FORMALIZED SCHEME FOR THE LIGHT HYDROCARBON FEEDSTOCK CONVERSION ON A ZEOLITE CATALYST

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The annual growth in the commercial petroleum products consumption is the reason for the search for alternative feedstock for processing. Selection of a catalyst based on its ecological safety, cost, activity and selectivity is important in the production of motor fuel. A promising feedstock for the motor gasoline high-octane components production is stable gas condensate, and a promising catalyst is zeolite. The Zeoforming process combines both components.

Forecasting and optimization Zeoforming light hydrocarbons of different composition requires a process mathematical model. A process mathematical model basis is a formalized scheme compilation for the substance's transformation.

Based on experimental data on samples individual hydrocarbon composition of stable gas condensate and products of their processing on a zeolite catalyst, a theoretically possible reactions list was compiled. The theoretically possible reactions total number is 805. Table 1 provides a theoretically possible reactions list.

Thermodynamic characteristics were determined for all theoretically possible reactions using quantum chemistry methods in the Gaussian software environment (GaussianView 5.0) [1]. The Gibbs energy values calculation was carried out under the conditions for the Zeoforming process implementation (process temperatures 375 °C (648 K); 400 °C (673 K); 425 °C (698 K) and pressure of 2.5 atm.).

According to the thermodynamic analysis results, it was established that 721 reactions are thermodynamically possible under conditions of zeo-

Table 1. Theoretically possible reactions list

Reaction type	Number of reactions
Isomerization of paraffinic hydrocarbons	102
Cracking of paraffinic hydrocarbons with the formation of olefins	34
Redistribution of hydrogen in olefins with the formation of aromatic hydrocarbons and n-paraffins	600
Redistribution of hydrogen in olefins with the formation of diolefins	22
Diene synthesis with the formation of cycloolefins	12
Redistribution of hydrogen in cycloolefins with the formation of naphthenes and aromatic hydrocarbons	7
Alkylation with the formation of naphthenes from olefins	21
Cracking of naphthenes with the formation of olefins and naphthenes	7

Table 2. Thermodynamically possible reactions list

Reaction type	Number of reactions
Isomerization of paraffinic hydrocarbons	51
Cracking of paraffinic hydrocarbons with the formation of olefins	28
Redistribution of hydrogen in olefins with the formation of aromatic hydrocarbons and n-paraffins	600
Redistribution of hydrogen in olefins with the formation of diolefins	4
Diene synthesis with the formation of cycloolefins	7
Redistribution of hydrogen in cycloolefins with the formation of naphthenes and aromatic hydrocarbons	7
Alkylation with the formation of naphthenes from olefins	21
Cracking of naphthenes with the formation of olefins and naphthenes	3

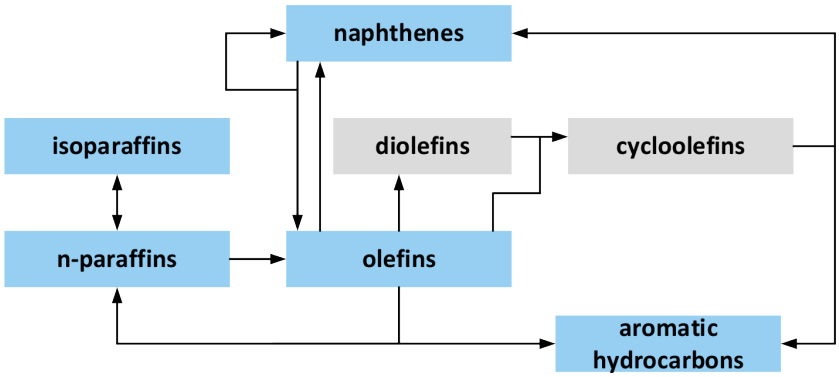

Fig. 1. *Formalized scheme for the light hydrocarbon feedstock conversion on a zeolite catalyst*

forming of a stable gas condensate. Table 2 provides a thermodynamically possible reactions list.

Based on the reactions list obtained, the hydrocarbon transformations formalized scheme will look like this (Figure 1).

References

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DEVELOPMENT OF AN ALGORITHM FOR RAW MATERIALS GROUP COMPOSITION CALCULATION IN A VACUUM GAS OIL HYDROTREATING MATHEMATICAL MODEL

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Hydrotreating is one of the main processes in petroleum feedstock refining, aimed to reduce significantly the content of heteroatomic compounds in petroleum products. Nowadays, significance of the catalytic cracking hydrotreating process of feedstock increases due to deteriorating resource base. With this process environmentally friendly fuel with almost zero sulfur content is obtained from heavy and high-sulfur oil. Also operating time of catalytic cracking catalysts increases due to the removal of catalytic poisons.

Various technical problems are solved with methods of mathematical modeling or by computer modeling systems at the modern level of digital development. At the same time, creation of an adequate model for vacuum gas oil hydrotreating is complicated due to the difficulty of identifying hydrocarbons groups and the lack of regular analyzes to determine the group composition of raw materials in factory laboratories, in contrast to analyzes for fractional composition, density and viscosity. Thus, the development of a methodology for the correlation of such parameters as regular indicators with the component composition of raw materials is relevant.

The purpose of this research is to develop an algorithm for calculation the group composition of hydrotreating feedstock based on plant data.

As a result, a calculation method was developed which is based on the API correlation [1]. In this case, the empirical formulas used in the calculation for determining the molecular weight and refractive index of the vacuum distillate take into account the degree of paraffin content of the fraction [2]. The calculation algorithm is shown in Figure 1.