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Modeling of Benzene with Ethylene Alkylation

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***Abstract*—The paper considers the benzene alkylation with ethylene model development with the use of zeolite catalyst. A list of reactions occurring in the alkylation reactor was made and the thermodynamic possibility of determination of these reactions by the change of Gibbs energy was defined. The paper presents the hydrocarbons transformation scheme, which includes the grouping of components on the basis of their reactivity and the degrees of compensation values of the corresponding reactions. Drawing on the obtained data the authors developed the kinetic model of the alkylation of benzene with ethylene.**

***Index Terms*—Alkylation, degree of compensation, modeling, zeolites.**

I. INTRODUCTION

Since the 70s of the last century it became possible to produce ethylbenzene with the use of heterogeneous zeolite catalyst on a commercial scale. Heterogeneous catalytic process gradually started to replace the old homogeneous catalytic technology. Nowadays most of the existing ethylbenzene production plants operate using the zeolite catalyst [1], [2]. According to the data of 2014 total world ethylbenzene production capacity is around 37 millions tons per year [3].

Technology of ethylbenzene production includes the stages of alkylation and transalkylation. The control of technological parameters such as benzene-to-ethylene ratio in the feed and temperature lets to conduct the process under the optimum conditions and monitor the output of ethylbenzene [4], [5].

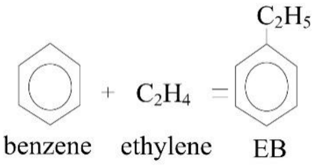
Although the technology developers provide their recommendations on the values of these parameters, the development of the model of ethylbenzene synthesis process and its subsequent modeling aimed at the increase of the resource and energy efficiency of the production plant is one of the most feasible ways of customization of the process to particular cases [6].

II. OBJECT OF THE RESEARCH

The ethylbenzene technology is developed for ethylbenzene production with the use of the liquid phase and zeolite catalyst.

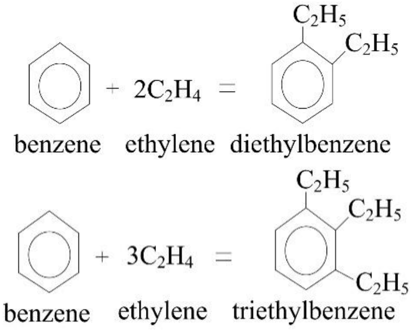
The industrial plant operates continuously and uses 2 different reactors for alkylation and transalkyation.

In alkylation reactor ethylene in its liquid phase goes through almost a complete reaction accompanied by the excess of benzene, which is necessary to form ethylbenzene (EB):



The process takes place at T = 220 - 255 ℃ and P=3.4 MPa. This reaction is exothermic, which leads to gradual temperature increase from one catalyst bed to the following one. This is the reason why alkylation reactors are typically equipped with intermediate coolers for keeping the total temperature rise.

Then ethylbenzene converts to produce small amounts of polyethylbenzenes (PEB):



These reactions are the main side ones and generate considerable quantities of heat being exothermic ones.

PEB are separated from ethylbenzene and then converted to EB in the transalkyation reactor at T = 190 - 220 ℃ and P = 3 - 3.5 MPa.

By now the chemistry of ethylbenzene synthesis is quite well understood [7], [8]. In addition to the main reactions leading to ethylbenzene formation it's known a number of side reactions. Altogether these reactions are a challenging task from the perspective of mathematical description and its subsequent use. Representation and adequacy of a mathematical model and its ability to be approximate enough to the real data depend on reaction scheme of the model. This scheme should be quite simple, but at the same time accurate enough to describe the process [9].

III. MODEL DEVELOPMENT

Reactions that occur in alkylation and transalkyation processes and that are based on different types of the zeolite catalyst were investigated by certain authors [10]-[12]. However, alkylation and transalkyation have different

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conversion processes schemes, and at the same time they have quite much in common. So the main task is to determine the pathway of the development of secondary reactions: transalkyation, disproportionation, dealkylation, cracking and other ones, the result of which is the formation of by-products. Some steps were taken to make up a detailed reaction scheme based on industrial data and the existing knowledge about the process [13]. We offer the method of designing of the math model that combines industrial data, research results and quantum-chemical calculation.

