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Creation of the Formalized Scheme of Chemical Transformations for Pentane, Hexane and Heptane in Case of Their Processing on ZSM-5 Type Zeolite Catalyst

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Abstract

The active development of the gas industry and an increase in the production and treatment of natural gas makes the problem of the effective use of the obtained by-products more and more actual, in particular, stable gas condensates, consisting mainly of hydrocarbons with5-7 carbon atoms. One of the promising areas for the use of stable gas condensates is their processing into components of motor fuels at low-tonnage autonomous units using zeolite catalysts. For the effective use of these technologies, a detailed study of the chemical conversion's directions, occurring on zeolite catalysts, is necessary. This research directly for the stable gas condensates is complicated by their diverse hydrocarbon composition. It is expedient to study the directions of chemical conversions for pure hydrocarbons, which make up most of the composition of stable gas condensates. In the work using a laboratory catalytic unit and the ZSM-5 structural type zeolite catalyst, the processing of pure n-pentane, n-hexane, and n-heptane was carried out. The process was carried out in the temperature range of 375-425°C with a step of 25°C, at a constant pressure of 0.35 MPa and a weight hour space velocity of 2 h^{-1}. For the obtained products, the hydrocarbon composition was determined by the gas chromatography method. Based on the chromatographic analysis data, as well as theoretical aspects about the mechanism of the occurring chemical conversions on the ZSM-5 type zeolites, a list of theoretically possible reactions (865 reactions) was formed, for which thermodynamic parameters were calculated using the Gaussian software package under the conditions of the process realization. According to the results of thermodynamic analysis, it was found that under the process realization conditions on a zeolite catalyst, 777 reactions are thermodynamically possible. Based on the obtained results, a formalized scheme of C_5-C_7 hydrocarbons chemical conversions on ZSM-5 type zeolite catalyst has been developed.

Keywords: *Conversion scheme; Zeolite catalyst; Stable gas condensate; Pentane; Hexane; Heptane.*

1. Introduction

Modern trends in the strategic development of the oil and gas processing industry are associated with an increase in the depth of processing of hydrocarbon feedstock as well as with an increase in the quality of produced motor fuels. All of this determines the growing requirements for the resource-efficient use of light hydrocarbon feedstock, in particular, stable gas condensates (SGC), which are a by-product of natural gas treatment. The volumes of SGC production are stably growing in connection with the development of new fields and the implementation of advanced gas projects such as Nord Stream, Nord Stream-2, Power of Siberia, Turkish Stream [1-5], as well as the plan for accelerated gasification of the Russian Federation territories [6]. In addition, the Russian Federation is actively developing the production of liquefied natural gas (LNG) (projects Sakhalin-2, Yamal LNG, Baltic LNG) [7-9], this industry will also increase the volume of SGC production. One of the promising directions for using SGC is its catalytic processing into components of motor gasoline [10].

At the same time, the large remoteness of oil and gas production areas (the main oil and gas producing enterprises are located at a distance of at least 2000-4000 km from major

cities), as well as the labor intensity and high cost of supplying fuel and lubricants, sets the task for the industry in providing motor fuel for its own needs at the fields.

A possible solution to this problem is the building of low-tonnage modular units in the field's areas using effective technologies based on the use of zeolite catalysts. Using such units shall it is possible to ensure the complex processing of light hydrocarbon feedstock and significantly reduce the prices of various motor fuels, including by reducing the cost of their transportation.

Nowadays zeolites are one of the most promising catalysts in the processes of obtaining and upgrading motor fuels, which is associated with their high activity and selectivity in cracking, isomerization and oligomerization reactions, low cost, and high resistance to the action of catalytic poisons – organic hetero-compounds of nitrogen and sulfur [11]. In addition, zeolite catalysts are used for biomass valorization processes to produce both biofuels and/or bio-based chemicals, which is an emerging and fast-expanding field [12]. The most widely used is zeolite catalysts with the ZSM-5 structure type. So in works [13] this type of catalysts is used for the synthesis of clean jet fuels by 1-hexene oligomerization, and in work [14] for oligomerization of olefins from light cracking naphtha for the production of high quality diesel fuel. In addition, zeolites of the ZSM-5 type are used in catalytic cracking processes. [15-17].

