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Development of 15-lump kinetic model of the catalytic cracking process

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The article presents the stages of development and primary results of calculation of the 15-component model of catalytic cracking of gasoil. Based on the analysis of models published in the literature, the advantages and disadvantages of each of them were identified, and on the basis of these data, a new model was proposed that allows taking into account both quantitative and qualitative characteristics of the products obtained. Initial calculations showed the convergence of the new model for most components, from which it can be concluded that the model can adequately describe the mechanism of the catalytic cracking process.

Keywords: Gasoline, catalytic cracking, kinetic model, reaction rate constant, direct and inverse kinetics problem, system of differential equations

Introduction. Today, the process of catalytic cracking occupies an important place in the oil refining industry. This process increases the depth of oil refining by obtaining from dark, heavy vacuum fractions components of commercial fuels and raw materials for petrochemical. Currently, the processes of catalytic cracking and catalytic reforming form the main fund of gasoline in factories. The increased interest in the process of catalytic cracking has revealed the problem of disadvantaged of theoretical scientific data, especially in terms of detailed schemes of chemical transformations. Detailed kinetic models will increase the depth of processing of vacuum gasoil. An important tool in the development of the theoretical foundations of schemes of chemical reactions of catalytic processes is the creation of mathematical models that allow the most complete description of the occurring processes [1].

The relevance of this work is complex, combining theoretical and experimental research. The Ufa State Petroleum Technical University (USPTU) conducts experimental kinetic work to identify the contribution of different groups of hydrocarbons (paraffin, naphthenic and aromatic) to the production of high-quality gasoline, as well as light and heavy catalytic gas oils [2-5].

Such a parallel approach, based on the reproduction of experimental kinetic data by mathematical modeling methods, will allow to develop recommendations for the optimal introduction of the process and to create new designs of devices for the implementation of catalytic cracking of vacuum gasoil. Thus, the study and improvement of the catalytic cracking process is an urgent task of modern technical science.

Review of existing kinetic models of catalytic cracking. There are a large number of research teams in which the process of catalytic cracking is studied in the laboratory [6-9]. Mathematical modeling is an equally important task. This article describes the kinetic models of

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catalytic cracking, available in Russian and foreign literature, as well as the results of calculations on the new proposed scheme of transformations.

A team of researchers led by Pitault in 1995 developed the 4-lump kinetic model of catalytic cracking presented in figure 1 [10]. Here, the transformation scheme includes a minimum number of components: gas, gasoline, vacuum gasoil, coke oven structures, and therefore the model calculated quite simply and quickly. The main chemical transformations occurring in the process of catalytic cracking taken into account: the decomposition of vacuum gasoil to produce gasoline and C_1-C_4 gases and coke formation. Note that the need to take into account the formation of coke is caused by its property of deactivation of the catalyst. Thus, the reaction affects the choice of reaction time and regeneration time by burning coke from the catalyst surface. However, the catalytic cracking process involves a large number of other reactions. The influence of the rate constants and activation energy of these reactions is not taken into account in this model; it must be taken into account when processing the results. Also, the scheme does not allow you to predict the performance of the resulting gasoline, since gasoline is represented by one component. Depending on the structural composition of the vacuum gasoil, which is also impossible to set for this model, gasoline will be obtained with different octane number, the content of standardized components. However, it should be noted that this is the simplest model for making process calculations. According to this model, it is convenient to obtain initial approximations for subsequent calculations on more complex transformation schemes.