The list of possible reactions for benzene alkylation was made with account of the quality of sources (ethylene and benzene), product composition and aspects of the process chemistry.

Thermodynamic possibility of these reactions has been confirmed by determination of the isobaric-isothermal parameter – the change of Gibbs energy ΔG at T=510 K and P=3.4 MPa. As for the target reaction Gibbs energy is equal to -43.4 kJ / mol and according to all defined ΔG of the considered reactions, thermodynamic possibility of these reactions is probable. The determination was performed with the use of *Gaussian-98* program by PM3 semi-empirical method.

The graphical description of the reactions pathway of benzene alkylation is shown in Fig. 1. Among them there are benzene alkylation of ethylene and propylene (ethylene feed impurity), toluene (benzene feed impurity) alkylation, next step of alkylation caused by the PEB formation, heavy by-product formation (diphenylethane) through the intermediate formation in the process of incomplete benzene alkylation.

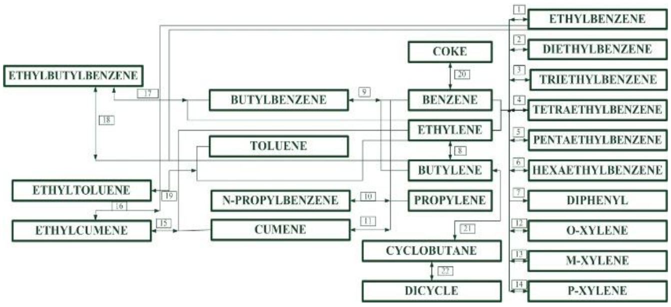

Fig. 1. Detailed scheme of hydrocarbons conversion in the process of alkylation of benzene with ethylene.

The scheme needs to be formalized (simplified) in order it could be used for future computations; at the same time it is to provide the highly accurate description of the process.

Formalization was performed by means of uniting individual substances into the pseudo-components having similar reactivity in respect of a particular reaction. The determination of compensation degree, which is characterized by the partial compensation of the energy expended on the breaking of the old bonds by the energy of the new bonds formation on the reaction route, was considerably helpful in solving the problems of catalytic action prediction.

Therefore, further step is to study the degree of compensation for the list of considered reactions.

$$H = \frac{\sum D_i - E_a}{\sum D_i} \cdot 100\% \tag{1}$$

where $\sum D_i$ – the energy of bounds breaking, kJ / mol, E_a – energy of activation, kJ / mol.

The main problem in calculation of the compensation energy is to determine the activation energy of the reaction.

As the first approximation, the activation energy was calculated according to Polanyi-Semenov equation for exothermic reactions [14].

$$E_a = 11.5 + 0.25 \cdot \Delta H \tag{2}$$

where E_a – energy of activation, kcal / mol, ΔH – heat of reaction, kcal / mol.

Enthalpy of the reactions was calculated with the use of quantum-chemical methods of thermodynamic functions determination. The calculated enthalpy of alkylation reaction of benzene with ethylene (-117.9 kJ / mol) was compared with the literature data (-113 kJ / mol) [15] as a proof of the relevance of the method for the unknown enthalpy of some reactions in the literature. All the considered reactions are exothermic.

Then the activation energy of the given reaction was calculated in first approximation with the use of the empiric equation. The value of the reaction mentioned above is 78.5 kJ / mol in comparison with 63.4 kJ / mol in [16]. It’s important to note that activation energy that was found for all reaction refers to the non-catalytic process, and it was good for the first approximation on next stage of the parameter estimation. The meanings of defined activation energy according to Polanyi-Semenov equation at T=510 K and P=3.4 MPa are represented in Table I. However, it might be improved with the use of literature sources of activation energy values for some reactions. After that the activation energy could be calibrated to the activation energy of the reaction.

