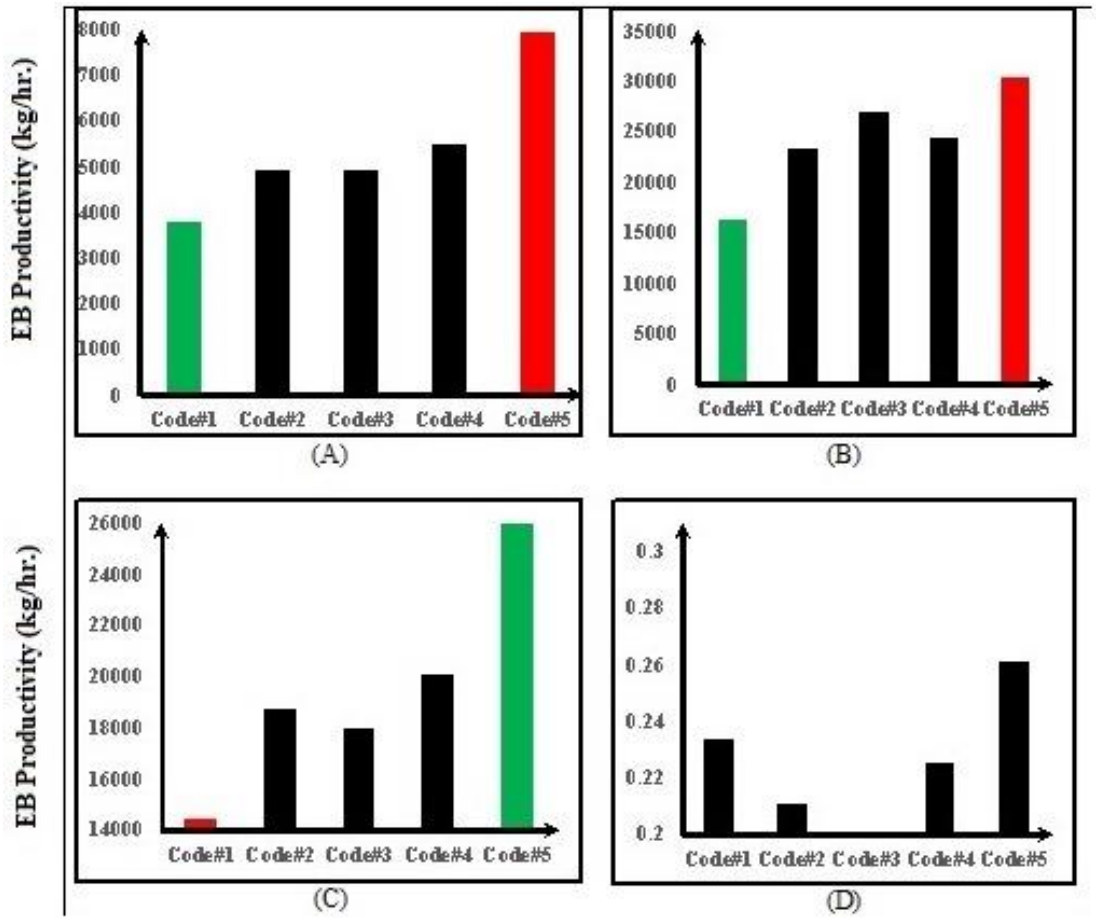


Figure 6. EB Productivity (kg/hr) comparison of various parameters between several arrangement scenarios; A:Ethylene consumption; B: Benzene consumption; C: Ethylbenzene production; D: Ratio of ethylene to benzene

Nomenclature

Abbreviations

ABS	Acrylonitrile Butadiene Styrene
BASF	BadischeAnilin und Sodafabrik
Benzene	BZ
BFD	Block Flow Diagram
DEB	diethylbenzene
EB	Ethylbenzene
HPS	High pressure steam
LLPS	Low-low pressure steam
Max.	Maximum
Min.	Minimum
PEB	Polyethylbenzenes
ppm	Part per million
-R-	Reactor
SBL	Styrene Butadiene Latex
SBR	Styrene Butadiene Rubber
S-DVB	Styrene-divinyl-Benzene
S-EB-S	Styrene-Ethylene/Butylene-Styrene
SIS	Styrene-isoprene-Styrene
-T-	Tower
TEB	triethylbenzene
Wt	Weight percent

Symbols

M.F.	Mass flow	kg/hr
P	Pressure	Pa
r_i	Kinetic rate	$\frac{\text{Kmol component i}}{\text{kg. cat. hr}}$
T	Temperature	^{0}C

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