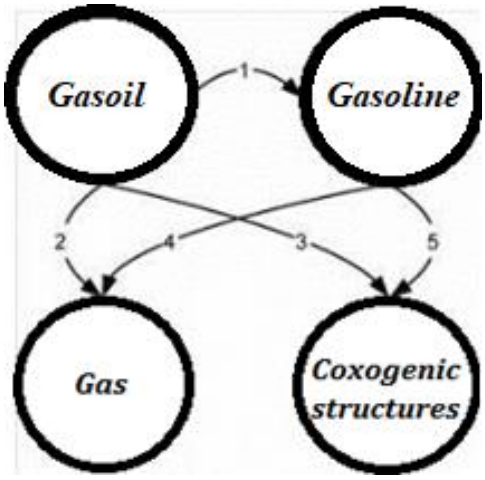

Fig. 1. Schematic representation of the 4-lump model of the catalytic cracking process

There is another important side reaction in the catalytic cracking process – the compaction reaction. In the previous 4-lump model, the reaction of coke formation was taken into account, but in the course of the reaction, other by-products are formed: light and heavy catalytic gasoil. The scientific team led by Serquiera [11] developed a 5-lump model of the catalytic cracking process, the scheme of transformations of which is shown in figure 2. This model differs from the previous one by introducing a new component – light aromatic oil (LCO), which includes compaction products other than coke. This is an important addition, as the yield of catalytic gasoil can reach a value of 50%.

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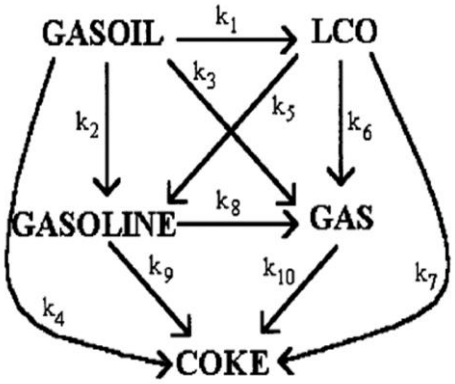

Fig. 2. Schematic representation of the 5-lump model of the catalytic cracking process

The article [12] describes a 6-lump kinetic model of catalytic cracking, which presents reactions with the production of gasoline from vacuum gasoil, light gaseous products of catalytic cracking. Light olefins C_2H_4 and C_3H_6 – valuable raw materials for petrochemistry-are especially distinguished. Two types of so-called coxogenic structures (KG1 and KG2) are also given. The process model is shown in figure 3. Note that this model describes the process of catalytic cracking, focused on the production of ethylene and propylene, which are valuable raw materials for petrochemistry. For example, they serve as raw materials for the synthesis of polymers: polyethylene, polypropylene, polystyrene, etc. However, to calculate the quality and quantity of gasoline, the depth of study proposed in this model is insufficient.

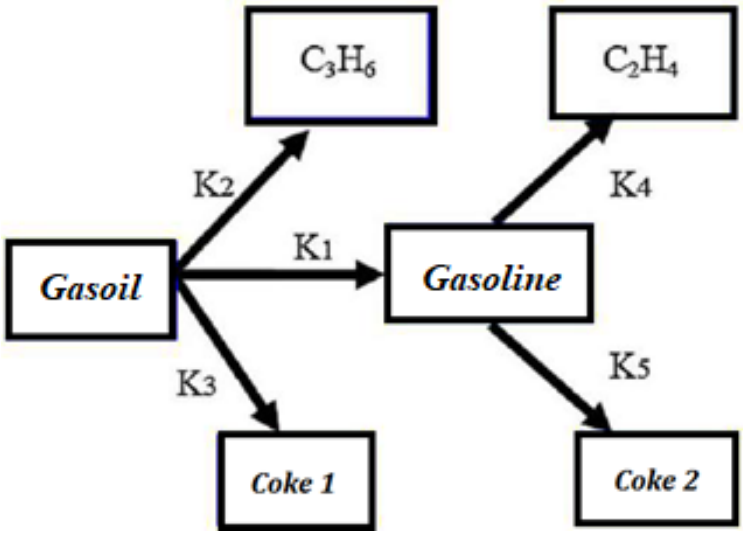

Fig. 3. Schematic representation of the 6-lump model of the catalytic cracking process taking into account the yield of light olefins

In the case of cracking of light hydrocarbon fractions on the Fe/HZSM-5 catalyst, a different 6-lump model [13] has been developed, the scheme transformation of which is shown in figure 4. This model is also applicable for the calculation of catalytic cracking process to obtain ethylene and propylene. Gasoline and catalytic gasoil are combined into one component – liquid hydrocarbons, as a result of which it is impossible to determine even the amount of gasoline produced in the process.