Activation energy values were determined without taking zeolitic alkylation catalyst action into account. The kinetic parameters for alkylation zeolite catalyst under similar process conditions were defined in literature data. According to sources, the activation energy for the reaction of diethylbenzene the activation energy is 47.03 kJ / mol.

To find the relationship between literature and defined values of activation energy according to Polanyi-Semenov equation, the linear correlation equation was determined (Fig. 2).

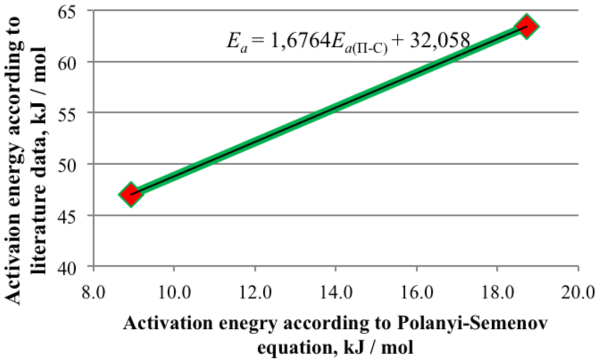

Fig. 2. The relationship between literature and defined values of activation energy according to Polanyi-Semenov.

E_a – literature activation energy; $E_{a(\text{П-С})}$ – activation energy according to Polanyi-Semenov equation.

Using the obtained relationship values of activation energy for the rest reactions were determined.

The next step in calculating the degree of compensation is the determination of the energy of bonds breaking. Let’s consider the methods based on the example of the main reaction (Fig. 3).

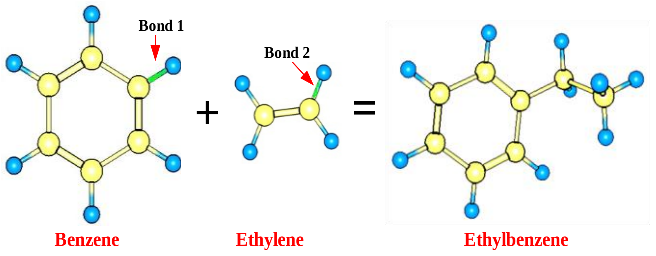

Fig. 3. Graphical representation of the main reaction.

To form ethylbenzene it’s necessary to break the two bonds: C-H bond in a molecule of benzene and C-H bond in a molecule of ethylene. The energies of these bonds have been calculated with the use of *Gaussian-98*.

The energy of the first bond was 433.8 kJ / mol, the energy of the second one was 215.5 kJ / mol. The energy of bonds breaking was equal to 649.3 kJ / mol. Similarly, the energy of bonds breaking was calculated for the rest of the reactions, and then the degree of compensation was calculated by the formula (1). The results are shown in Table I. The literature values of the energy of bonds breaking and their comparison with the determined values are also shown in Table I.

Computation results show the good comparability of the determined values of energy of bonds breaking with the literature data.

Similar work was carried out for the transalkylation process.

Relations between literature and defined values of activation energy according to Polanyi-Semenov equation for transalkylation is shown in Fig. 4.

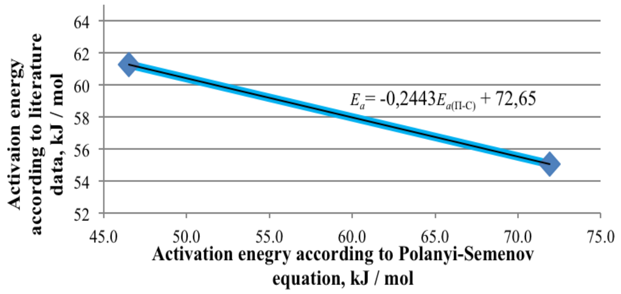

Fig. 4. The relationship between literature and defined values of activation energy for transalkylation.

Reactions and their characteristics are listed in Table II.

