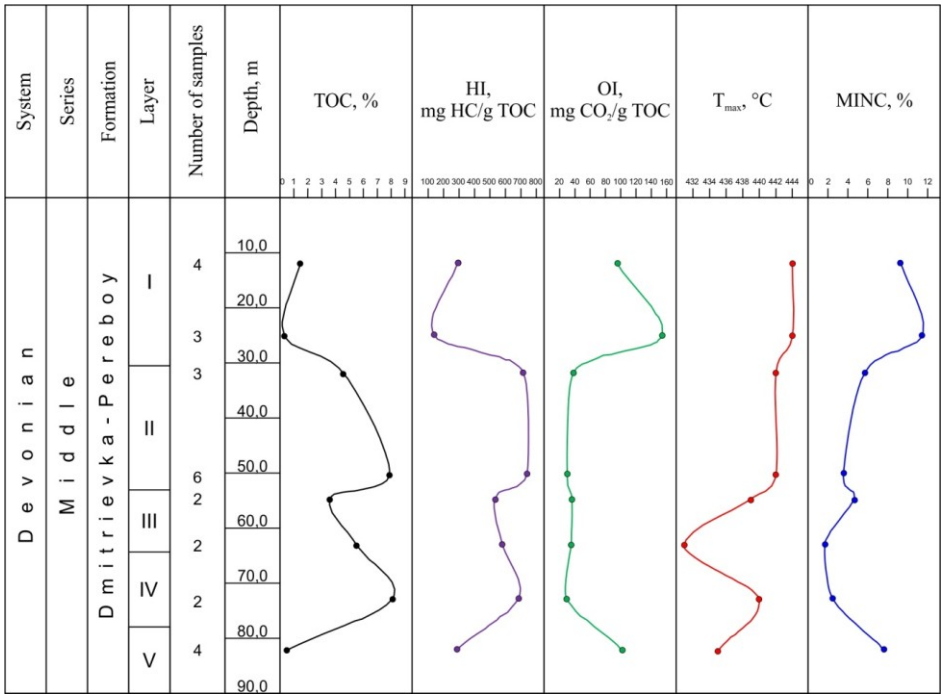

Fig. The geological and geochemical section of the Dmitrievskoe deposit

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QUANTUM-CHEMICAL CALCULATIONS OF THE THERMODYNAMIC PROPERTIES OF N-PARAFFINS HYDROCRACKING REACTIONS

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Every year the share of heavy and high-sulfur oils in the total volume of oil produced increases. Due to the peculiarities of climatic conditions and geographical location, the production of winter and Arctic brands of diesel fuel with corresponding low-temperature and environmental characteristics is of particular importance for Russia [2].

Long-chain paraffins of normal structure (C_{12}-C_{27}) have a significant influence on the low-temperature properties of diesel fuel. The main characteristics of the low-temperature properties of paraffins are: the cold filter plugging point, the freezing point and cloud point. The solidification temperature of long-chain n-paraffins varies from –10 °C for n-dodecane (n-$C_{12}H_{26}$) to +60 °C for n-heptacosan (n-$C_{27}H_{56}$).

In oil refining, the solution of problems to increase the yield, composition and quality of the obtained products, depending on the composition of raw materials and technological conditions of the process, is carried out using mathematical models that are developed on the basis of the physical and chemical regularities of the studied processes [5].

Currently, in order to conduct research on hydroprocesses, models based on grouping of components by fractions have been developed [4], as well as more detailed models based on combining reactants by groups: paraffins, naphthenes, and aromatic hydrocarbons [3]. However, these models do not take into account the distribution of n-paraffins and their reactivity in the target hydrocracking reaction.

To predict the low-temperature properties of the obtained diesel fuels, it is necessary to determine the number of long-chain n-paraffins in their composition. It is also established that n-paraffins in hydrocracking reactions have different reactivity [1]. In addition, during the hydrocracking reaction of n-paraffins, there is a different probability of breaking the bond in a particular position in the molecule, which also affects the yield and the ratio of the obtained products (gas, naphtha and diesel fraction, unconverted residue).

