to the CFPP values, all the obtained blends conform the requirements [2] for grade S (Summer) (the permissible value is not higher than –5 °C).

Thus, we can conclude that, despite the negative effect on the physicochemical properties when BioDF is involved in the blend, a positive effect on CFPP is observed. This affect is explained by the distinctive structure of BioDF molecules, which do not freeze when the temperature decreases, but take a gelatinous form in blend, which in turn is pumped through the filter. From the viewpoint of the production of blend DF grade S (Summer), it is significant that it is possible to involve BioDF obtained from various oils in an amount of up to 20 % vol., which will increase the commercial DF production.

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QUANTUM-CHEMICAL MODELING IN ASSESSING THE INTERACTION OF DIESEL FRACTIONS HYDROCARBONS WITH A DEPRESSANT AND DEPRESSANT-DISPERSANT ADDITIVE

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In the conditions of the modern Arctic climate, it becomes urgent to improve the low-temperature characteristics of diesel fuel (DF) by adding depressant-dispersant (DD) additives. Intermolecular interactions arising between hydrocarbons (HC) of diesel fuel and the additive have a significant effect on the amount of additive required to improve the properties of diesel fuel.

In this work, a quantum-chemical simulation of DF hydrocarbons with DD additive was carried out. Vinylacetate was chosen as a depressant, and undecylamine itaconic acid was chosen as a dispersant. The construction of HC groups of diesel fractions (DF) and the calculation of intermolecular interactions were carried out in the Gaussian software package at standard temperature and pressure. Were selected HC groups, such as: paraffins, aromatic HCs and naphthenes, with the number of carbon atoms from C_8 to C_{12}. Such characteristics as the energy and enthalpy of intermolecular interaction were calculated. For comparative assessment, the values of intermolecular interactions of HC groups were averaged. Low-temperature characteristics, such as cloud point (CP), cold filter plugging point (CFPP), and pour point (PP) were determined using the «INPN» device. The results are shown in Tables 1, 2.

Table 1. Energy and enthalpy of intermolecular interactions between groups of hydrocarbons of diesel fractions with vinyl acetate and undecylamine of itaconic acid

Hydrocarbon group	E of interactions, kJ/mol	E of interactions, kJ/mol
Paraffins	14.91	–25.00
Naphthene substituted	13.54	–30.15
Benzene substituted	13.53	–26.83

The smallest enthalpy of interaction with the additive is observed for aromatic hydrocarbons, which indicates that diesel fuel containing the largest amount of aromatic hydrocarbons will be the most responsive to DD additive. The highest enthalpy of interaction is observed for paraffinic hydrocarbons, which indicates that diesel fuel containing the largest amount of paraffinic hydrocarbons will negatively affect the injectivity of diesel fuel to the DD additive.

Earlier, the hydrocarbon composition of DF was determined (Table 3) [1].

The highest content of aromatic hydrocarbons is observed for DF №3 (26.55 %), therefore, with the addition of an additive of 0.01 %, the greatest decrease in PP (21 °C) is observed. For DF №1, a similar situation is observed (a decrease of 19.8 °C). The largest amount of paraffins is observed for DF №4 (63.46 %) and DF №5 (62.60 %), therefore, with the addition of 0.01 % additive, the smallest decrease in PP is observed, 7.2 °C for DF №4 and 12.9 °C for DF №5.

For DF №2, there is also a high content of paraffins (62.58 %), and a low content of aromatics (16.90 %), which should indicate the poor injectivity of diesel fuel to the DD additive. However, there is a large decrease in PP. This is due to the fact that, in contrast to DF №1, 3, 5, in DF №2 the ratio of aromatics to naphthenes is < 0.8 (0.79). Thus, the content of aromatics more than 20 % and the ratio of aromatics to naphthenes < 0.8 have the greatest influence on the injectivity of diesel fuel to DD additive. The content of paraffins in the composition of diesel fuel > 60 % worsens the injectivity of diesel fuel to DD additive.

Table 2. Low-temperature properties of DF, depending on the concentration (Cad) of the depressant-dispersant additive

Cad, %	DF №1			DF №2			DF №3		
	CP, °C	CFPP, °C	PP, °C	CP, °C	CFPP, °C	PP, °C	CP, °C	CFPP, °C	PP, °C
0	–25.4	–27	–33.9	–25.5	–26.4	–36.7	–25.4	–26.7	–34.8
0.009	–24	–35.2	–53.1	–25.7	–37	–55.5	–22.5	–33	–49.7
0.01	–23.9	–36	–53.7	–24.5	<–25.8	–54.2	–23	<–24.4	–56

Cad, %	DF №4			DF №5		
	CP, °C	CFPP, °C	PP, °C	CP, °C	CFPP, °C	PP, °C
0	–2.5	–6.1	–13.4	–16.2	–21.2	–24.5
0.009	–4.5	–17.7	–28.2	–17.7	–27.5	–34.2
0.01	–2.3	–11.4	–20.6	–17.2	–29.1	–37.4

Table 3. Hydrocarbon composition of diesel fractions

Hydrocarbon, % wt	DF №1	DF №2	DF №3	DF №4	DF №5
Paraffins, %	49.74	62.58	58.72	63.46	62.60
Aromatics, %	24.85	16.90	26.55	17.03	22.38
w(aromatics)/w(naphtenes)	1.16	0.79	1.96	0.95	2.95

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