TABLE I: RESULTS OF DETERMINED DEGREES OF REACTION COMPENSATION

Reaction	Ea (Polanyi-Semenov), kJ / mol	$\sum D_i$, kJ/mol	$\sum D_i$, kJ / mol (liter.)	$\Delta\sum D_i$, %	H, %
Benzene + Ethylene = Ethylbenzene	78.5	649.3	715.0	9.2	90.2
Ethylbenzene + Ethylene = Diethylbenzene	86.1	633.5	715.0	11.4	92.6
Diethylbenzene + Ethylene = Triethylbenzene	90.7	617.7	715.0	13.6	88.9
Triethylbenzene + Ethylene = Tetraethylbenzene	84.4	602.0	715.0	15.8	89.1
Tetraethylbenzene+ Ethylene = Pentaethylbenzene	84.8	586.2	715.0	18.0	88.8
Pentaethylbenzene + Ethylene = Hexaethylbenzene	93.2	570.4	715.0	20.2	87.9
2Benzene + Ethylene= Diphenylethane + Hydrogen	94.1	1083	1100.0	1.5	93.6
Ethylene + Ethylene = Butylene	77.7	882.2	955.0	7.6	92.8
Benzene + Butylene = Butylbenzene	105.8	762.9	685.0	11.4	90.3
Benzene + Propylene = n-Propylbenzene	99.1	788.2	685.0	15.1	90.9
Benzene + Propylene = Cumene	107.9	788.2	685.0	15.1	90.5
Benzene + Ethylene = o-Xylene	63.8	1298	1428.0	9.1	95.6
Benzene + Ethylene = m-Xylene	55.0	1298	1428.0	9.1	95.8
Benzene + Ethylene = p-Xylene	55.0	1298.7	1428.0	9.1	95.8
Cumene + Ethylene = Ethylcumene	94.5	633.0	715.0	11.5	89.0
Ethylbenzene + Propylene = Ethylcumene	123.5	772.3	715.0	8.0	89.5
Butylbenzene + Ethylene = Ethylbutylbenzene	92.8	635.4	715.0	11.1	89.1
Ethylbenzene + Butylene = Ethylbutylbenzene	120.5	747.1	715.0	4.5	89.3
Toluene + Ethylene = Ethyltoluene	108.4	747.6	715.0	4.6	89.9
6Benzene = Coronene + Hydrogen	1179.8	5206.0	4980.0	4.5	90.3
Butylene = cis-Butene	183.1	952.5	1014.0	6.1	89.0
cis-Butene + cis-Butene = Dicyclobutane + Hydrogen	166.3	809.6	830.0	2.5	87.8

TABLE II: REACTIONS OCCURRED DURING THE TRANSALKYLATION

Reaction	ΔH, kJ / mol	Ea (Polanyi-Semenov), kJ / mol
Benzene+ Diethylbenzene= 2Ethylbenzene	-60.6	46.5
2Benzene+Triethylbenzene = 3Ethylbenzene	-95.0	24.4
Benzene+Tetraethylbenzene= Triethylbenzene+Ethylbenzene	-101.6	22.8
2Benzene+Pentaethylbenzene= Triethylbenzene+2Ethylbenzene	-123.8	17.2
3Benzene+Hexaethylbenzene= Triethylbenzene+3Ethylbenzene	-22.2	42.6
Benzene+Ethyltoluene= Ethylbenzene+Toluene	-44.2	37.1
Benzene+Buthylbenzene= 2Ethylbenzene	-24.4	42.1
Benzene+Buthylbenzene= n-Propylbenzene+Toluene	-84.4	27.1
Benzene+Buthylbenzene= Cumene+Toluene	-92.1	25.2
Ethyltoluene+Hydrogen= o-Xelene+Methane	-25.3	41.9
Ethyltoluene+Hydrogen= m-Xelene+Methane	-33.1	39.9
Ethyltoluene+Hydrogen= p-Xelene+Methane	-33.3	39.9
Ethylbuthylbenzene+Benzene= Ethylbenzene+Buthylbenzene	-13.4	44.8
Ethylcumene+Benzene= Ethylbenzene+ Cumene	-14.9	44.5
2Benzene+Ethylene= Diphenilethane+Hydrogen	-280.3	21.9

IV. RESULTS AND DISCUSSIONS

In order to formalize the transformation schemes, reactions were divided into two groups by the criterion of the similarity of their values of compensation degree (Table III). The degree of compensation for the same group of reactions differs approximately by 1% [17]-[19].

