By combining the ML model with GA, we identified most effective NPs with selective antimicrobial properties, screening approximately 500 candidates per second. As a proof of concept, we identified CuO NP (with the main parameters: NP obtained with green synthesis, nanorods in shape, the average NP size of 30 nm, and the reaction time of 2 hours) as one of the top selectively antimicrobial NP. It showed minimal bactericidal concentration (MBC) of 62.52 µg/ml against *Staphylococcus aureus* whereas it achieved MBC of 455.37 µg/ml for *Bacillus subtilis*. Hence, the selectively antimicrobial CuO NP demonstrated higher toxicity against pathogenic *Staphylococcus aureus* compared to non-pathogenic *Bacillus subtilis*, with a concentration difference of 392.85 µg/ml. The antimicrobial selectivity of NPs may be attributed to a complex interaction between the NPs and diverse microbial strains. This research marks a significant advancement in exploring selectively toxic NPs, presenting a novel avenue for precision medicine and customized therapeutic approaches to combat pathogenic infections.

Reference

1. *Dadgostar P. Antimicrobial Resistance: Implications and Costs // Infect Drug Resist. – 2019. – V. 12. – P. 3903. – doi: 10.2147/IDR.S234610.*
2. *Ramadan N. et al., Nanotechnology as a Promising Approach to Combat Multidrug Resistant Bacteria: A Comprehensive Review and Future Perspectives // Biomedicines. – 2023. – Vol. 11. – № 2. – P. 413. – doi: 10.3390/BIOMEDICINES11020413.*
3. *Amaro F., Morón Á., Díaz S., Martín-González A. and Gutiérrez J.C. Metallic Nanoparticles-Friends or Foes in the Battle against Antibiotic-Resistant Bacteria? // Microorganisms. – 2021. – V. 9. – № 2. – P. 1–11. – doi: 10.3390/MICROORGANISMS9020364.*

PRODUCTION OF MOTOR FUEL COMPONENTS USING A COMPLEX CATALYST: HYDROTREATING AND ZSM-5 ZEOLITE

Y. S. Kokorina, I. A. Bogdanov, A. A. Altynov, D. V. Sosnina
Scientific supervisor – assistant I. A. Bogdanov
Linguist – I. A. Bogdanov

National Research Tomsk Polytechnic University
ysk14@tpu.ru

One of important renewable resources for reducing dependence on petroleum products and decrease carbon footprint are vegetable oils. The production and use of fuels obtained from vegetable oils can reduce emissions of carbon oxide, carbon dioxide and other toxic gases into the atmosphere, which contributes to the overall fight against climate change [1].

In this work, corn, sunflower and rapeseed oils were processed using the Al–Co–Mo complex hydrotreating catalyst and the ZSM-5 zeolite catalyst.

Processing of vegetable oils were carried out at the laboratory catalytic unit with fixed-bed catalyst. Table 1 shows the technological parameters of processing.

Catalysts (10 cm^3) were alternately loaded into the reactor in equal volumes. In the reactor, vegetable oil first go through the hydrotreating catalyst and then go through the zeolite catalyst. The catalysts were pre-calcined for 3 hours in a hydrogen current at 375 °C. The fraction of zeolite catalyst has sizes ranging from 0.5 to 1 mm.

Table 1. Technological parameters of oils processing

Technological parameter	Value
Pressure, mPa	7
Temperature, °C	375
Hydrogen consumption, ml/min	35
Feedstock space velocity, ml/min	0.08

Table 2. Group composition of products of catalytic processing of vegetable oils

Group	Content, % wt.		
	Corn oil product	Sunflower oil product	Rapeseed oil product
Iso-paraffins	17.63	18.75	3.14
N-paraffins	7.58	5.95	3.47
Naphthenes	6.86	6.37	1.81
Olefins	2.23	2.31	1.99
Alkynes	0.05	0.04	–
Aromatic hydrocarbons	48.27	48.58	68.31
Oxygen-containing	2.33	2.31	1.45
Not Identified	15.04	15.69	19.83

Table 3. Fractional composition of the product obtained by catalytic processing of rapeseed oil

Fraction of distillation fraction, % vol.	Temperature, °C
The beginning of boiling	38
10	61
20	84
30	110
40	133
50	154
60	180
70	270
80	307
90	322

As a result of the processing of vegetable oils, liquid products with a water content of 16–18 % by weight were obtained.

To determine the group composition of catalytic processing products, chromathomas-spectrometric analysis was carried out on the Chromatec Crystal 5000.2 device with an HP-1-MS column (30 m; 0.25 mm; 0.25 micrometers). The results of determining the group composition of products are presented from Table 2.

Based on the results from Picture 1, aromatic hydrocarbons account for a large share. Moreover, in the product of rapeseed oil processing, aromatic hydrocarbons are 20 % by weight. more than in the products of corn and sunflower oil processing. For further research, the product of catalytic processing of rapeseed oil was selected as the most promising.

The fractional composition was analyzed in accordance with the method [2] and the product of catalytic processing of rapeseed oil was divided into fractions. The results of the analysis of the fractional composition of the resulting product are presented in Table 2.

From the obtained results, it follows that the sample has a wide fractional composition and includes gasoline (boiling limits: IBP-180 °C) and diesel (boiling limits: 180 °C-EBP) fractions. Moreover, the separation into gasoline and diesel fractions occurs in approximately equal proportions of the total amount of the product under study, which indicates the profitability of catalytic processing.

Reference

1. *Evteev V.K., Vasil'ev F.A. Vozmozhnosti primeneniya topliva na osnove vegetablenogo masle v Irkutskoy oblasti [Possibility of using fuel based on vegetable oil in the Irkutsk region] // Topical Issues of Agrarian Science. – 2018. – № 29. – P. 5–12.*
2. *GOST 2177-99 Petroleum Products. Methods for determining fractional composition. – Moscow : Standartinform, 2006. – 23 p.*