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Application of GA in Optimization of Modified Benzene Alkylation Process

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Abstract
A genetic algorithm is used to optimize the modified benzene alkylation process. Based on the previous studies, the modified process increases ethylbenzene selectivity and decreases energy consumption at the same time. The inlet ethylene flow rate of each alkylation reactor is optimized in order to reduce the chance of transalkylation reactions but increase ethylbenzene selectivity. The byproduct trans-ethylbenzene concentration is used as the fitness variable in the optimization process to confine undesired reactions throughout the process. The obtained optimal values of ethylene flow rate for the adiabatic reactors are 3.50, 2.94, 2.58, and 0.36 m3/hr. The ethylbenzene selectivity has been increased by applying the optimized values indicating the current unit is not operating under optimal conditions. Temperature profile within the alkylation reactors and temperature and concentration profiles through the towers of the fraction unit under the optimized conditions of the modified process are also presented.
Key words: Genetic Algorithm, Optimization, Modified Process, Temperature Profile, Ethylbenzene

Introduction
The alkylation of aromatic hydrocarbons with olefins is applied on a large scale in the chemical industry [1]. Benzene alkylation is one of the most important processes for ethylbenzene (EB) production. The production of EB in 2010 was about 34 million metric tons [2]. EB is an important raw material in the petrochemical industry for the manufacture of styrene. Styrene monomer is used in the production of synthetic rubber, synthetic plastics, and resins. Also, EB has a limited use as a solvent in the production of dyes [3].
Several alkylation processes have been proposed to enhance the benzene alkylation processes [4-7]. Degnan et al. provided an overview of various industrial alkylation processes for the production of EB and cumene [1]. They proposed that zeolite catalysts have begun to displace the conventional aluminum chloride and solid phosphoric acid.
The effects of operational parameters and process variables have been investigated by many researchers. For instance, the effects of temperature and feed composition on the catalytic activity and product distributions were studied by Li et al. [5]. Craciun et al. proposed a liquid phase alkylation of benzene over three USY zeolites [8]. They showed that the alkylation rate will increase when the average acid strength is higher. Cavani et al. investigated the effects of temperature, contact time, and feed composition on the catalytic performance of transalkylation of diethylbenzene with benzene [9]. Sharanappa et al. studied the selective alkylation and disproportionation of EB in the presence of other aromatics [10]. Xu et al. developed a composite catalyst of ZSM-5/ZSM-11 co-crystallized zeolite for the alkylation of dilute ethylene with benzene in EB production [11]. Al-Kinany et al. have shown that trifluoromethanesulfonic (triflic) acid could be used for the transalkylation of o-diethylbenzene with benzene to EB at low temperatures and atmospheric pressure [12]. Many other attempts have been made to study the effects of operational parameters on alkylation process [13-16].
In this paper, a genetic algorithm is used to optimize the inlet ethylene flow rate in a modified EB production process. The concentration of the produced trans-ethylbenzene is considered as the objective variable to regulate the flow rate and confine the undesired reactions. The temperature and concentration profiles through the towers of the fraction unit are presented. Also, ethylene selectivity increased when the first three alkylation re actors

where kept at their maximum allowable temperature.

Production Process Description

The simulated EB production unit is an industrial working unit. The unit provides the needed EB for the juxtaposed styrene monomer unit. In this commercial process, the alkylation reactors are designed for the 100% conversion of ethylene. EB synthesis could be done based on the following alkylation reaction:

$$C_6H_6 + C_2H_4 \rightarrow C_6H_5{-}C_2H_5,\ \Delta H^{\circ}_{298} = -114\ \frac{kJ}{mol} \qquad (1)$$

A complete benzene alkylation could be occurring under the atmospheric pressure and at a temperature of 500 °C [17]. However, side reactions, especially successive alkylation, cause trans-ethylbenzene production. Due to these restrictions, the industrial alkylation processes should be done in a catalytic bed and at low temperatures.

Figure 1 shows a simple diagram of the EB production process in a real working unit. As it can be seen from Figure 1, the process encompasses three packed bed adiabatic reactors in series. The first two reactors (R-1 and R-2) both have two Y type zeolite packed beds used as catalysts for the alkylation of benzene. The third reactor (R-3) with three packed beds is used for the transalkylation processes.