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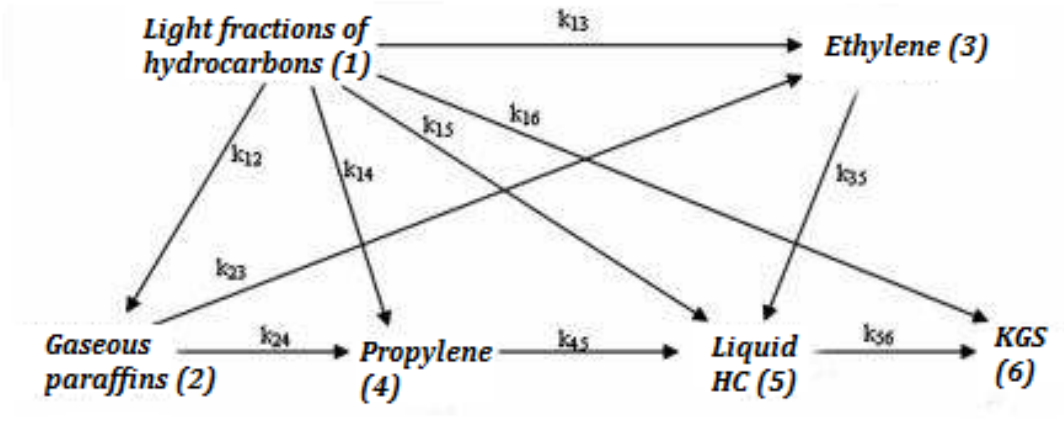

Fig. 4. Schematic representation of the 6-lump model of the catalytic cracking process

The paper [14] presents a model of catalytic cracking with 9-lump. The model takes into account the aromatization reactions of unsaturated gasoline components obtained in the process of catalytic cracking. The components are divided into groups depending on their structure: n-paraffins, iso-olefins, olefins, aromatic hydrocarbons, coke-gene structures, light hydrocarbons (C1-C4) and hydrogen-gas. The kinetic model is represented by a large number of different types of transformation between these components, for example, cracking of low molecular weight hydrocarbons, and isomerization, cyclization and dehydrogenation of paraffins. For simplicity, the least important reactions were excluded from the transformation scheme. The scheme of transformations according to this model is shown in figure 5. In comparison with the above models, the breakdown into components in this model is carried out in detail, which allows us to calculate the catalytic cracking process with sufficient accuracy. It should be noted that iso-paraffins and aromatic hydrocarbons have a high octane number, thus, with an increase in their content in gasoline, its commodity indicators increase [15]. Calculation of the content of aromatic hydrocarbons and olefins in gasoline is relevant due to the limitation of their content according to Russian and international standards [16].

