## **COMMERCIAL DIESEL FUEL PRODUCTION** USING BIODIESEL SYNTHESIZED FROM VARIOUS PLANT FEEDSTOCK

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The transition to a low-carbon economy and renewable energy sources is becoming a popular direction in the energy industry development [1]. The increasing diesel fuel (DF) distribution also entails the alternative direction development - biodiesel fuel (BioDF) production.

BioDF is a blend of fatty acids monoalkyl esters obtained as a result of the renewable biological resources transesterification reaction (oils, fats, waste, algae, etc.).

In this work was investigated the BioDF effect on the DF properties, regulated by [2], such as density  $(\rho)$ , kinematic viscosity (v), cold filter plugging point (CFPP).

BioDF was synthesized by transesterification reaction from various vegetable oils: sunflower (SBioDF), linseed (LBioDF), mustard (MBioDF), and rapeseed (RBioDF). The transesterifying agent was ethyl alcohol, the catalyst – sodium hydroxide. The oil: ethanol ratio was 1:6, the catalyst concentration – 1.75% by vegetable oil weight. The synthesis was carried out for 1 hour at 45 °C.

The results of studying the DF characteristics and the obtained BioDF are presented in Table 1.

BioDF does not conform the requirements [2] for commercial DF, due to its high viscosity and density, hereat BioDF is used as an additive to DF at a certain concentration [3]. As part of the work, blends with various BioDF concentrations were prepared. The following designations were assigned to the blends: B5, B10, B15, B20, where the figure denotes the BioDF content in the blend in %vol. The determined characteristics results of DF blends with BioDF are presented in Tables 2 and 3.

As can be seen from Table 2, the addition of BioDF to DF negatively affects the physicochemical properties of the latter. It should be noted that all the obtained blends conform the requirements [2] in terms of density (no more than 863.4 kg/m<sup>3</sup>) and viscosity (permissible limits 3.0-6.0 mm<sup>2</sup>/s) for grades S (Summer) and E (Inter-season). According

Table 1. Characteristics of DF and obtained BioDF						
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Table 1

Characteristic	DF	SBioDF	LBioDF	MBioDF	RBioDF
$\rho$ at 15 °C, kg/m <sup>3</sup>	837.3	888.2	897.1	891.1	900.1
<i>v</i> at 20 °C, mm <sup>2</sup> /s	3.96	9.62	8.88	11.53	20.18
CFPP, °C	-5	-6	-11	-14	-14

Characteristic		SBi	oDF		LBioDF			
	B5	B10	B15	B20	B5	B10	B15	B20
$\rho$ at 15 °C, kg/m <sup>3</sup>	839.4	841.9	844.5	846.9	839.8	843.4	846.2	849.5
v at 20 °C, mm <sup>2</sup> /s	4.13	4.33	4.53	4.74	4.31	4.28	4.44	4.62
CFPP, °C	-7	-7	-7	-11	-10	-10	-10	-12

Characteristics of DF blends with MBioDF and RBioDF Table 3.

Characteristic	SBioDF			LBioDF				
	B5	B10	B15	B20	B5	B10	B15	B20
$\rho$ at 15 °C, kg/m <sup>3</sup>	839.6	842.3	845.1	847.7	840.3	843.2	846.6	849.7
v at 20 °C, mm <sup>2</sup> /s	4.28	4.54	4.62	4.87	4.29	4.62	4.98	5.41
CFPP, °C	-7	-11	-11	-11	-11	-11	-12	-12

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

## References

- 1. Special report: global warming of 1.5 °C https://www.ipcc.ch/sr15/chapter/spm/ (application date: 17.02.2021).
- 2. USS 305-2013 "Diesel fuel. Specifications", 2014. 10 c.

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 inter						
	actions between groups of hydrocarbons of						
	diesel fractions with vinyl acetate and un-						
	decylamine of itaconic acid						

Hydrocar- bon group	E of interac- tions, kJ/mol	E of interac- tions, kJ/mol				
Paraffins	14.91	-25.00				
Naphthene substituted	13.54	-30.15				
Benzene sub- stituted	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