The fraction unit has four towers. The first one is the benzene column, (T-1), which is used for the separation of benzene from EB. There is a benzene drag tower, (T-2), for the treatment of benzene from undesired lighter products. EB is taken out from the third tower, (T-3), where EB is separated from trans-ethylbenzene and other undesired heavier products. In the last tower, (T-4), trans-ethylbenzene is separated from the flux oil products and recycled to the transalkylation reactor for EB production.

The input ethylene is ramified into four streams and each is fed to the each bed of R-1 and R-2. The R-1 outlet stream is cooled down to the R-2 feed temperature in a heat exchanger (E-1). The input benzene is a mixture of fresh benzene and the recycled stream from the T-1 in the fraction unit. The ratio of the recycled benzene to the benzene required for a stoichiometric alkylation is 6:1. The excess benzene helps regulate the temperature and reduce the transalkylation reactions.

Rate expressions are vital for the simulation, analysis, and design of chemical reactors. Therefore, they should be carefully selected for an accurate simulation. Reactions 1-3 and Equations 4-5 are the main reactions and reaction rates in the alkylation of benzene with ethylene [18].

$$C_6H_5C_2H_5 + C_2H_4 \rightarrow C_2H_5\text{-}C_6H_4\text{-}C_2H_5 \qquad (2)$$

$$C_2H_5\text{-}C_6H_4\text{-}C_2H_5 + C_2H_4 \rightarrow C_2H_5\text{-}\underset{\displaystyle C_2H_5}{\overset{\displaystyle C_6H_4}{\overset{|}{\underset{|}{}}}}\text{-}C_2H_5 \qquad (3)$$

$$r_1 = \frac{k_r.C_{Et}}{1 + k_{EB}C_{EB}}$$

$$k_r = 0.69\times10^{6}\exp\left(\frac{-6.344\times10^{4}}{RT}\right) \qquad (4)$$

$$k_{EB} = -1.5202\times10^{-2}\exp\left(\frac{-3.933\times10^{3}}{RT}\right)$$

$$r_2 = 2.80\times10^{2}\exp\left(\frac{-4.7030\times10^{4}}{RT}\right)C_{EB}.C_{ET} \qquad (5)$$

where, r_1 and r_2 are the rates of reactions 1 and 2 respectively. k_r is the rate constant and k_{EB} is the adsorption coefficient for EB. R, T, C_{Et}, and C_{EB} are the ideal gas constant, temperature, and ethylene and EB concentrations respectively. It must be mentioned that the amount of produced three-EB is negligible, so the reaction rate for Equation 3 is overlooked.

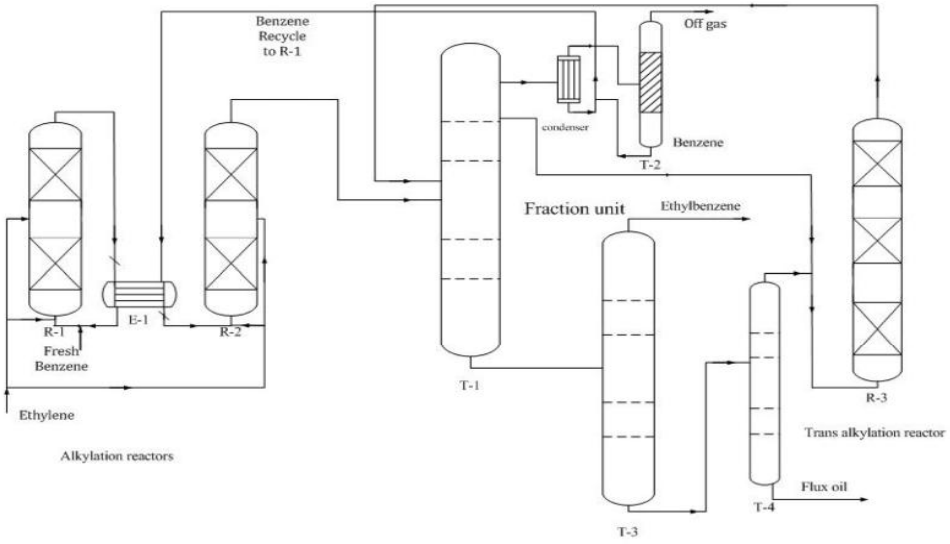

Figure 1- A simple schematic diagram of the EB production process in the real working unit

R-2 outlet stream is sent to T-1 in the fraction unit. The transalkylation reactions are carried out in R-3. A mixture of benzene stream, which is taken out from T-1 and trans-ethylbenzene flow from T-4, is fed to R-3 for the transalkylation reactions purpose. The R-3 outlet stream is then sent to T-1 in the fraction unit. Equations 6 and 7 are the main transalkylation reactions and the relevant rate expression [17].