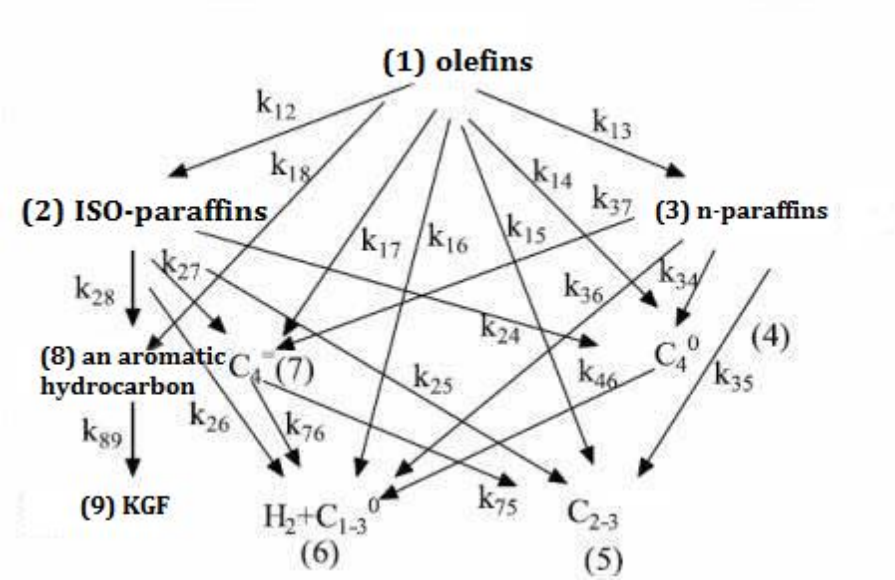

Fig. 5. Schematic representation of the 9-lump model of the catalytic cracking process

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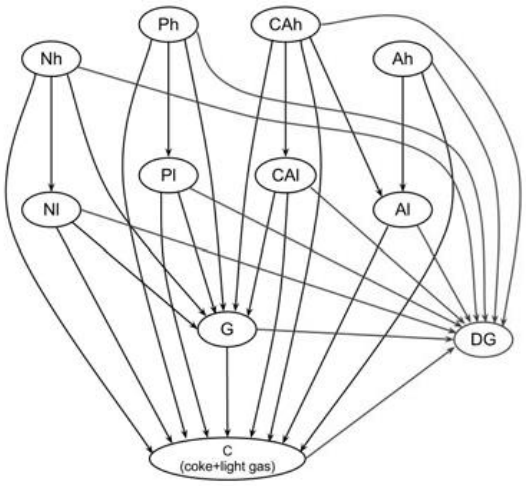
Figure 6 shows an 11-lump model of catalytic cracking [17]. In contrast to the previous model, the structural groups of hydrocarbons are divided into heavy and light, which will allow more accurately calculate not only the qualitative but also quantitative indicators of the resulting products. In the 9-lump model, due to the lack of division of hydrocarbons into light and heavy, it was impossible to determine the structural composition of gasoline and catalytic gasoils. In this model, the physical and chemical properties of homologous hydrocarbons are taken into account, namely: density, heat capacity, viscosity, thermal conductivity, heat of formation and molecular weight. Since the eleven-component model contains a single group describing both coke and light greenhouse gases, their characteristics have been determined as a weighted average of these varieties. The coke content of 30% and 70% of light hydrocarbon gas was confirmed. However, as practice shows, it is impractical to unite these components.



Ah – Heavy aromatic
Al – Light aromatic
C – Coke and light gases
CAh – Heavy aromatic substituents
CAl – Light aromatic substituents
DG – Dry gas
G – Gasoline
Nh – Heavy naphthenic
Nl – Light naphthenic
Ph – Heavy paraffinic
Pl – Light paraffinic

Fig. 6. Schematic representation of 11-lump model of catalytic cracking process

Figure 7 shows a 12-lump kinetic model of the catalytic cracking process, developed by the previously mentioned scientific team under the leadership of Serquiera [11]. In fact, the 5-lump model is a simplification of the twelve-component model. It can be assumed that simplification is permissible only under certain conditions of the process and under a certain type of catalysis, and therefore the five-component model should be used with caution, as a first approximation in the calculations of kinetic problems. Compared to the previous model, gas and coke are separated into different components. Separation of reaction products by mass and structure allows evaluating the quality and properties of the resulting products.

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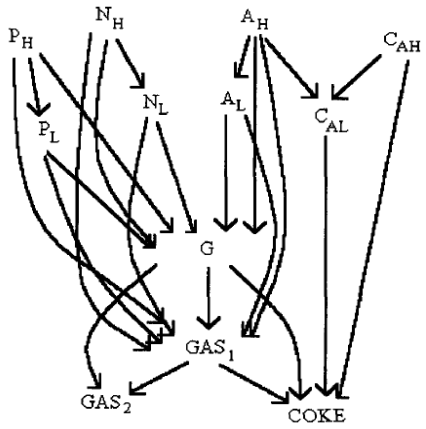
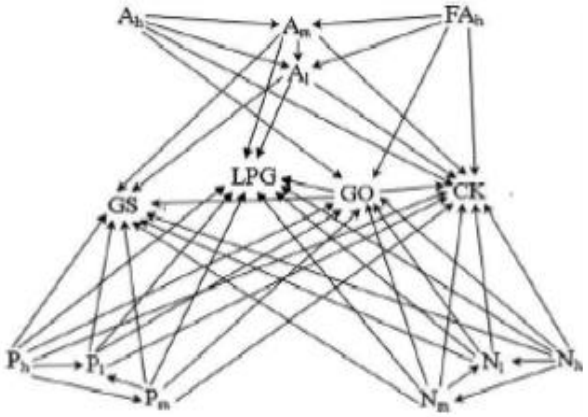


