METHOD OF CALCULATING HYDROCARBON COMPOSITION OF RAW MATERIAL OF THE DEWAXING PROCESS

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The production of winter and arctic diesel fuel is an urgent problem for Russia. High demand is associated with huge northern territories, more than 2/3 of the territories of the Russian Federation refer to territories with conditions of the Far North. Demand for diesel fuel increases every year due to the growth of cargo transportation by truck, with an increase in the vehicle fleet and an increase in the share of diesel car [1]. In addition, in the near future, demand will increase due to the active development of the Arctic territory of the country, as the region is rich in minerals.

The process of dewaxing finds a wider application for the production of diesel fuels because:

- the process allows to receive winter Arctic diesel fuel, which meets the requirements of GOST R 55475-2013;
- a relatively inexpensive catalyst (in comparison with catalytic isomerization) is used in the process;
- the process is well integrated with the process of deep desulfurization;
- it is possible to involve some amount of atmospheric gas oil (temperature of the end boiling point is 360 ˚C) in the dewaxing feedstock, as well as a certain amount of visbreaking gasoline, which allows increasing the depth of oil refining and increasing the output of the target diesel fraction (i.e. the process is also promising from the point of view of the Russian oil refining industry development strategy developed by the government RF).

Mathematical modeling is a powerful and effective tool for researching a wide variety of systems from different areas of human activity. The method of mathematical modeling is an objective necessity for increasing the efficiency and processes of the chemical industry, since the possibilities of the physical modeling method are limited, especially when optimizing the chemical-technological systems, predicting the activity level of the catalysts. The need for modeling the process of dewaxing is dictated by the urgency of the problems of catalyst deactivation, the forecasting of the inter-regeneration cycle, and the calculation of the technological parameters of the corresponding optimal activity.

At the development stage of the dewaxing model in order to reduce the number of calculations, a reasonable assumption was made. It consisted in the fact that for the system of equations of the concentrations of non-individual substances were taken, but concentrations of hydrocarbon groups and averaged reaction rate constants. The scheme for the transformation of hydrocarbons, embedded in the model, is shown in Fig.1. The material balance is represented in the form of a system of ordinary differential equations, the solution of which is realized by the Euler method, the heat balance is similarly represented (see equation (1)) [3].

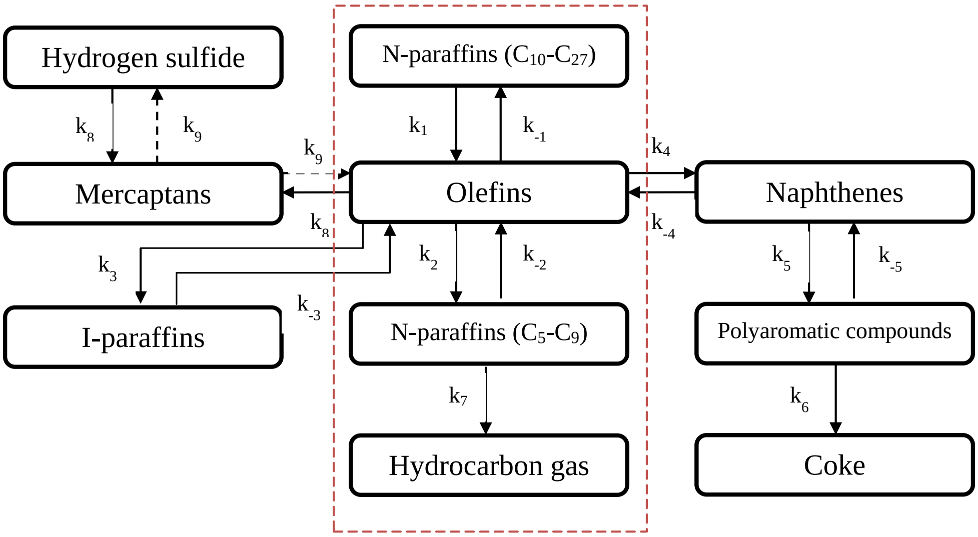

Fig. 1 Scheme of hydrocarbon transformations

$$\begin{cases} G\cdot\dfrac{\partial C_i}{\partial z}+G\cdot\dfrac{\partial C_i}{\partial V}=\sum\limits_{j=1}^{m}a_j\cdot W_j \\ G\cdot\dfrac{\partial C_i}{\partial z}+G\cdot\dfrac{\partial T}{\partial V}=\dfrac{1}{\rho\cdot C_p^{см}}\sum\limits_{j=1}^{m}Q_j\cdot a_j\cdot W_j \end{cases} \qquad (1)$$

During the implementation of the mathematical model of the dewaxing process, a problem arose due to the incomplete availability of the data of the group hydrocarbon composition of incoming raw materials to the plant. This problem was overcome by calculating the change in the content of hydrocarbon groups (n-paraffins, aromatic hydrocarbons, naphthenes, isoparaffins) in raw materials, depending on the density and fractional composition. Functional dependence has the following form:

$$\omega_i = A \cdot \rho + B \cdot T(10\%) + C \cdot T(50\%) + D \cdot T(90\%) + E$$

ω_i – mass concentration of i-th group of hydrocarbons in raw materials; A, B, C, D, E are coefficients to be determined by the method of least squares; ρ – density of raw materials, kg/m3; T (10%), T (50%), T (90%) are the boiling points of 10%, 50%, 90% of the raw meal volume, respectively.

When determining the values of the coefficients A, B, C, D, E using the regression analysis of each hydrocarbon group, experimental data were used for 22 points per group (that exceeds five times the number of variables entering into the equation).

Table 1 shows the calculation of hydrocarbon groups using the equations obtained by regression analysis. The points presented in the table were not used when finding the coefficients A, B, C, D, E. The calculated values of the mass concentrations of the hydrocarbon groups were compared with the experimental values (Table 1).

Table 1

Comparison of calculated and experimental data

Date	The content of the hydrocarbon group, mass. %, experimental values	The content of the hydrocarbon group, mass. %, calculated values	Absolute error, Δ
aromatic hydrocarbons			
01.03.2012	30,2	31,5	1,3
12.03.2012	30,7	31,5	0,8
15.01.2014	33,2	30,7	2,5
21.01.2014	33,0	30,8	2,2
25.01.2016	28,2	29,5	1,3
03.02.2016	27,8	26,9	0,9
n-paraffins			
01.03.2012	16,6	16,4	0,2
12.03.2012	14,8	16,4	1,6
15.01.2014	14,9	16,4	1,5
21.01.2014	21,7	19,6	2,1
25.01.2016	18,1	18,2	0,1
03.02.2016	18,6	18,9	0,3
isoparaffins + naphthenes			
01.03.2012	48,5	46,8	1,7
12.03.2012	49,8	48,7	1,1
15.01.2014	46,1	44,7	1,4
21.01.2014	39,8	41,6	1,8
25.01.2016	49,0	48,4	0,6
03.02.2016	45,4	45,4	0,0

The error in the calculations does not exceed the reproducibility limit indicated in the corresponding methods for determining each group of hydrocarbons, which indicates a sufficient degree of reliability of the results obtained and the possibility of their application in calculations.

References

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