$$C_2H_5 - C_6H_4 - C_2H_5 + C_6H_6 \rightarrow 2C_6H_5 - C_2H_5 \quad (6)$$

$$r_3 = \frac{2.378\times10^2 \exp(\frac{-6.128\times10^{24}}{RT}) C_{DEB} C_{BZ}^{1.0218}}{1+3\times10^6 C_{BZ}} \quad (7)$$

where, r_3 is the rate of Reaction 6 and C_{BZ} and C_{DEB} are the EB and DEB concentrations respectively.

Optimization

Recently, we have proposed a modified benzene alkylation process to reduce the total energy consumption [13]. The modified process is shown in Figure 2.

In this study, the genetic algorithm is applied to reduce the transalkylation reactions by the simultaneous regulation of ethylene flow rate to each backed bed.

Genetic Algorithm

Inspired by Darwin's theory of survival of the fittest, Genetic Algorithm (GA) was developed to find the approximate solution to optimization and search problems as a global search technique [18].

In genetic algorithm, an initial set of random candidate solutions called population is postulated in the beginning. Each individual in the population, which is called a chromosome, is a set consisting of various segments or genotypes.

A so called fitness function evaluates the fitness of chromosomes at each generation. Different chromosomes are sorted based on their fitness values. Now for the generation of offspring, two chromosomes from a set of chromosomes (called mating pool) are chosen. The higher fitness of chromosome, the better chance of selection for that chromosome. This assures that chromosomes with better fitness value have priority to participate in the creation of offspring [19]. Using crossover and/or mutation operators, two selected chromosomes produce two new offsprings.

Exchanging information between parent chromosomes to create two new chromosomes is the basis for crossover operator, while making random changes on the selected genes of each newly obtained chromosome is done by mutation operator [20].

Results and Discussion

The goal of any optimization problem is to either maximize or minimize the objective function. In GA, a particular type of objective function called fitness variable is used. Fitness variable quantifies the optimality of a solution (chromosome). Since in GA better chromosomes should have a higher chance in creating offspring, sorting out all chromosomes based on the fitness variable is an important step in optimization. In this paper, the fitness variable is the concentration of the by-product trans-ethylbenzene. This concentration should be kept as minimum as possible throughout the process. Table 1 shows GA parameters used in this study.

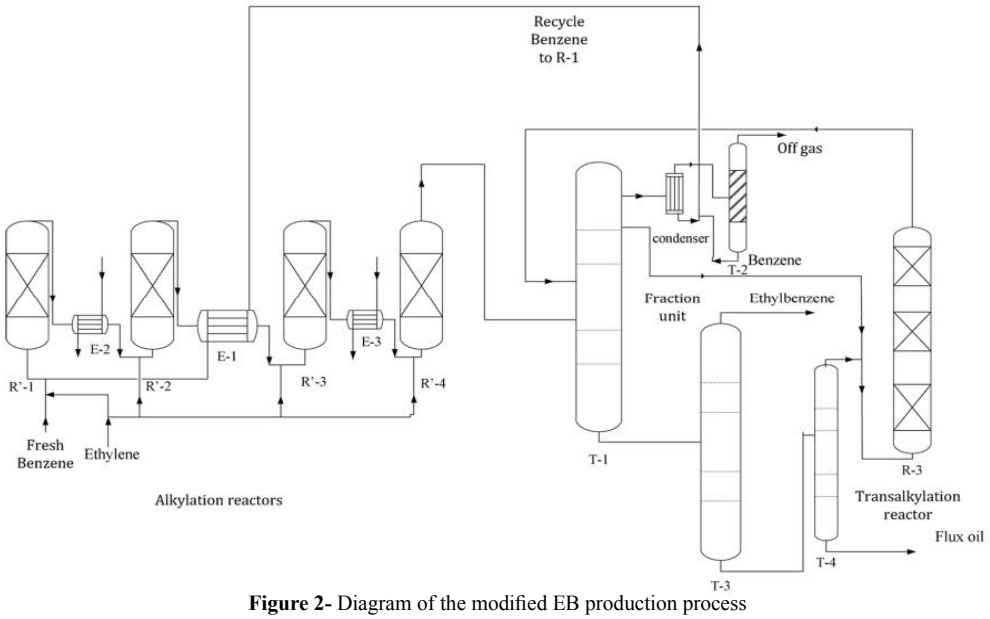

Figure 2- Diagram of the modified EB production process

Table 1- Applied GA parameters

Population	Max No of Generations	Crossover Type	Crossover Rate	Mutation Rate	Hybrid
50	100	Scattered	0.70	0.04	Pattern search

The inlet ethylene flow rate to each alkylation reactor in the modified process is used as a decision variable in order to reduce the transalkylation reactions and increase EB selectivity. Figure 3 illustrates fitness values for all generations.