It should also be noted the trend of digitalization of industrial production and the active creation of digital twins of technological processes. However, the develop a mathematical description of a chemical technological process, it is necessary to understand the chemistry of the process, i.e. the main ongoing chemical transformations, as well as the thermodynamic and kinetic parameters of reactions.

The hydrocarbon composition of SGC is diverse, represented by several hundred individual hydrocarbons and largely depends on the field of production and production technology. However, according to [18], paraffinic hydrocarbons prevail in the composition of SGC, their part is from 40 to 70% wt., while the main part (from 15 to 30% wt.) is paraffins with the number of carbon atoms from 5 to 7 (C_5-C_7). It is the C_5-C_7 paraffinic hydrocarbons that actively participate in the transformations taking place on the acid sites of zeolite catalysts, which lead to the formation of high-octane components of motor gasoline (aromatic hydrocarbons, isoparaffins). To develop a mathematical model of the processing of SGC on a zeolite catalyst, it is most important to study the directions of these hydrocarbon's conversion. This work aim is to create the formalized scheme of chemical transformations for pentane, hexane and heptane in case of their processing on ZSM-5 type zeolite catalyst.

2. Materials and methods

In the work, the process on a zeolite catalyst was realized using the chemically pure n-pentane, n-hexane, n-heptane (paraffins C_5-C_7), as well as a zeolite catalyst of the structural type ZSM-5, grade KN-30, produced by PJSC "Novosibirsk Chemical Concentrates Plant". The specific surface area of the KN-30 catalyst is more than 300 m^2/g, composition: SiO_2 – 90.0-97.6% wt.; Al_2O_3 – 1.4-2.7% wt.; Na_2O – less than 0.1% wt.; Fe_2O_3 – 0.35-1.25% wt. The hydrocarbon composition of products in the work was determined by the gas-liquid chromatography method using a Chromatek-Crystall 5000 chromatograph (with a quartz capillary column 25 m × 0.22 mm, stationary phase – SE-54, carrier gas – helium), according to [19].

The calculation of thermodynamic parameters in this work was carried out using quantum-chemical calculation methods in the Gaussian software package. The nonempirical Density Functional Theory (DFT) method was used as a calculation method. The theoretical approximation was the B3LYP model (the theory of the Becke density functional (B3), using the electronic correlation of Lee Yang and Steam (LYP)), the basis 3-21G [20]. The calculations were carried out under the conditions (temperature, pressure) of the laboratory processing on a zeolite catalyst.

The processing of C_5-C_7 hydrocarbons on a zeolite catalyst was carried out on a laboratory catalytic unit "CATACON". The technological scheme of the unit, as well as the scheme of the reactor, are presented in the earlier works of the author's team [21].

At the stage of preliminary preparation, the catalyst was ground in a mortar and sieved through sieves to select a fraction of 0.5-1.0 mm^2. After that 10 cm^3 zeolite catalyst was

loaded into the reactor of a laboratory catalytic unit. At the next stage, the catalyst was activated to remove adsorbed moisture and organic matter from the catalyst surface. During activation, the catalyst was calcined for eight hours at a temperature of 500°C in a stream of nitrogen.

The processing of C_5-C_7 hydrocarbons on a zeolite catalyst was carried out at the technological parameters presented in Table 1.

Table 1. Technological parameters of the C_5-C_7 hydrocarbons processing on a zeolite catalyst

Test number	Temperature, °C	Pressure, MPa	Weight hour space velocity, h^{-1}
1	375	0.25	2
2	400		
3	425		

3. Results and discussion

Figure 1 shows the results of determining the group hydrocarbon composition of the n-pentane processing products on a zeolite catalyst, obtained under conditions of varying the process temperature in the range of 375-425°C.