A_H-heavy aromatic hydrocarbons
A_L-light aromatic hydrocarbons
C_{AH}-heavy aromatic substituents
C_{AL}-light aromatic substituents
N_H-heavy naphthenes
N_L-light naphthenes
P_H-heavy paraffins
P_L-light paraffins
GAS_1 is the primary gaseous products
GAS_2-secondary gaseous products
G-light gasoline
COKE-coke

Fig. 7. Schematic representation of the 12-lump model of the catalytic cracking process

A 14-lump kinetic model [18] used to describe catalytic cracking reactions is presented in figure 8. Of all the models considered, this model most fully describes the process of catalytic cracking. With this model, you can evaluate both the yield and the quality of the resulting products. It is accepted that light hydrocarbon fractions contain paraffins, naphthenes and aromatic hydrocarbons in their composition. Reactions of conversion of aromatic hydrocarbons into paraffin are considered. It is worth noting that aromatic hydrocarbons do not enter into cracking reactions with the formation of gaseous products, since these transformations are impossible in the conditions of the catalytic cracking process. Due to the high temperature in the catalytic cracking reactor, products with a sufficiently high molecular weight are subjected to secondary cracking reactions. The conversion of olefins into liquid hydrocarbons by oligomerization and aromatization is also taken into account.



A_H -heavy aromatic hydrocarbons
A_M-medium aromatic hydrocarbons
A_L-light aromatic hydrocarbons
F_{AH}-heavy aromatic hydrocarbons in resins and asphaltenes
N_H-heavy naphthenes
N_M-medium naphthenes
N_L-light naphthenes
P_H-heavy paraffins
P_M-medium paraffins
P_L-light paraffins
GO-gasoline
LPG-liquefied petroleum gas
GS-dry gas
CK – coke

Fig. 8. Schematic representation of the 14-lump model of the catalytic cracking process

Comparison and analysis of existing kinetic models. The considered models differ in the number of components and the necessary equilibrium constants of chemical transformations between the components. The analysis of models is given in table 1 [19].

Table 1. Comparison of the studied kinetic models of catalytic cracking

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Number of components	The number of equilibrium constants	The Target component of the model	The Ability to assess the quality of gasoline
4-lump model	5	Gasoline	Absent
5-lump model	10	Gasoline	Absent
6-lump model [7]	5	Ethylene, propylene	Absent
6-lump model [8]	10	Ethylene, propylene	Absent
10-lump model	20	Gasoline	Exists
11-lump model	29	Gasoline	Exists
12-lump model	23	Gasoline	Exists
14-lump model	46	Gasoline	Exists

As you can see, the more components, the more complex the calculation of the model. In addition, there is a complexity in the form of a large number of necessary equilibrium constants. These constants can only be obtained experimentally, and differ for different types of catalysts. Also, the equilibrium constants depend on the temperature and pressure of the process (for reactions involving the gas phase). In addition, simple models without taking into account the structural components do not allow to assess the quality of the resulting products, which is a significant drawback. But, for the primary approximation, the use of these models can be justified and appropriate.

Thus, it can be argued that currently there are a large number of different approaches to modeling the process of catalytic cracking. Different models are determined by the composition of raw materials, technological conditions of the process, different types of catalysts and designs of reaction apparatus. Currently, the problem of modeling the catalytic cracking process is an urgent one.