In this paper, the functional dependence of the Gibbs energy change in the course of hydrocracking reactions of n-paraffins when the bond is broken at different positions in the molecule is determined. The results obtained are shown in figures 1,2.

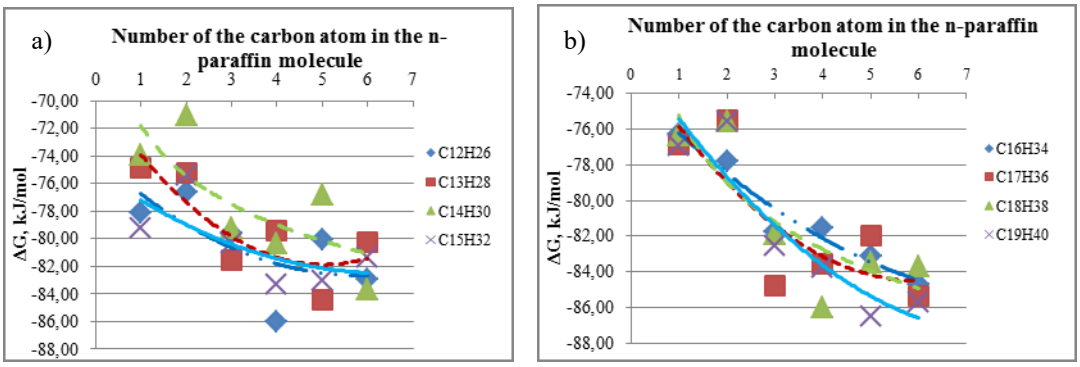

Fig. 1 Function of the Gibbs energy change during the hydrocracking reaction of n-paraffins a) $C_{12} – C_{15}$, b) $C_{16} – C_{19}$ when the bond is broken in different positions

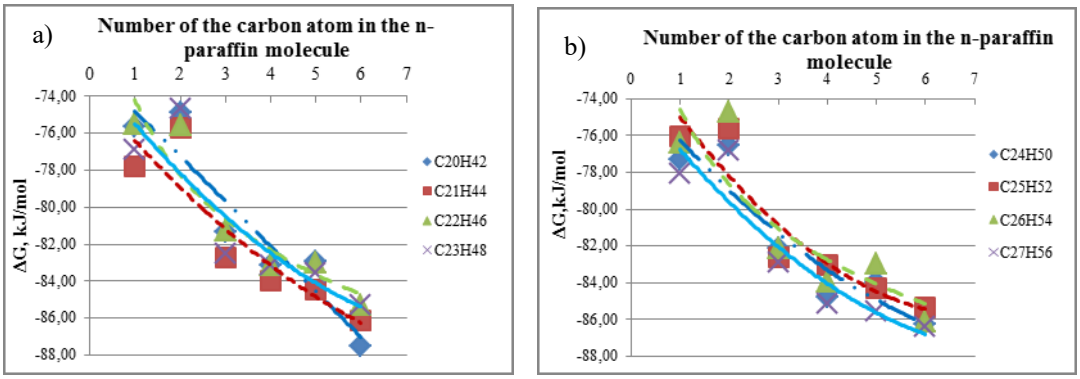

Fig. 2 Function of the Gibbs energy change during the hydrocracking reaction of n-paraffins a) $C_{20} – C_{23}$, b) $C_{24} – C_{27}$ when the bond is broken in different positions

Based on the results presented, it can be concluded that with an increase in the number of atoms in the paraffin molecule, an increase in the reactivity of paraffins is observed. Quantitatively, reactivity of n-paraffins in hydrocracking reaction is added to the model through the matrix of bond breakage in different positions in the molecule. Table 1 shows a fragment of the matrix of the thermodynamic probability of breaking the bond in the hydrocracking reaction at different positions of the bond in the n-paraffin molecule.