Thus, it is possible to identify the number of pseudo-components: the heavy compounds which are composed of individual components such as tetra-, penta-, hexaethylbenzene and diphenylethane; monoalkylates (butylbenzene, n-propylbenzene, cumene), dialkylates (ethylcumene, ethylbutylbenzene), xylenes (o-, m-, p-xylene), cyclic and dicyclic hydrocarbons. Formalized scheme of hydrocarbons transformations is shown in Fig. 5.

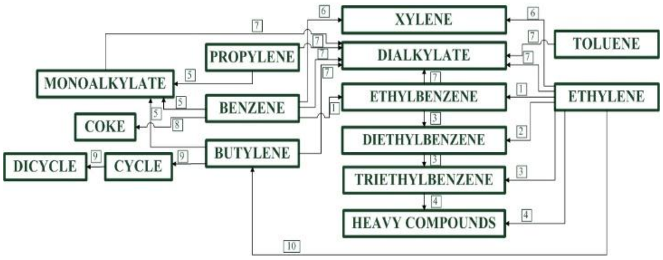

Fig. 5. Formalized scheme of hydrocarbons transformations in benzene in process of its alkylation with ethylene.

TABLE III: ALKYLATION REACTIONS GROUPING BY THEIR DEGREES OF COMPENSATION

Reaction group	Average H, % for reaction group
1. Ethylbenzene formation	90.2
Benzene + Ethylene = Ethylbenzene	
2. Diethylbenzene formation	92.6
Ethylbenzene + Ethylene = Diethylbenzene	
3. Triethylbenzene formation	88.9
Diethylbenzene + Ethylene = Triethylenebenzene	
4. Heavy compounds formation	89.8
Triethylbenzene + Ethylene = Polyethylenebenzene	
2Benzene + Ethylene = Diphenylethane + Hydrogen	
5. Other monoalkylates formation	90.6
Benzene + Butylene = Monoalkylate	
Benzene + Propylene = Monoalkylate	
6. Xylene formation	95.7
Benzene + Ethylene = Xylene	
7. Other dialkylates formation	89.4
Ethylbenzene + Propylene = Dialkylate	
Ethylbenzene + Butylene = Dialkylate	
Monoalkylate + Ethylene = Dialkylate	
Toluene + Ethylene = Dialkylate	
8. Coke formation	90.3
6Benzene = Coke + Hydrogen	
9. Cyclo and dicyclo formation	88.4
Butylene = cis-Butene	
cis-Butene + cis-Butene = Dicyclobutane + Hydrogen	
10. Butylene formation	92.8
Ethylene + Ethylene = Butylene	

According to the law of mass action the expressions of the rates of alkylation and transalkylation reactions can be put as follows (see Table IV).