On the basis of the presented literary review the comparative characteristic of these models was made.

Table 2. Comparison of models presented in the literature

The number of components	Accounting for the influence of the composition of raw materials	Accounting for the molecular weight of components (number of categories)	Accounting for the structure of components	Ability to determine the yield of ethylene and propylene	Ability to determine the yield of gasoline	Ability to determine the quality of gasoline (octane number, content olefins and aromatic compounds
4	-	-	-	-	+	-
5	-	-	-	-	+	-
6	-	-	-	+	-	-
6	-	-	-	+	-	-
9	-	-	+	+	-	-
10	-	-	+	-	+	+
11	+	+ (2)	+	-	+	-
12	+	+ (2)	+	+	+	-
13	+	-	+	-	+-	+-
14	+	+ (3)	+	-	+	+-

The development of a 15-lump kinetic model. Taking into account the disadvantages and advantages of these models, we have compiled and analyzed several schemes of transformation of components in the process of catalytic cracking [20, 21]. As a result of the analysis, we propose a

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15-lump kinetic model, which will allow us to estimate not only the amount of the target product-catalytic cracking gasoline, but also its quality-structural, fractional composition, octane number. Also on this model it is possible to estimate an output of raw materials valuable for petrochemical productions propane-propylene and butane-butylene fractions, and also quantity and qualitative indicators of fraction of light catalytic gasoil which is components of diesel fuel.

The scheme of transformations, which is used in the proposed model, is shown in figure 15.

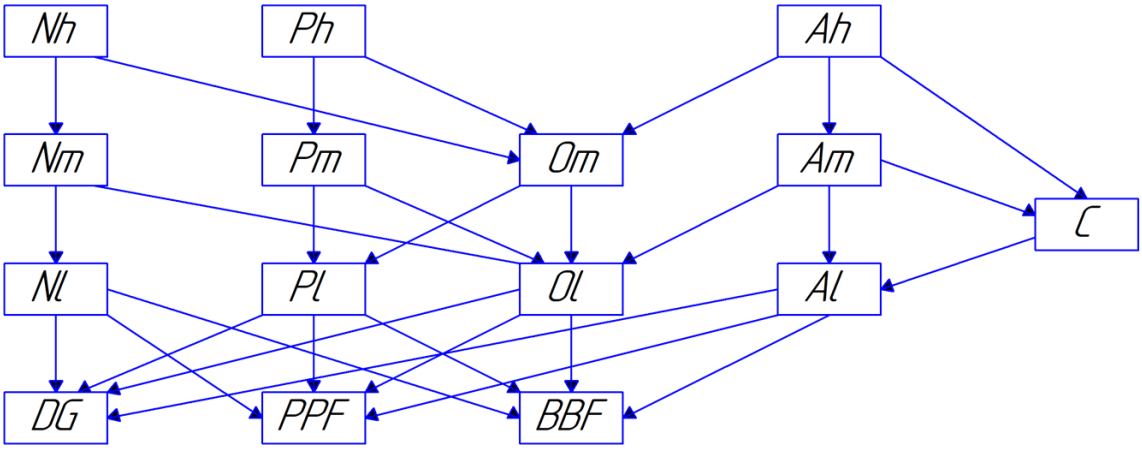

Fig. 9. 15-lump kinetic model

The designations in this scheme are given in table 2.

Table 2. Designations in the kinetic model of catalytic cracking

The marking	Component	The Average molecular weight, kg/kmol	Belonging to the product
Nh	Heavy naphthenes (C_{24}-C_{40})	400	Heavy catalytic gasoil
Ph	Heavy paraffins (C_{24}-C_{40})		
Ah	Heavy aromatics (C_{24}-C_{40})		
Nm	Medium naphthenes (C_{13}-C_{23})	200	Light catalytic gasoil
Pm	Medium paraffins (C_{13}-C_{23})		
Om	Medium olefins (C_{13}-C_{23})		
Am	Medium aromatics (C_{13}-C_{23})		
Nl	Light naphthenes (C_5-C_{12})	100	Gasoline
Pl	Light paraffins (C_5-C_{12})		
Ol	Light olefins (C_5-C_{12})		
Al	Light aromatics (C_5-C_{12})		
DG	Dry gas	16	-
PPF	Propane-propylene fraction	43	-
BBF	Butane-butylene fraction	57	-
C	Resin + coke	600	-