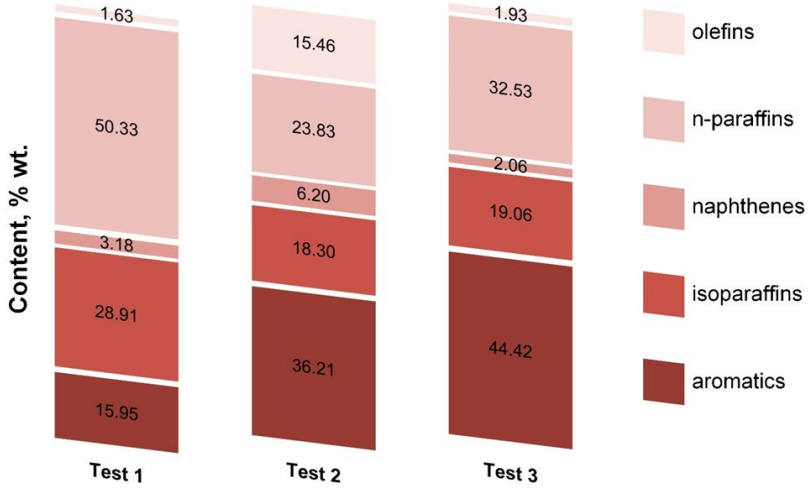

Fig. 1. Group hydrocarbon composition of the n-pentane processing products, obtained under different process temperature

According to the obtained results, with an increase in the temperature of n-pentane processing, the following trends are observed for the obtained products:

1. The content of aromatic compounds increases. The main representatives of aromatic hydrocarbons at all temperatures of the process are toluene and xylenes.
2. The isoparaffins content is maximum at a process temperature of 375°C. The main product at 375°C is isopentane. At process temperatures of 400 and 425°C, the content of isopentane and its contribution to the total content of isoparaffins decreases, but remains the highest.
3. The maximum content of naphthenes is observed at a process temperature of 400°C, moreover, half of these naphthenes are heavy C_{9+} hydrocarbons (more than 9 carbon atoms in a molecule), which are practically not formed at process temperatures of 375 and 425°C.
4. The content of n-paraffins in obtained products has a minimum at a process temperature of 400°C. This result is explained by the fact that a significant part of the initial n-pentane does not react at a process temperature of 375 °C (the content of n-pentane in the product of its processing at 375°C is 35.00% wt.). An increase in the content of n-paraffins at a process temperature of 425°C relative to the content at a temperature of 400°C occurs mainly due to an increase in the content of heavy C_{9+} n-paraffins in the products, with a simultaneous decrease in the content of n-pentane. This fact indicates the occurrence of

hydrogen transfer reactions in olefins with the formation of unsaturated hydrocarbons and heavy n-paraffins.

5. The olefin content in the obtained products has a maximum at a process temperature of 400°C. The main part of olefins at all temperatures of the process is heavy C_{8+} hydrocarbons. Olefins in the system are formed as a result of cracking reactions and then participate in hydrogen transfer reactions with the formation of heavy paraffins and aromatic compounds. The obtained distribution of the olefin content allows us to assume that at a process temperature of 375°C, the cracking of n-pentane is the limiting stage of the described sequence of transformations, and at a temperature of 400 °C the reaction of hydrogen transfer in olefins.

Figure 2 shows the results of determining the group hydrocarbon composition of the n-hexane processing products on a zeolite catalyst, obtained under conditions of varying the process temperature in the range of 375-425°C.