TABLE IV: REACTION RATE IN ALKYLATION AND TRANSALKYLATION

Reaction group	Reaction rate expression
1. Ethylbenzene formation	$W_1 = k_{0(1)} \cdot e^{-Ea(_1)/RT} \cdot C_{benzene} \cdot C_{ethylene}$
2. Diethylbenzene formation	$W_2 = k_{0(2)} \cdot e^{-Ea(2)/RT} \cdot C_{ethylbenzene} \cdot C_{ethylene}$
3. Triethylbenzene formation	$W_3 = k_{0(3)} \cdot e^{-Ea(3)/RT} \cdot C_{diethylbenzene} \cdot C_{ethylene}$
4. Heavy compounds formation	$W_{4.1} = k_{0(4)} \cdot e^{-Ea(4.1)/RT} \cdot C_{triethylbenzene} \cdot C_{ethylene}$ $W_{4.2} = k_{0(4)} \cdot e^{-Ea(4.2)/RT} \cdot C^2_{benzene} \cdot C_{ethylene}$
5. Other monoalkylates formation	$W_{5.1} = k_{0(5)} \cdot e^{-Ea(5.1)/RT} \cdot C_{benzene} \cdot C_{butylene}$ $W_{5.2} = k_{0(5)} \cdot e^{-Ea(5.2)/RT} \cdot C_{benzene} \cdot C_{propylene}$
6. Xylene formation	$W_6 = k_{0(6)} \cdot e^{-Ea(6)/RT} \cdot C_{benzene} \cdot C_{ethylene}$
7. Other dialkylates formation	$W_{7.1} = k_{0(7)} \cdot e^{-Ea(7.1)/RT} \cdot C_{ethylbenzene} \cdot C_{propylene}$ $W_{7.2} = k_{0(7)} \cdot e^{-Ea(7.2)/RT} \cdot C_{ethylbenzene} \cdot C_{butylene}$ $W_{7.3} = k_{0(7)} \cdot e^{-Ea(7.3)/RT} \cdot C_{monoalkylate} \cdot C_{ethylene}$ $W_{7.4} = k_{0(7)} \cdot e^{-Ea(7.4)/RT} \cdot C_{toluene} \cdot C_{ethylene}$
8. Coke formation	$W_8 = k_{0(8)} \cdot e^{-Ea(8)/RT} \cdot C^6_{benzene}$
9. Cyclo and dicyclo formation	$W_{9.1} = k_{0(9)} \cdot e^{-Ea(9.1)/RT} \cdot C_{butylene}$ $W_{9.2} = k_{0(9)} \cdot e^{-Ea(9.2)/RT} \cdot C^2_{cis\text{-}butene}$
10. Butylene formation	$W_{10} = k_{0(10)} \cdot e^{-Ea(_{10})/RT} \cdot C^2_{ethylene}$

TABLE V: KINETIC MODELS OF ALKYLATION AND TRANSALKYLATION

The kinetic model of alkylation	**The kinetic model of transalkylation**
$\begin{cases} \frac{dC_{benzene}}{dt} = -W_1 - 2W_{4.2} - W_{5.1} - W_{5.2} - \\ -W_6 - 6W_8 \\ \frac{dC_{ethylene}}{dt} = -W_1 - W_2 - W_3 - W_{4.1} - \\ -W_{4.2} - W_6 - W_{7..3} - W_{7.4} - 2W_{10} \\ \frac{dC_{butylene}}{dt} = -W_{5.1} - W_{7.2} - W_{9.1} + W_{10} \\ \frac{dC_{propylene}}{dt} = -W_{5.2} - W_{7.1} \\ \frac{dC_{cis\text{-}butene}}{dt} = W_{9.1} - 2W_{9.2} \\ \frac{dC_{dicyclobutane}}{dt} = W_{9.2} \\ \frac{dC_{hydrogen}}{dt} = W_8 + W_{4.2} + W_{9.2} \\ \frac{dC_{ethylbenzene}}{dt} = W_1 - W_2 - W_{7.1} - W_{7.2} \\ \frac{dC_{diethylbenzene}}{dt} = W_2 - W_3 \\ \frac{dC_{triethylbenzene}}{dt} = W_3 - W_4 \\ \frac{dC_{heavy\_compounds}}{dt} = W_{4.1} + W_{4.2} \\ \frac{dC_{monoalkylate}}{dt} = W_{5.1} + W_{5.2} - W_{7.3} \\ \frac{dC_{dialkylate}}{dt} = W_{7.1} + W_{7.2} + W_{7.3} + W_{7.4} \\ \frac{dC_{xylene}}{dt} = W_6 \\ \frac{dC_{toluene}}{dt} = -W_{7.4} \\ \frac{dC_{coke}}{dt} = W_8 \end{cases}$	$\begin{cases} \frac{dC_{benzene}}{dt} = -W_1 - W_2 - W_3 - W_{4.1} - \\ -W_{4.2} - W_{5.1} - 6W_7 - 2W_8 \\ \frac{dC_{ethylene}}{dt} = W_8 \\ \frac{dC_{diethylbenzene}}{dt} = -W_1 + W_2 \\ \frac{dC_{triethylbenzene}}{dt} = -W_2 + W_3 \\ \frac{dC_{polyethylbenzene}}{dt} = -W_3 \\ \frac{dC_{ethylbenzene}}{dt} = 2W_1 + W_2 + W_3 + 2W_{4.1} + W_{5.1} \\ \frac{dC_{butylbenzene}}{dt} = -W_{4.1} - W_{4.2} \\ \frac{dC_{monoalkylate}}{dt} = 2W_{4.2} + W_{5.1} \\ \frac{dC_{dioalkylate}}{dt} = -W_{5.1} - W_{5.2} \\ \frac{dC_{hydrogen}}{dt} = -W_{5.2} + W_6 + W_7 + W_8 \\ \frac{dC_{xylene}}{dt} = W_{5.2} \\ \frac{dC_{methane}}{dt} = W_{5.2} \\ \frac{dC_{cis\text{-}butene}}{dt} = -2W_6 \\ \frac{dC_{dicyclobutane}}{dt} = W_6 \\ \frac{dC_{diphenylethane}}{dt} = W_8 \\ \frac{dC_{coke}}{dt} = W_7 \end{cases}$