As it can be seen from Figure 3, the mean fitness value reaches a steady state condition after 9 iterations. However, the best fitness remains constant after the fourth generation. The oscillations in the mean fitness curve are caused by the mutation parameter.

As it was mentioned before, the inlet ethylene flow rates are used as decision variables to minimize the trans-ethylbenzene production and increase EB selectivity. The operational and optimal ethylene flow rates for each alkylation reactor are presented in Table 2.

The operational ethylene flow rates are constant for the first pair of the alkylation reactors. However, the optimal ethylene flow rates decrease monotonically through reactors. Since there is no EB in the inlet stream of first reactor, there is no chance for transalkylation reactions and as a result, the maximum ethylene flow rate is assigned to R-1. Table 3 compares the output compositions of the optimal conditions of the modified process results with those obtained from the simulation of the modified process.

As it can be seen from Table 3, under the optimal conditions of the modified process, there is a considerable reduction in the trans-ethylbenzene production while the EB concentration increases a little bit. As a result, EB selectivity increases when GA is applied for the optimization. Temperature profile within the alkylation reactors under the optimal conditions of the modified process are demonstrated in Figure 4.

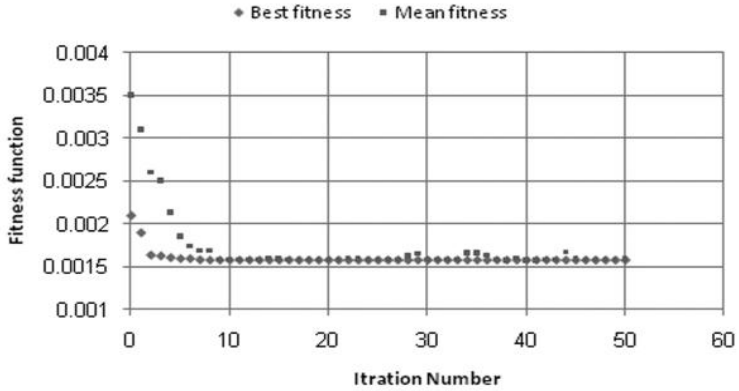

Figure 3- Best and mean fitness values for all generations

Table 2- Operational and optimal value of ethylene flow rate (m^3/hr)

.Reactor No	Operational Value	Optimal Value
R-1	2.81	3.50
R-2	2.81	2.94
R-3	1.87	2.58
R-4	1.87	0.36

Table 3- Comparison between the outlet compositions of the modified process and its optimal conditions

Component	Modified process (mole fraction %)	Optimal conditions (mole fraction %)
Trans-ethylbenzene	0.326	0.151
EB	34.243	34.563

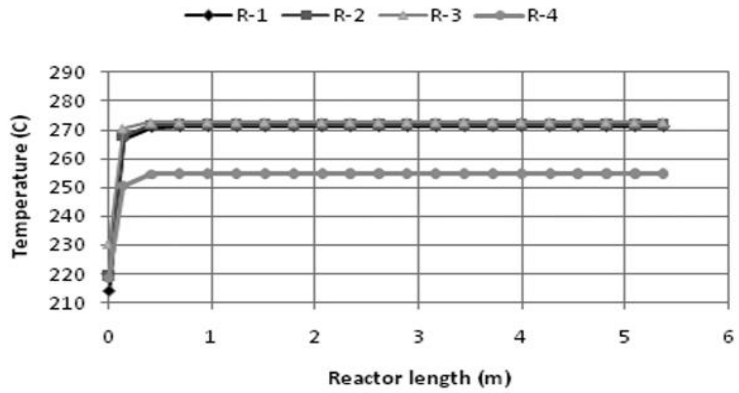

Figure 4- Temperature profile through the alkylation reactors under the optimal conditions of the modified process

The desired operational temperature range for the alkylation reactors in the real unit is 250–270 °C. Since alkylation reactions are exothermic, temperature rise increases EB selectivity [13]. The final temperatures are still within the desirable operational ranges. As it can be seen from Figure 4, the first three alkylation reactors are working at their maximum allowable temperature. However, since the ethylene flow rate for the last alkylation reactor is low, the reactor temperature reaches the maximum value at 255 °C. The temperature and concentration profiles through the towers of the fraction unit are shown in Figures 5 and 6 respectively.

