analysis indicate the dominance in the product of three crystalline phases: silicon carbide, silicon and graphite.

According to the presented data the product consists mainly of the cubic phase of silicon carbide (48,1 %) graphite carbon structures differing in the parameters of the unit cell (46,5 %) and silicon (5,4 %).

It can be concluded that it is possible to obtain a composite dispersed material based on carbon fibers and the cubic phase of silicon carbide in a DC arc discharge plasma. Within the framework indicated in this paper, studies are being conducted on the control of phase composition of the product and its consolidation into high-density ceramics with given properties. According to the literature review, evidence of obtaining such materials was not found without the use of vacuum-gas equipment to protect components and synthesis products from oxidation. As a result, this approach leads to positive economic effect and relatively high method performance.

References

1. *R.A. Andrievski // Nano-sized silicon carbide: synthesis, structure and properties, 2009.– 78(9).– P.821–831.*
2. *Wu R., Zhou K., Yue CY, Wei J, Pan Y. // Recent progress in synthesis, properties and potential applications of SiC nanomaterials. Progr. Mater.Sci., 2015.– Vol.72.– P.1–110.*
3. *Pak A.Y., Rudmin M.A., Mamontov G.Y., Bolotnikova O.A. Electroarc Synthesis and Cleaning from Carbon Impurities of Cubic Silicon Carbide in the Air Atmosphere. Journal of Superhard Materials, 2018.– №40.– P.157–163.*

MATHEMATICAL MODELING OF CATALYTIC REFORMING PROCESS

I.R. Dolgov
Scientific adviser – Candidate of Engineering sciences, Associate Professor N.S. Belinskaya;
Candidate of Engineering sciences, Associate Professor M.V. Kirgina
Linguist – Doctor of Philological sciences, Associate Professor I.A. Matveenko

National Research Tomsk Polytechnic University
634050, Russia, Tomsk, 30 Lenin Avenue, ilya.dolgov94@mail.ru

At present, the main tasks of the oil refining industry are increasing production volumes of petroleum products, the expansion of product range, and quality improvement [1]. Changing in petroleum refining technology are due to an increase in the share of refined sulfur, high-sulfur and high-paraffin oils. Simultaneously, the requirements for modern gasoline quality are getting severer. In this regard, secondary processes, especially catalytic ones, have taken increasing priority, among which the catalytic reforming process is of particular importance [2].

The method of mathematical modeling has found wide application in chemical technology. It enables to carry out computational experiments of complex chemical processes at low costs [3], to monitor the operation of industrial facilities and to carry out optimization.

The purpose of this research was to design a mathematical model of the catalytic reforming process. The research objects were three catalytic reforming units.

At the first stage of research, six main types of reactions were considered to develop a formalized scheme of chemical transformations taking place in the catalytic reforming process: six-membered naphthene dehydrogenation, five-membered naphthene dehydroisomerization, paraffin dehydrocyclization, paraffin, naphthene and aromatic isomerization, hydrocracking, hydrodealkylation. All theoretically possible chemical reactions were registered. The result was a list of 948 theoretically possible reactions.

At the second stage of research, the chromatograms of hydrogenate (raw material) and stable catalyzate (product) within the period from 2015 to 2016 years were analyzed. Substances, which concentration was less than 1 wt.%, were combined and presented as pseudo-components. As a result, a list of 55 components (40 individual and 15 pseudo-components) involved in catalytic reforming process was made. Thus, after aggregation the list of chemical reactions was shortened to 505.

The next step was the calculation of the thermodynamic parameters of chemical reactions in the

Gaussian software package (GaussView 3.0; Gaussian 09 W). The calculation was carried out at the temperatures of 753 K (480 °C) and 793 K (520 °C) and at a pressure of 14 atm (1.4 MPa). After calculation, the total number of thermodynamically possible reactions ($\Delta G < 0$) was reduced to 305.

The research has contributed to the development of formalized scheme of substances transformations in the catalytic reforming process. The scheme includes 55 components (40 individual and 15 pseudo-components) and 305 thermodynamically possible reactions.

The selected high detail level will ensure the high sensitivity of the mathematical model to changes in the composition of raw materials and high accuracy of calculations.

References

1. *Ivanchina E.D., Kirgina M.V., Chekantsev N.V., Sakhnevich B.V., Sviridova E.V., Romanovskiy R.V. Complex modeling system for optimization of compounding process in gasoline pool to produce high-octane finished gasoline fuel // Chemical Engineering Journal, 2015.– Vol.282.– P.194–205.*
2. *Dyusembaeva A.A., Vershinin V.I. Modeling of Reforming of Straight-Run Gasoline (Fraction 85–140 °C) with Allowance for Deactivation of the Platinum Catalyst // Kataliz v promyshlennosti, 2016.– 16(5).– P.24–29.*
3. *Belinskaya N.S. Mathematical modeling and optimization of catalytic dewaxing of diesel oil cuts and atmospheric gas oil // Petroleum and Coal, 2016.– Vol.58(1).– P.126–134.*

GRAMICIDIN S COMPOSITION WITH SURFACTANTS FOR LIQUID DRUG FORMULATION

A.A. Drannikov[1,2]

[1]National Research Tomsk Polytechnic University
634050, Russia, Tomsk, 30 Lenin Avenue, a.drannikov@pfk-obnovlenie.ru

[2]JSC «PFK Obnovlenie»
630096, Russia, Novosibirsk, 80 Stancionnaya st.

New antibiotics investigation has been the subject of recent years fundamental and applied research in the ever-growing resistance of microorganisms towards antimicrobial agents [1]. Despite all the efforts recent WHO report demonstrates that the threat of antimicrobial resistance is always increasing in current conditions [2].

Gramicidin S is a natural peptide which exhibits strong antibiotic activity towards Gram-negative and Gram-positive bacteria and several pathogenic fungi as well interacting with the cell-membranes to make the canals for ion-erosion [3].

However, due to low solubility Gramicidin S formulation is generally fabricated in solid state dosage form [4].

In the present work, Gramicidin S was solubilized forming the microemulsion based on tween-80 as surfactant since it has the appropriate properties for peptide solubilization as determined previously [5].

The main aim was to form a stable Gramicidin S composition that saves its antimicrobial activity and demonstrates no more side-effects comparing to tablets.

The resulting emulsion showed poor stability and lost its homogeneity in several months which resulted in phase separation.

Next step was to add co-surfactant in order to stabilize tween-80 loaded with gramicidin S in water with propylene glycol used as a co-surfactant.

The obtained emulsion demonstrated enhanced stability being stored under room temperature.

Also the antimicrobial properties were enhanced comparing to ethanoic solution of gramicidin S that can be described by the presence of surfactants in ready formulation [6].

Forward studies let us find the optimal rate of the components in the microemulsion obtained that provides the system stability for the longest time.

The structure of the resulting composition was characterized using DLS and SEM methods which have proved the stable emulsion formation.

As a result gramicidin S loaded in tween-80 microemulsion can be regarded as promising composition for liquid drug formulation of the peptide for oral and topical application.