where W_i – rate of i – group reaction; $k_{0(i)}$ – pre-exponential factor for i – group reaction; $E_{a(i,j)}$ – activation energy of j - subgroup for i – group reaction.

Similar work was carried out with the transalkylation process. Kinetic models of alkylation and transalkylation are presented in Table V.

Initial conditions are: $t=0$, $C_i=C_{0i}$, where i –corresponding hydrocarbon.

The kinetic models presented in the paper are to become the basis for the computer simulation of the ethylbenzene production system development.

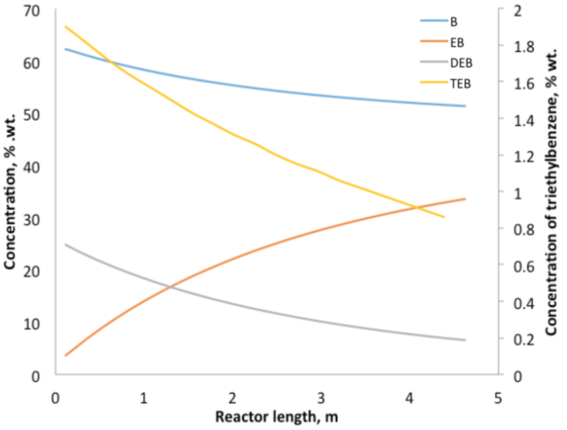

Fig. 6. The concentration changing of the major components along the reactor length (B-benzene, EB-ethylbenzene, DEB-diethylbenzene, TEB-triethylbenzene).

At the current stage model of transalkylation was tested. Parameters adjustment and their determination were carried out according to data operation of the industrial alkylation plant with liquid phase transalkylation process.

A 6 months operations plant data were taken as a basis. The parameters of equations (Table IV) were defined in *MathCAD* by least squares. Modeling was carried out in *HYSYS* using the kinetic model and the results according to parameters - constants of the equations give the changing of consumption and accumulation of basic substances along the reactor length (see Fig. 6).

V. CONCLUSION

Thermodynamic analysis of alkylation and transalkylation reactions were performed with the use of quantum-chemical methods of calculating thermodynamic functions. The method of formalization of the hydrocarbons transformation scheme which consists in the grouping of components by their reactivity drawing on the compensation degree values of the corresponding reactions, was developed. The correctness of the determination of the energy of bonds breaking in the reagent's molecules is confirmed by comparison of its results with the literature data. The kinetic models of alkylation of benzene with ethylene and polialkylbenzenes transalkylation were developed on the basis of the formalized transformations schemes. The primary data of the activation energies approximation and results of transalkylation reactor simulation were obtained.

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