The basis of the kinetic model is the following system of differential equations:

$$\frac{d[y_1]}{dt} = -k_1[y_1] - k_8[y_1]$$

$$\frac{d[y_2]}{dt} = -k_2[y_2] - k_9[y_2]$$

$$\frac{d[y_3]}{dt} = -k_3[y_3] - k_{10}[y_3] - k_{15}[y_3]$$

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$$\frac{d[y_4]}{dt} = k_1[y_1] - k_4[y_4] - k_{11}[y_4]$$
$$\frac{d[y_5]}{dt} = k_2[y_2] - k_5[y_5] - k_{12}[y_5]$$
$$\frac{d[y_6]}{dt} = k_3[y_3] - k_6[y_6] - k_{13}[y_6] - k_{16}[y_6]$$
$$\frac{d[y_7]}{dt} = k_8[y_1] + k_9[y_2] + k_{10}[y_3] - k_7[y_7] - k_{14}[y_7]$$
$$\frac{d[y_8]}{dt} = k_4[y_4] - k_{18}[y_8] - k_{19}[y_8] - k_{20}[y_8]$$
$$\frac{d[y_9]}{dt} = k_5[y_5] + k_{14}[y_7] - k_{21}[y_9] - k_{22}[y_9] - k_{23}[y_9]$$
$$\frac{d[y_{10}]}{dt} = k_6[y_6] - k_{17}[y_{10}] - k_{24}[y_{10}] - k_{25}[y_{10}] - k_{26}[y_{10}]$$
$$\frac{d[y_{11}]}{dt} = k_{11}[y_4] + k_{12}[y_5] + k_{13}[y_6] + k_7[y_7] - k_{27}[y_{11}] - k_{28}[y_{11}] - k_{29}[y_{11}]$$
$$\frac{d[y_{12}]}{dt} = k_{15}[y_3] + k_{16}[y_6] + k_{17}[y_{10}]$$
$$\frac{d[y_{13}]}{dt} = k_{18}[y_8] + k_{21}[y_9] + k_{24}[y_{10}] + k_{27}[y_{11}]$$
$$\frac{d[y_{14}]}{dt} = k_{19}[y_8] + k_{22}[y_9] + k_{25}[y_{10}] + k_{28}[y_{11}]$$
$$\frac{d[y_{15}]}{dt} = k_{20}[y_8] + k_{23}[y_9] + k_{26}[y_{10}] + k_{29}[y_{11}]$$

The results of calculations on the 15-lump model. To calculate the reaction rate constants describing the chemical transformation in the catalytic cracking reactor, we used the production data from the article [22], which relate to the section C-200 at the catalytic cracking unit KT-1/1 of OAO «Gazpromneft-Omsk oil refinery».

The raw material of the process is vacuum gasoil containing heavy naphthenic, paraffin and aromatic compounds. Taking into account the production data, the initial concentrations of the components at the beginning of the reaction were calculated:

– heavy naphthenes: 0.1849 g/ml;

– heavy paraffins: 0.4065 g/ml;

– heavy aromatic compounds: 0.3129 g/ml.

Next, we calculated the concentration of products in the reaction mixture. The calculation results are given in table 3.