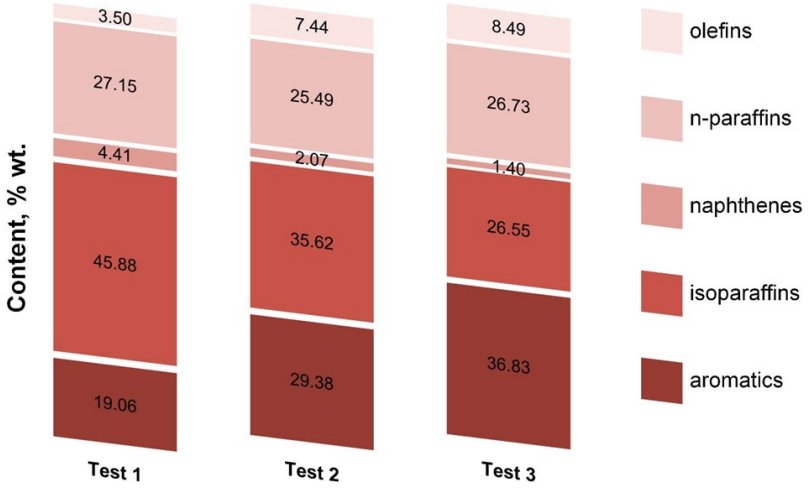

Fig. 2. Group hydrocarbon composition of the n-hexane processing products, obtained under different process temperature

According to the obtained results, with an increase in the temperature of n-hexane processing, the following trends are observed for the obtained products:

1. The content of aromatic compounds in the obtained products increases. The main aromatic hydrocarbons observed in products are toluene and xylenes, with the toluene : xylenes ratio increasing with increasing process temperature.
2. The content of isoparaffins decreases. Note that at a process temperature of 375°C, the most common isoparaffins are 2-methylpentane and dimethylpentanes; at a temperature of 400°C – 2-methylpentane, isopentane, isobutane and dimethylbutanes; at a temperature of 425°C – isobutane and isopentane, however, the part of 2-methylpentane and dimethylbutanes remains significant. Thus, a decrease in the content of isoparaffins with an increase in the process temperature is associated with a decrease in the stability of C_{6+} isoparaffins.
3. The content of naphthenes decreases, the main representatives of which at all studied process temperatures are methylcyclopentane and dimethylcyclopentane.
4. The total content of n-paraffins changes slightly. At the same time, for a process temperature of 375°C, the main representative of paraffins (9.30% wt.) is n-butane, less common are n-pentane, propane, and heavy n-paraffins. With an increase in the process temperature, the yield of light C_3-C_4 n-paraffins practically does not change, the yield of C_5-C_8 n-paraffins decreases, and the yield of heavy C_{9+} n-paraffins, which are one of the products of the hydrogen transfer reactions in olefins, increases. In contrast to the processing of n-pentane, where the conversion of the feedstock at a process temperature of 375°C was only 65%, the conversion of n-hexane exceeds 96% at all process temperatures.

5. The content of olefins in the obtained products increases. The main representative of this class of hydrocarbons at a process temperature of 375°C is methylenecyclopentane, and at temperatures of 400 and 425°C – 1,3,5-hexatriene. These compounds contain six carbon atoms, as does the n-hexane feedstock molecule, which explains their relatively high yield at appropriate temperatures. Since these compounds were not found in the products of n-pentane and n-heptane processing (where benzene, isoparaffins, and naphthenes with six carbon atoms are present), it can be assumed that they are intermediate compounds for the transformation chains, which are characteristic for the n-hexane processing.

Figure 3 shows the results of determining the group hydrocarbon composition of then-heptane processing products on a zeolite catalyst, obtained under conditions of varying the process temperature in the range of 375-425°C.

