τ is the reaction time.

Constraints allowed to replace variables, that were made on the rate constants, based on the available information [4]:

$$k = \frac{k_{upp} - k_{low}}{\frac{k_{upp} - k_0}{k_0 - k_{low}} e^{-\xi} + 1} + k_{low}$$

where k_{upp} and k_{low} are respectively the upper and lower limits of the variation of the corresponding rate constant; k_0 is its initial value; ξ is a new variable that varies from $-\infty$ to $+\infty$, which minimizes.

Following data determined by computer analysis: the theoretical curve of conversion-time, a theoretical curve linked with the concentration of the Ru-carbene complex and theoretical weight average molecular mass. Imposed values limitations of elementary polymerization events made it possible to describe the experimental data. The calculated values of the rate constants of initiation and chain growth were as follows: $k_i = 5{,}4 \bullet 10^{15} \bullet e^{\frac{-92800}{RT}}$ and $k_p = 8{,}3 \bullet 10^{11} \bullet e^{\frac{-65200}{RT}}$ $L \bullet mol^{-1} \bullet s^{-1}$.

In fig. 1 the experimental conversion-time curves relevant to the polymerization of 5-Norbornene-2,3-dicarboximide-N-methyl acetate in the presence of Hoveyda-Grubbs II catalytic system at two different temperature are directly compared with the computed ones.

References

1. *Leal A.M.M., Kulik D.A., Smith W.R., Saar M.O. An overview of computational methods for chemical equilibrium and kinetic calculations for geochemical and reactive transport modeling. Pure and Applied Chemistry, 2017.– 89(5).– 597–643.*
2. *Gear C.W. Maintaining solution invariants in the numerical solution of ODEs. SIAM Journal on Scientific and Statistical Computing, 1986.– 7(3).– 734–743.*
3. *Nordsieck A. On numerical integration of ordinary differential equations. Mathematics of Computation, 1962.– 16.– 22–49.*
4. *Polak L.S., Goldenberg M.Ya., Levitsky A.A. Computational methods in chemical kinetics.– Nauka, Moscow, 1984.– 280p.*

GASOLINE PRODUCTION USING THE ZEOFORMING PROCESS PRODUCTS AND STABLE GAS CONDENSATE AS FEEDSTOCK

A.M. Temirbolat, A.A. Altynov

Scientific adviser – PhD student A.A. Altynov

Linguistic advisor – PhD-student A.A. Altynov

National Research Tomsk Polytechnic University

634050, Russia, Tomsk, 30 Lenin Avenue, aset_temirbolat@mail.ru

Stable gas condensate (SGC) is a blend of liquid hydrocarbons (C_{5+}), it was obtained as a by-product at fields, in the process of removing condensed hydrocarbon from natural gas. SGC is used as a feedstock in petrochemistry, as well as a blending component in the production of motor fuels.

The Zeoforming process allows the production of high-octane motor fuels by catalytic processing of low-octane gasoline fractions of various origins on zeolite catalysts [1].

The purpose of this work is to study the possibility of using zeoforming products (ZP) as blending components for the gasoline production. ZP were obtained under various process conditions and using SGC like a process feedstock.

In the course of the work, on the laboratory catalytic unit, the Zeoforming process was carried out, using a KN-30 zeolite catalyst. Test conditions are given in table 1.

Further, using the "Compounding" software [2], and based on various ZPs, recipes for blending gasoline AI-92 brand were developed (table 2). SGC, toluene and methyl tert-butyl ether (MTBE) were used as additional blending components. Characteristics of gasolines, obtained according to the developed recipes are presented in table 3. As can be seen from the table 3, all gasolines obtained according to the developed recipes meet the requirements of [3].

As can be seen from the data presented in Table 2, the most preferable is the recipe for blending

Table 1. Test conditions of the Zeoforming process

Product	ZP 1	ZP 2	ZP 3
Temperature, °C	375	400	425
Pressure, mPa	2.5		
Feedstock rate, ml/min	0.33		

Table 2. Recipes of blending AI-92 gasoline brand

Component, % wt.	ZP	SGC	Toluene	MTBE
ZP 1	70	6	24	0
ZP 2	22	41	25	12
ZP 3	18	45	25	12

Table 3. Characteristics of the gasoline

Characteristic	ZP 1	ZP 2	ZP 3	**Norm [3]**
RON	92.4	92.1	92.0	**92.0**
MON	84.6	83.4	83.2	**83.0**
SVP, kPa	43.8	57.5	58.4	**35.0–100.0**
Density 15 °C, kg/m^3	732.1	745.4	741.8	**725.0–780.0**
Benzene, % vol.	0.15	0.95	0.95	**1.00**
AH, % vol.	26.87	26.27	25.45	**35.00**
Olefins, % vol.	3.75	1.64	1.38	**18.00**

RON – octane number, research method; MON – octane number, motor method; SSP – saturation vapour pressure; AH – aromatic hydrocarbons.

AI-92 gasoline based on ZP 1 (maximum content of ZP and zero content of expensive MTBE). Thus, the optimum temperature for carry out the process of SGC zeoforming, from the point of view of the gasoline production, is a temperature of 375 °C.

References

1. *Nourcuk.ru [Electronic resource].– Electron is given. URL: http://www.nourcuk.ru/61-business/techraz/223-tseoforming, access free. – The date of circulation is January 31, 2019.*
2. *Altynov A.A., Bogdanov I., Kirgina M.V. Study of the possibility of using stable gas condensate as a component of automobile gasolines // Problems of Geology and Subsurface Development: Proceedings of the 22th International Scientific Symposium of students, Postgraduates and young Scientists Part II / Tomsk Polytechnic University.– Tomsk: TPU Publishing House, 2018.– P.369–370.*
3. *USS 32513-2013 "Automotive fuels. Unleaded petrol. Specifications".– M .: Standardinform, 2014.– P.16.*

THERMODYNAMIC ASPECTS OF REALIZATION OF COUPLED PROCESSES FOR THE ENERGY-SAVING SYNTHESIS OF ETHYL FORMATE

M.A. Trofimova, A.A. Sadaev
Scientific adviser – is PhD, Associate Professor M.A. Trofimova
Linguist – is PhD, Associate Professor M.A. Trofimova

Saint Petersburg State University
198504, Russia, Saint Petersburg, Peterhof, Universitetsky prospect, 26, m.trofimova@spbu.ru

Energy- and resource-saving environmentally friendly technologies are essential part of current chemical industry, which is explained by a tendency to comply with the principles of green chemistry and smart use of natural resources. Nowadays postulates of environmental compatibility and energy efficiency [1] is laid in the basis of development of new industrial chemical processes and optimizing of existing ones. Coupled processes joining phase transition with chemical reaction correspond to the above mentioned postulates and therefore they are important element of modern energy- and resource-saving technologies of the chemical industry. Inclusion in industrial production of such coupled processes as, for example, reactive distillation, which unites the stages of chemical reaction and distillation separation of substances, allows to achieve a significant increase in the conversion degree of reagents, re-