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

1. *Ochterski J.W. Thermochemistry in Gaussian. Gaussian, Inc., 2000. – 19 c.*

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

S.B. Arkenova[1], D.A. Afanasyeva[1], T.A. Kaliyev[1,2]
Academic advisers – Doctor of Engineering Sciences, professor E.N. Ivashkina[1];
Candidate of Engineering Sciences, research scientist N.S. Belinskaya[1]
Linguist – Candidate of Engineering Sciences, research scientist N.S. Belinskaya[1]

[1]*National Research Tomsk Polytechnic University*
634050, Russia, Tomsk, 30 Lenin Avenue

[2]*«Pavlodar oil chemistry refinery» LLP*
Kazakhstan, Pavlodar, arkenova19@gmail.com

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.
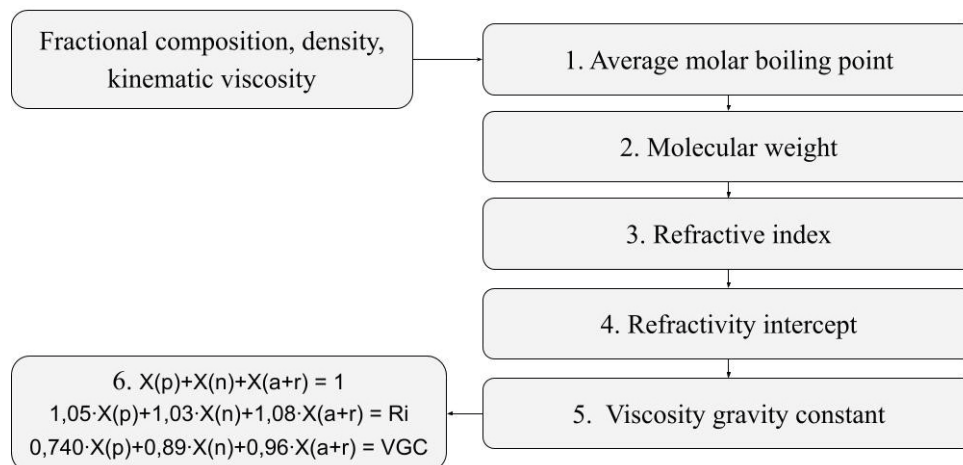
Fig. 1. *Diagram of the algorithm for calculation the group composition of hydrotreating feedstock*

The developed methodology is based on a system of three equations (Figure 1): the first equation is the molar balance of the group composition of vacuum gas oil, the second and third equations are the additivity law for the refraction intercept and the viscosity-weight constant, respectively [3].

The developed technique was tested using a dataset from one of the existing oil refineries. It was found out that with an increase of the average molar boiling point, the mass fraction of saturated hydrocarbons decreases, as shown in Figure 2, but on the other hand, mass fraction of aromatic hydrocarbons and resins increases.

Thus, an algorithm was proposed for assessing the component composition of the feedstock of the hydrotreating process. The calculation error does not exceed 5%. The calculation module based on this algorithm is incorporated into the kinetic model of vacuum gas oil hydrotreating, which will make it possible to recommend the optimal technological
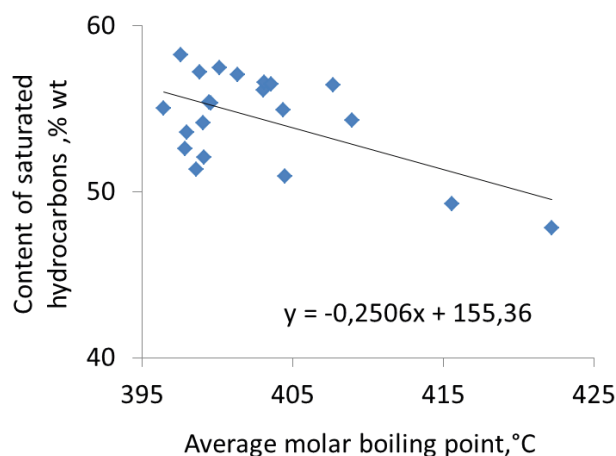

Fig. 2. *Correlation between the mass concentration of saturated hydrocarbons and the average molar boiling point of the vacuum distillate*

mode of operation of the vacuum gas oil hydrotreating unit, depending on the composition of the processed feedstock.

References

1. Dhulesia H. // Oil & Gas Journal, 1986. – Vol. 84. – P. 51–54.
2. El-Hadi D., Bezzina M. // Fuel, 2005. – Vol. 84. – P. 611–617.
3. Riazi M.R., Daubert T.E. // Ind. Eng. Chem. Process Des. Dev., 1980. – Vol. 19. – P. 289–294.