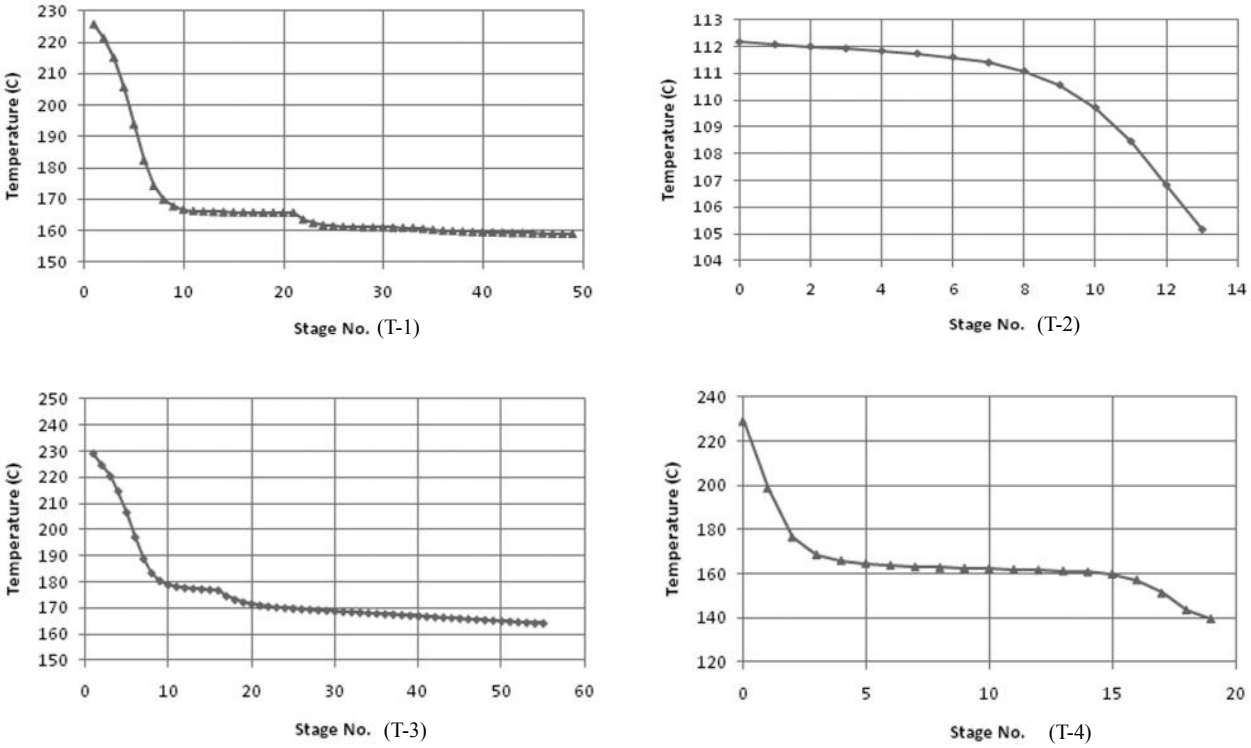

Figure 5- Temperature profile through the towers of the fraction unit under the optimal conditions of the modified process