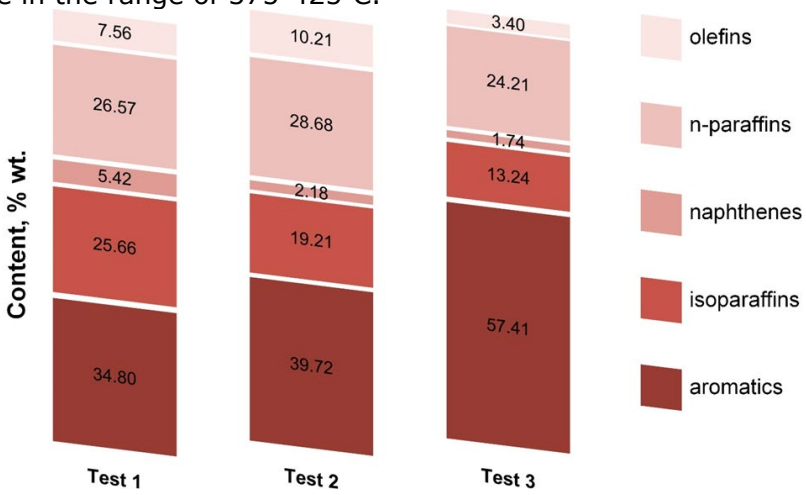

Fig. 3. Group hydrocarbon composition of the n-heptane processing products, obtained under different process temperature

According to the obtained results, with an increase in the temperature of n-heptane processing, the following trends are observed for the obtained products:

1. The content of aromatic compounds increases. Moreover, at a process temperature of 375°C, a significant content of heavy C_{9+} aromatic compounds is observed, which is not typical for process temperatures of 400 and 425°C, and is also not observed in the previously considered processing products of n-pentane and n-hexane. The main representatives of aromatic hydrocarbons are toluene and xylenes.
2. The content of isoparaffins decreases. At a process temperature of 375°C, this class of compounds is mostly represented by isopentane, heavy C_{9+} isoparaffins, isobutane, methylpentanes. The content of isopentane and isobutane increases with an increase in the process temperature, and the part of heavy C_{9+} isoparaffins decreases due to an increase in the rate of cracking reactions.
3. The content of naphthenes decreases, the representatives of which are methylcyclopentane, dimethylcyclopentane, ethylcyclopentane, C_8 naphthenes, as well as heavy C_{9+} compounds. This is explained by the fact that with an increase in the process temperature, the equilibrium of the hydrogen transfer reaction changes towards the formation of reaction products:

$$O + N \rightarrow A + P$$

where O – olefin, H – naphthene, A – aromatic hydrocarbon, P – n-paraffin.

4. The content of n-paraffins changes insignificantly, passing through a maximum at a process temperature of 400°C. At all temperatures under study, the main components are heavy C_{9+} n-paraffins (products of the hydrogen transfer reaction) and also n-butane and n-pentane, which are present in the products due to the relatively high stability of C_5-C_4 hydrocarbons in the temperature range of 375-425°C.

5. The olefin content passes through a maximum at a process temperature of 400°C. Unlike the products of n-hexane processing, where olefins were mainly represented by C_6 compounds, heavy C_{8+} compounds are the most common olefins among the products of n-heptane processing.

Among the general trends typical for the processing of C_5-C_7 hydrocarbons on a zeolite catalyst, it should be noted that with an increase in the process temperature, the yield of aromatic compounds, represented to the greatest extent by toluene and xylenes, increases significantly. With an increase in process temperature, the content of isoparaffins in the obtained products decreases due to cracking reactions of C_{6+} isoparaffins, while isopentane remains stable in the temperature range of 375-425°C. The yield of naphthenes decreases with an increase in the process temperature due to a change in equilibrium in the reactions of hydrogen transfer towards the formation of products. The content of n-paraffins in the products practically does not depend on the process temperature, however, as the temperature rises, the content of heavy C_{9+} paraffins increases and the content of C_6-C_8 n-paraffins decreases. Olefins are intermediate compounds and their yield significantly depends on the feedstock composition.

Based on the analysis of the composition of the processing products of hydrocarbons C_5-C_7 on the zeolite catalyst, as well as theoretical ideas about the mechanism of the occurring chemical transformations on high-silicon zeolites of the ZSM-5 type, a list of theoretically possible reactions was formed (Table 2). The complete list consists of 865 theoretically possible chemical reactions.

