

sider salting out effect. In addition, different cases of rectification block organization was compared – from simple distillation to pure aniline separation and intermediate rectification that gives a possibility to determine specification of upper product stream. These variants are shown in fig. 2.

Rectification (C in fig. 2) is optimal for polyamine synthesis because it allows overhead prod-

uct recycling and its utilization for washing stage. Thus, overall freshwater consumption by the technology could be minimized. For this case, optimal column number of stages and feed stage that allows minimizing reboiler heat duty was determined. Also column dimensions and hydraulics calculation was done for internals that are available in Aspen Plus database.

References

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STUDY OF CARBON NANOPOWDER FLUORINATION

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Fluorine and carbon compounds are widely used in industry, such as fluorolefins and freons. Fluorolefins are used as monomers for the synthesis of thermo- and chemically resistant polymers and copolymers, such as fluoroplasts and fluorocarbons, which have been widely used in engineering because of their properties. Freons, in turn, are used as refrigerants, feedstocks for industrial production of fluorolefins, for aerosols, etc. In addition, fluorocarbon compounds (perfluorocarbons) can potentially be used for terraforming, I don't know what makes them strategic substances.

These facts about fluorocarbon compounds make them quite important in technology and industry, so we decided to investigate the synthesis of new such substances, namely the possibility of creating a substance with the general formula C_xF_y , and $x \geq y$.

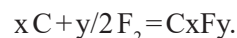
During the experiment, the carbon nanoparticle was fluorinated with elemental fluorine at a mass delivery rate of 1.4 g/h. The results are shown in Figure 1.

After interpolating the chart, the function is:

$$y = -0.151 \cdot \exp(-0.00276 \cdot x) + 0.2.$$

The order-one reaction graph and type-one adsorption isotherm can be described in terms of the time increase of the sample.

The general equation of reaction can be written as:



The increase in mass of the sample is then equal to the mass of fluorine reacted at time t.

Then, by comparing the resulting equation with the general linear record of the first-order reaction equation, the reaction rate constant is 0.00214 s^{-1} .

The kinetic equation of adsorption curves is described by the equation:

$$a_1 = a_\infty (1 - \exp(-K \cdot t))$$

a_1 , a_∞ – current and equilibrium absolute values of adsorption, respectively; K – adsorption coefficient [1].

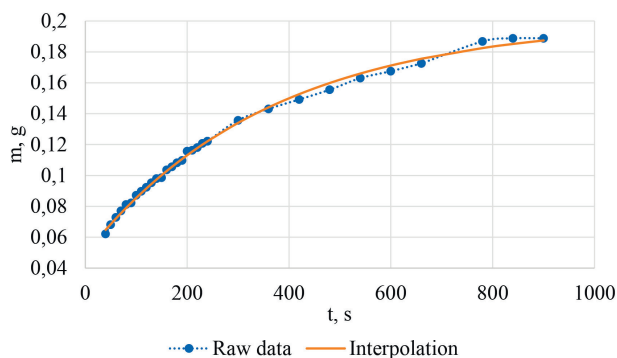


Fig. 1. Graph of the relationship of the carbon mass increase with the reaction time

Thus, it is difficult at the moment to judge the nature of the interaction. The results suggest that both chemical reaction and fluorine adsorption can be performed on the carbon surface. Further research will focus on the nature of the interaction and

its properties and criteria. One such experiment will be a multi-temperature reaction kinetics study that classifies this interaction as chemical. In case of adsorption, the type and laws of adsorption (chemical or physical adsorption) must also be defined.

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MODELING OF STABLE GAS CONDENSATE ZEOFORMING

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Nowadays, the oil refining industry produces a significant part of marketable products and semi-finished products, which constitute an important share of Russia's GDP. The production plants of this industry are usually based on catalytic chemical processes that use multicomponent mixtures of organic substances as feedstock.

Mathematical models of such processes, which sufficiently fully consider the process thermobaric conditions, the reactor's geometry, and the loss of catalyst activity, can provide significant support at the design stage.

This work describes the kinetic model development for the process of stable gas condensate on a zeolite catalyst. Gas condensate is a relatively light hydrocarbons that are in a supercritical state in reservoir conditions (in the gas phase). Stable gas condensate is obtained after removing light gases from gas condensate.

It is necessary to collect a theoretical and experimental information from the literature for the first developing stage of mathematical model. The collection of experimental data was carried out,

which were obtained on a laboratory catalytic unit of a flow type. The information about feedstock composition and (or) the content of the main components in products are also required for developing a kinetic model.

The hydrocarbon blends compositions were described by a list including 50 components. Based on the complex analysis of materials, a formalized scheme of chemical transformations was compiled. This scheme represents 180 thermodynamically possible chemical reactions. The system of differential equations was written in Python to perform calculations according to the law of mass action.

Using the evolutionary algorithm proposed by John Holland in 1975 [1], the inverse kinetic problem was solved by selecting the rate constants values of chemical reactions, which are included as coefficients in the system of differential equations describing the reaction rates.

Kinetic constants were matched for experiment, which was carried out with technological parameters: temperature of 375 °C, pressure of 0.25 MPa, feedstock volumetric flow rate 2 h⁻¹.

Table 1. The group compositions of the product

Component group	Sample 1 (exp.)	Sample 1 (calc.)	Sample 2 (exp.)	Sample 2 (calc.)
isoparaffins	40.004	41.520	42.000	42.365
n-paraffins	24.101	24.497	30.551	26.204
olefins	2.197	2.283	4.984	2.201
aromatic compounds	24.136	22.587	13.291	21.240
naphthenes	9.554	9.112	9.175	7.991