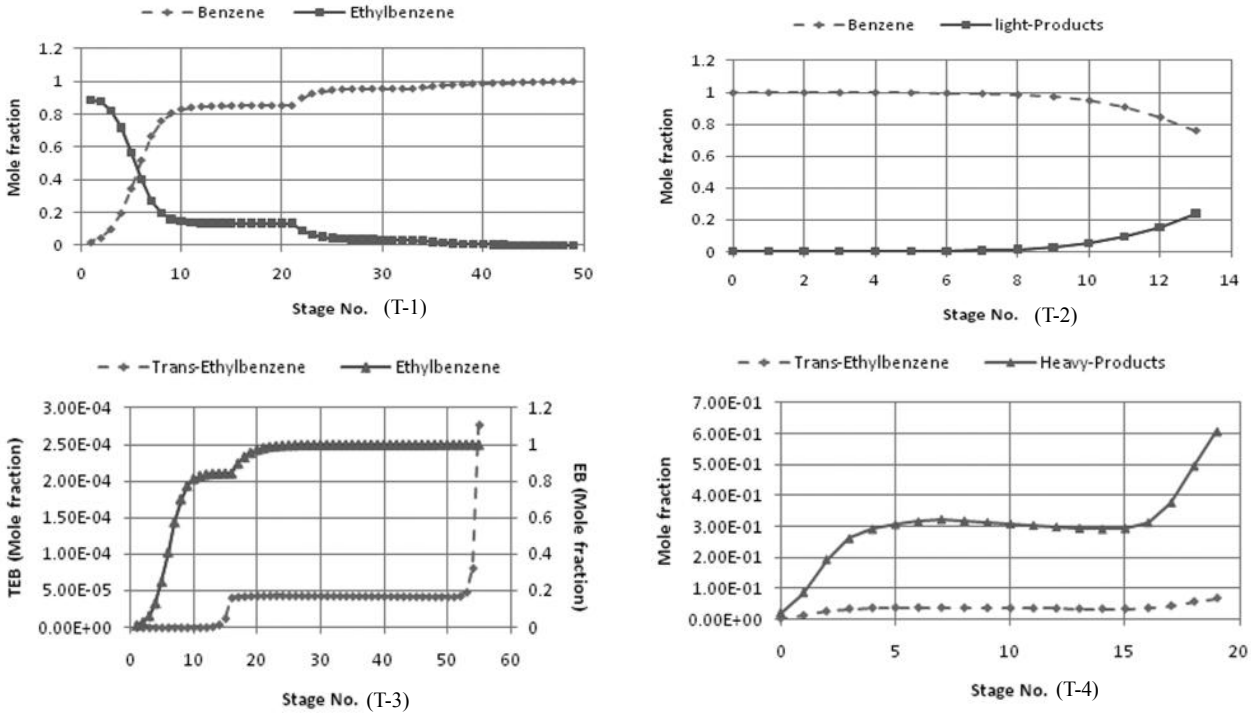

Figure 6- Concentration profile through the towers of the fraction unit under the optimal conditions of the modified process

As mentioned before, the fraction unit has four towers. T-1 is used for the separation of benzene from EB. It has 49 equilibrium stages beside reboiler and condenser. It must be mentioned that the trays are numbered from bottom to top. The main feed stream with the temperature of 258 °C enters tray 21 and increases the benzene concentration (see Figure 6-a). The temperature curve shows a sharp increase at the bottom of the tower where reboiler is located (Figure 5-a). The temperature profile within the benzene drag tower is plotted in Figure 5-b. The tower has 13 trays and since there is no reboiler, mass transfer causes a smooth temperature change at the top of column. Benzene is completely separated from the lighter products at the bottom of tower (Figure 6-b).

The separation of EB from trans-ethylbenzene is done in T-3 with 55 equilibrium stages. Temperature profile and concentration variation of T-3 are shown in Figures 5-c and 6-c respectively. Temperature profile has a sharp trend in the vicinity of reboiler while there is a constant temperature decrease for the remaining trays. Also, the feed stream of the third tower, with a temperature of 234 °C, enters at 16th tray causing an oscillation in both temperature and concentration profiles.

In the last tower, trans-ethylbenzene is separated from the flux oil products and is recycled to the transalkylation reactor for EB production. As it can be seen from Figure 5-d, the temperature profile is sharpened when it reaches the vicinity of reboiler or condenser. However, mass transfer and heat of mixing are the major factors for the heat transfer in the middle of tower where temperature profile is smooth (Figure 6-b).

Conclusion

In this paper, GA is used to obtain the optimal values of the ethylene flow rate to increase EB selectivity in a modified EB production process. The desired operational temperature range for the alkylation reactors is 250–270 °C. It is found that EB selectivity could reach its maximum value when the first three alkylation reactors work at their maximum allowable temperature and the ethylene flow rates for the adiabatic reactors are fixed at the values of 3.50, 2.94, 2.58, and 0.36 m^3/hr for reactors 1-4 respectively. The EB selectivity increases by applying the optimal values indicating current unit is not working under the optimal conditions. The temperature profiles within the alkylation reactors show a sharp increase due to being in contact with fresh catalyst at the beginning of each reactor. Also, temperature and concentration profiles through the towers of the fraction unit under the optimal conditions of the modified process are presented.

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