

are characterized by poor flammability. Additives are added to diesel fuels from naphthenic base oils, as well as to fuels from gas condensates, distributed in oil production sites [2].

In this paper, the effect of a cetane-increasing additive on such parameters of diesel fuel as Free Energies, Enthalpies, Entropies, heat capacity and total energy is considered.

In this work using quantum-chemical methods the influence of hydrocarbons of diesel range and cetane improving additive was studied through such parameters as Gibbs free energy, enthalpy, entropy

Calculations on the effect of the additive on the parameters of diesel fuel were carried out using the software product Gaussian. As an additive, isopropyl nitrate was used. The process conditions are

shown in Table 1. The results of the calculations in Table 2.

Since the value of the energy of isopropyl nitrate interaction with the studied isoparaffins under standard conditions was positive, it indicates the presence of an energy barrier for the formation of intermolecular bonds between these molecules of compounds of 65–67 kJ. That testifies, on the one hand, about possible other mechanism (radical) of interaction of isopropyl nitrate with isoparaffins, and on the other – about possible need of change of thermobaric conditions (temperature, pressure) for increase of reception of isopropyl nitrate to isoparaffins in diesel fuels that will become a subject of further researches.

References

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USING COMPUTER MODELING SYSTEM TO STUDY THE INFLUENCE OF PRESSURE ON THE PROCESS OF CATALYTIC DEWAXING

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The process of catalytic dewaxing is aimed to produce diesel fuel, having low freezing temperature from -18°C to -60°C . The fuel in this case is called winter diesel fuel and arctic diesel fuel [1].

The freezing temperature is mainly determined by the content of long straight-chain paraffins [2]. These normal paraffins undergo the reaction hydrocracking in the process of catalytic dewaxing to form short-chain normal paraffins and iso-paraffins, which have much lower freezing points [3].

The aim of this work is to study the influence of pressure on the process of catalytic dewaxing.

To perform calculations, computer modeling system of the catalytic dewaxing process was applied. This system is based on the mathematical model of the process.

As the initial data, two different feedstock compositions were used. The feedstock differs by the content of long-chain normal paraffins. The content

of n-paraffins in the first feedstock is 14 wt. %. The content of n-paraffins in the second feedstock is 21 wt. %. For each of these feedstock compositions the study of pressure influence on the process of catalytic dewaxing was studied. Technological parameters for the calculations were taken as: feedstock flow rate was $280\text{ m}^3/\text{h}$, flow rate of hydrogen-containing gas was $20000\text{ m}^3/\text{h}$, temperature was 340°C .

As a result, the following relations were obtained:

1. Relation between the pressure and the content of n-paraffins $C_{10}-C_{27}$ in the product for the first (fig. 1a) and the second (fig. 1b) composition.
2. Relation between the pressure and the cold filter plugging point of the product for the first (fig. 2a) and the second (fig. 2b) composition.
3. Relation between the pressure and the yield of the product for the first (fig. 3a) and the second (fig. 3b) composition.

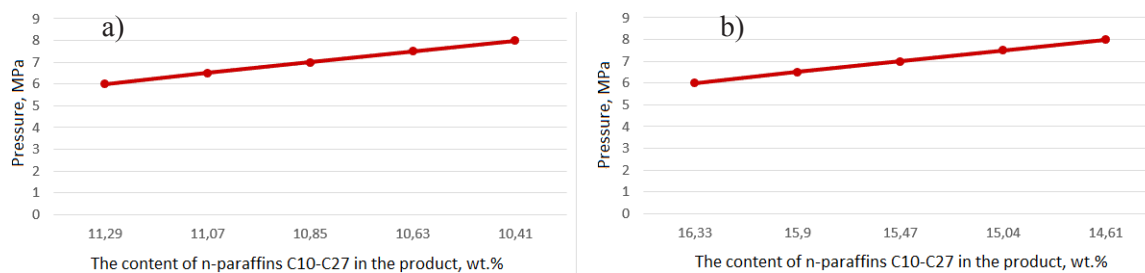


Fig. 1.

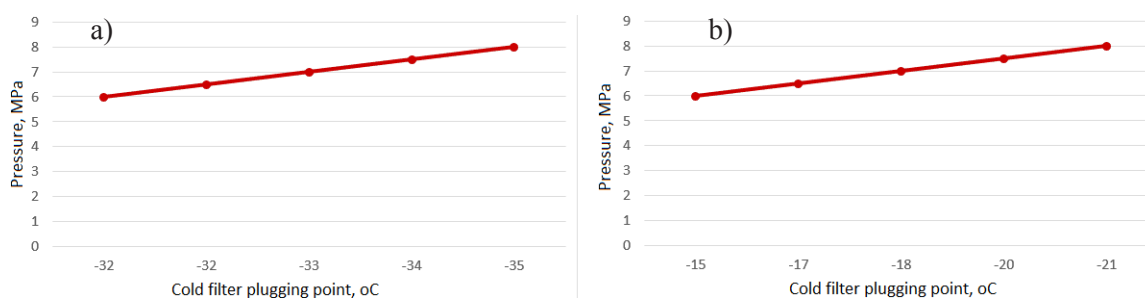


Fig. 2.

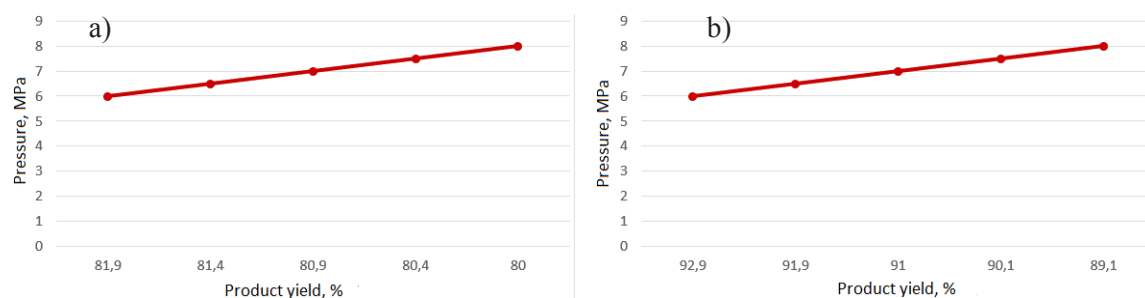


Fig. 3.

According to the obtained results, the following conclusions were made:

1. Increase in the pressure of the catalytic dewaxing process provides increasing in the conversion level. This in turn provides improving cold filter plugging point of the target diesel product.

2. Computer modelling helps to predict the composition and properties of the product at different operating conditions. Moreover, using mathematical models allows determining optimal operating parameters depending on the feedstock composition and requirements to the final product.

References

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