Table 3. Production values of concentrations in the reaction mixture

Component	Concentration, g / ml	Belonging to the product
C_{Nh}	0,0057	Heavy catalytic gasoil
C_{Ph}	0,0011	
C_{Ah}	0,0670	
C_{Nm}	0,0039	Light catalytic gasoil
C_{Pm}	0,0187	
C_{Am}	0,0802	
C_{Om}	0,0032	
C_{Nl}	0,0565	Gasoline
C_{Pl}	0,1905	
C_{Al}	0,1850	

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C_{ol}	0,1024	
C_{KOKC}	0,0387	Coke
C_{DG}	0,0498	Dry gas
C_{PPF}	0,0458	Propane-propylene fraction
C_{BBF}	0,0506	Butane-butylene fraction

We used Matlab software in our calculations. To solve the Cauchy problem, the Runge-Kutta method of order 4 (direct problem) was used. The reaction rate constants were obtained from the minimum condition of the function $z(k_1, \dots, k_{15}) = \sum_1^{15} |y_i - y_{\exp i}|$, where $y_{exp\ i}$ – the value of the concentration of components in the reaction mixture obtained from production data. The direct search method was used to find the minimum of this function (inverse kinetics problem) [23-24]. Methods of parallelization of the problem were also used to reduce the calculation time [25].

The results of the calculations are given in tables 4,5.

Table 4. Calculated values of chemical reaction rate constants of catalytic cracking process

№	k_i	№	k_i	№	k_i	№	k_i
1	4,7980	9	0,0060	17	0,4451	25	0,0022
2	5,9953	10	0,0063	18	0,0010	26	0,0353
3	2,4359	11	7,7201	19	0,0020	27	0,0047
4	4,9773	12	1,3014	20	0,0012	28	0,6194
5	7,6523	13	0,0014	21	0,5010	29	0,5672
6	3,0133	14	1,2955	22	0,1625		
7	4,8848	15	0,1240	23	0,2250		
8	1,0010	16	0,2461	24	0,0010		

Table 5. Calculation Error

№	Component	Error, %
1	Heavy naphthenes (C_{24}-C_{40})	0,00
2	Heavy paraffins (C_{24}-C_{40})	0,00
3	Heavy aromatics (C_{24}-C_{40})	0,00
4	Medium naphthenes (C_{13}-C_{23})	0,00
5	Medium paraffins (C_{13}-C_{23})	0,00
6	Medium olefins (C_{13}-C_{23})	0,00
7	Medium aromatics (C_{13}-C_{23})	0,00
8	Light naphthenes (C_5-C_{12})	0,00
9	Light paraffins (C_5-C_{12})	25,88
10	Light olefins (C_5-C_{12})	32,48
11	Light aromatics (C_5-C_{12})	5,74
12	Wet gas	0,00
13	Propane-propylene fraction	0,00
14	Butane-butylene fraction	0,00
15	Coke	0,00

Conclusion. Thus, on the basis of the analysis of the literature data, a scheme of chemical transformations for the catalytic cracking process was made, which allows to assess the quality and

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quantity of target and by-products: gasoline, propane-propylene and butane-butylene fractions, light and heavy catalytic gas oils. The calculation of the production data showed the convergence of this model for 12 of the 15 components. Errors in calculations may be due to the fact that light paraffins, naphthenes and aromatic compounds are associated with a large number of reactions. Perhaps it is necessary to change the order of calculations-the inverse problem to start calculating with these components. Also, the model does not take into account stoichiometric coefficients at the first approximation. In the future, they will be calculated and added to the model. Nevertheless, there is reason to believe that this model can adequately describe the process of catalytic cracking, and it will be possible to explore and develop ways to improve the process of catalytic cracking in the future.

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Разработка пятнадцатикомпонентной кинетической модели процесса каталитического крекинга

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В статье приведены этапы разработки и первичные результаты расчета пятнадцатикомпонентной модели каталитического крекинга вакуумного газойля. На основе анализа опубликованных в литературе моделей были выявлены достоинства и недостатки каждой из них, на основе этих данных предложена новая модель, которая позволяет учесть и количественные, и качественные характеристики получаемых продуктов. Первоначальные расчеты показали сходимость новой модели по большинству компонентов, из чего можно сделать вывод, что модель может адекватно описывать химизм процесса каталитического крекинга.

Ключевые слова: бензин, каталитический крекинг, кинетическая модель, константа скорости реакции, прямая и обратная задача кинетики, система дифференциальных уравнений.

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