SiC-based ceramics composition and a method for production thereof.

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DEVELOPMENT OF MATHEMATICAL MODEL OF CATALYTIC CRACKING TAKING INTO ACCOUNT THE IRREVERSIBILITY CRITERION OF REACTIONS

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Currently, the development of secondary refining processes for increasing the refining depth and production of high-octane motor fuels is typical for oil refining industry. Computer modeling of chemical-engineering processes is one of the effective methods for studying of the complex systems. Improving the efficiency of the oil refining units and the optimization of technological modes is possible to be carried out using mathematical modeling method.

The majority of mathematical models of oil refining and petrochemistry processes are built on the basis of equations describing the kinetics of chemical conversions in reactor. However, the specificity of hydrocarbons conversions of petroleum feedstock in the forward and reverse directions is not fully taken into account many models. It reduces the accuracy of calculations and the efficiency of the mathematical model application.

The aim of research is the development of the catalytic cracking mathematical model taking into account the reversibility of reaction in the height of riser.

According to [1] the correct criterion of thermodynamic irreversibility of some stage in the chain of chemical transformations is the significant change in the chemical potential during the conversion of the reactants corresponding to this stage:

$$A_{ij} = -\Delta_r G_{ij} = \mu_i - \mu_j > RT$$

here A_{ij} – chemical attraction J/mol; $\Delta_r G_{ij}$ – Gibbs energy change, J/mol; R – gas constant, J/(K • mol); T – current temperature of process, K.

This approach allows to take into account the direction reactions at current time depending on the current concentrations and technological mode. Figure 1 shows the chart for implementation of this approach at the mathematical modeling of the catalytic cracking.

Thus, the values of the Gibbs energy change of the reactions calculated using quantum-chemistry methods were used for determination of thermodynamic reversibility of the catalytic cracking reactions at the initial time (an average initial temperature of reaction is 848 K). According to [1] only the isomerization reactions of paraffins are reversible at the initial temperature of reaction.

Furthermore, the chemical attraction is determined depending on the current concentrations of reactants and current temperature in riser. If the condition is satisfied, the reaction is irreversible (the reaction rate constant of the reverse reaction is $k_{-j} = 0$) and vice versa, if the reaction is reversible, the reaction rate constant is determined by the expression $k_{-j} = k_j / \mathbf{exp}(A_{ij}/RT)$.

The calculation on the model shows that the isomerization of paraffins (A_{ij} = –14.01 kJ/mol)

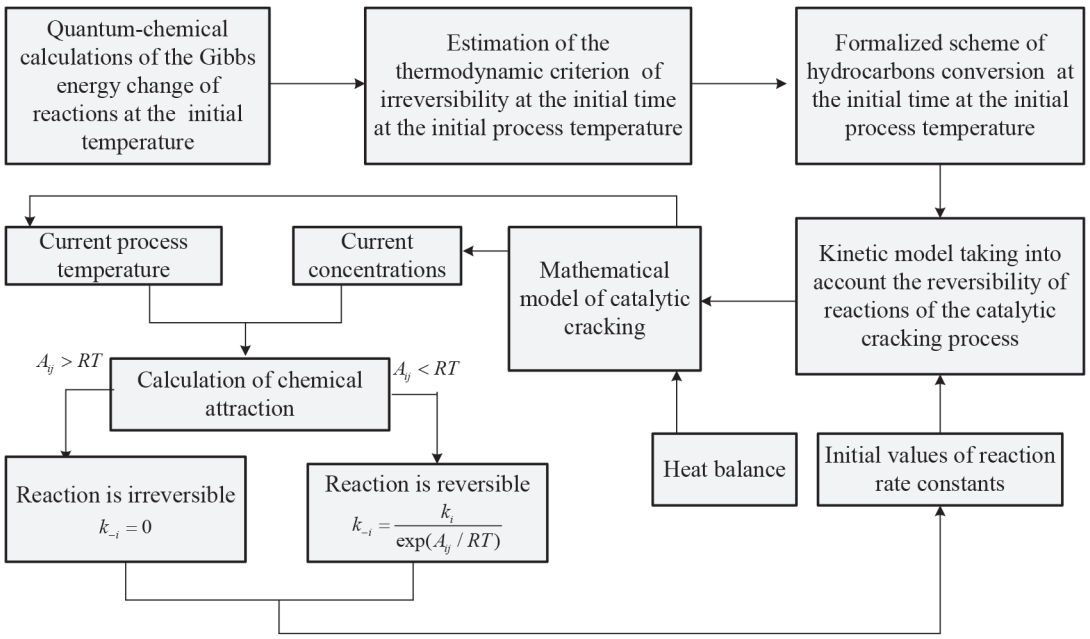

Fig. 1. *The chart for implementation of this approach at the mathematical modeling of the catalytic cracking*

and cyclization of olefins with hydrogen transfer (A_{ij}=4.62 kJ/mol) are reversible at the process temperature 794 K during the processing of vacuum distillate with saturated to aromatic ratio 1.88 unit and reaction temperature range is 848–794 K. In addition, the reversibility of cracking olefins take into account as the direct reaction of olefins aromatization in formalized scheme of hydrocarbon conversion due to the high reactivity of olefins according to the classical concepts of the catalytic cracking [2] and results of the quantum chemical calculation (ΔG=–92.2 kJ/mol).

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COMPARATIVE EVALUATION OF DIFFERENT RADICAL INITIATORS, USED FOR PRODUCTION OF GRAFT COPOLYMERS, BASED ON ATACTIC POLYPROPYLENE

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Introduction. Nowadays the demand for production of polypropylene is extremely high in the world. Polypropylene takes the 3rd place by volume of consumption now, and this number has increased from 200 to 1200 thousand tons per year in Russia in 2000–2015. It's obvious that the need of this polymer will keep growing, therefore the technologies of production should be developed and the volume of it ought to be increased.

Relevance. Polypropylene is most commonly produced by propylene polymerization in presence of the Ziegler–Natta catalyst [1, 2], yet at the end of the chemical process 2–3 % of the final product is an atactic polypropylene (abbreviated APP). This material has much lower quality in comparison with the isotactic polypropylene; therefore it isn't used in industry and is commonly utilized. A hypothesis was made [3] that a modification of APP with different graft copolymers could improve its characteristics and makes it suitable for using in industry. This approach might also contribute to a solution of economic and ecological questions in the subject of