Table 1

Matrix of probability of bond breakage in different position in n-paraffin molecule in hydrocracking reaction

№ carbon atom (the position of a disconnection)	$C_{12}H_{26}$	$C_{13}H_{28}$	$C_{14}H_{30}$	$C_{15}H_{32}$	C_iH_{i+2} $i = 16÷26$	$C_{27}H_{56}$
1	0,087	0,085	0,083	0,086		0,082
2	0,089	0,088	0,088	0,088		0,084
3	0,091	0,090	0,091	0,089		0,087
4	0,093	0,092	0,092	0,091		0,089
5	0,093	0,093	0,094	0,092		0,090
6	0,094	0,094	0,094	0,093	…	0,092
7	-	-	0,094	0,093		0,093
8	-	-	-	-		0,094
…	…	…	…	…		…
14	-	-	-	-		0,097

As a result of the study, the reactivity of n-paraffins was studied, which is proportional to the number of carbon atoms in the n-paraffin molecule. The probability of breaking bonds in different positions in the molecule during hydrocracking of n-paraffins was estimated. Based on the results obtained, a matrix of the probability of breaking bonds in the hydrocracking reactions of n-paraffins was composed, on the basis of which a mathematical model of the hydrodewaxing process will be improved.

This approach to modeling will allow us to study in more detail the processes of catalytic dewaxing, to predict the yield and low-temperature properties of the obtained diesel fuels depending on the composition of the raw materials and

technological conditions of the process, and to determine the degree of catalyst deactivation depending on the volume of processed raw materials.

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ALGORITHM OF CALCULATING THE DIMENSIONS OF FRACTURES DUE TO HYDRAULIC FRACTURING IN SEDIMENTARY ROCKS

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The exploitation of an oil deposit consists in bringing the hydrocarbons to the surface by natural depletion under the best conditions. As soon as production becomes insufficient despite large reserves in place, new recovery techniques are introduced to improve productivity and the characteristics of well, one of these techniques is known as acid fracturing.

This technique artificially creates permeable drains by injecting treatment fluid which is acid (HCl) into the reservoir. The study of the injection of an acidic solution (HCl) in a porous medium is therefore of capital interest the aim of which is to predict the formation or not of wormholes, their size, the modification of the resulting permeability as well as the role of the different parameters on the final result. [2]

The success of such an operation depends very much on the parameters chosen and the decisions made in order to avoid any failure or any additional expense and have a good return on the operation.

The aim of our paper is to study the operation of acid fracturing in carbonate rocks and write an algorithm which calculates the main key parameters which indicate the success or failure of the process.

Carbonate rocks:

Represent all the sedimentary rocks which contain a large amount of carbonate minerals during their formation, among these the two main ones are calcite and dolomite, although their intermediates also exist (dolomitic limestone, limestone dolomite). [2]

Like sandstone, carbonate rocks are sedimentary rocks. The vast majority of these sediments are composed of the skeletons of marine organisms. Over time, carbonate sediments are subject to physical and chemical modification in order to reach a stable form such as calcite, limestone, the most abundant carbonate, when the sediment remains in contact with a fluid containing a lot of magnesium for a long time, it forms dolomite (CaMg (CO3) 2). [3]

Definition and Meaning of the damage:

The damage represents all the incrustations, whether mineral or organic, which can alter the natural permeability by their deposition inside the tank or by sealing the perforations or even the production tubing. This damage can be located in the different parts of the effluent path, from the tank to the surface. [1].

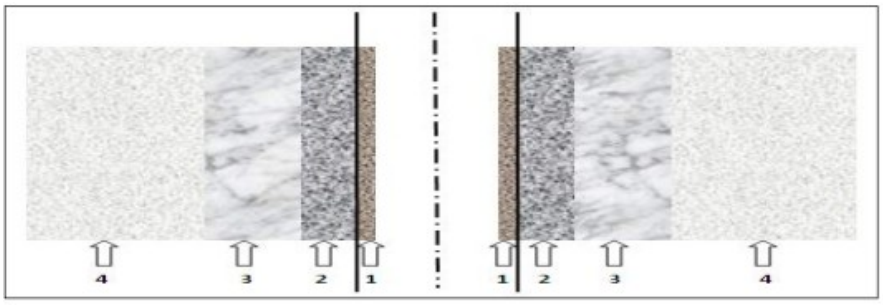

Fig.1 Location of damage