Table2. The number of theoretically possible and thermodynamically probable reactions occurring during the processing of C_5-C_7 hydrocarbons on a zeolite catalyst

No.	Reaction type	Number of reactions	
		Theoretically possible	Thermodynamically probable
1	Paraffins isomerization	52	19
2	Cracking of paraffins to form of olefins	41	34
3.1	Hydrogen transfer in olefins with the formation of aromatic hydrocarbons and n-paraffins	675	675
3.2	Hydrogen transfer in olefins with the formation of diolefins	22	4
4	Diene synthesis with the formation of cycloolefins	12	7
3.3	Hydrogen transfer in cycloolefins with the formation of naphthenes and aromatic hydrocarbons	7	7
5	Alkylation to form naphthenes from of olefins	28	26
6	Dealkylation of naphthenes to form of olefins and naphthenes	28	5

The calculation of the thermodynamic parameters of various reactions of the conversion of n-pentane, n-hexane and n-heptane on a zeolite catalyst was carried out for the conditions of the laboratory implementation of the process: temperature – 648-698 K with a step of 25 K, pressure – 2.5 atm.

According to the results of thermodynamic analysis, it was found that under the study conditions of the processing C_5-C_7 hydrocarbons on a zeolite catalyst, 777 reactions are thermodynamically possible (Table 2).

The conducted thermodynamic analysis revealed the following trends:

1. Among the C_5-C_7 n-paraffins cracking reactions, the most probable is the occurrence of reactions with the predominant formation of gaseous hydrocarbons C_3-C_4 due to the cracking of the weak C-C bond with the formation of olefins with a shorter chain length and the position of the double bond at the second carbon atom.

2. From a thermodynamic point of view, among the reactions of n-paraffins isomerization, the formation of such high-octane components as 2-methylbutane, 2-methylpentane, 2,2-dimethylpentane, 2,3-dimethylpentane, and 2-methylhexane is most likely by catalytic isomerization of the carbenium ion on acid sites of zeolite in β-position.
3. Among the reactions of hydrogen transfer in olefins with the formation of aromatic compounds and paraffinic hydrocarbons, the most thermodynamically probable reactions are those involving light C_2-C_3 olefins with C_5-C_7 olefins. It is in these reactions that a tendency towards a decrease in Gibbs energies is observed with increasing temperature, while in all other reactions this thermodynamic index tends to zero with increasing temperature.
4. Of the 22 reactions occurring with the formation of diolefins, only the reactions of the formation of hexadiene-1,3, hexadiene-2,4 and heptadiene-3,5 are thermodynamically possible. Also, according to the results of thermodynamic analysis, it was found that the formation of conjugated and isolated diolefins is more likely than the formation of cumulated diolefins.
5. The thermodynamic probability of diene synthesis reactions decreases with an increase in the number of carbon atoms in molecule and branching of cycloolefin side chains, as well as with an increase in the process temperature.
6. More thermodynamically favorable in the processing on a zeolite catalyst for alkylnaphthenic hydrocarbons is the abstraction of the entire alkyl group with the formation of olefins and naphthenes without a side chain.

Based on the obtained results, a formalized scheme of chemical transformations for pentane, hexane and heptane on a zeolite catalyst was created. Figure 4 shows the formalized scheme.

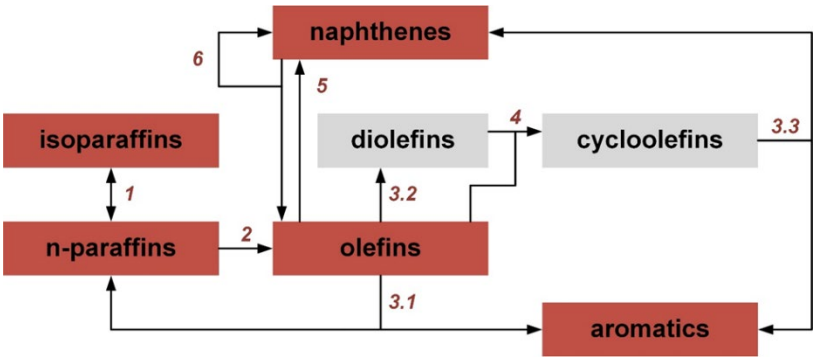

Fig. 4. Formalized scheme of chemical transformations for C_5-C_7 hydrocarbons on a zeolite catalyst

The formalized scheme of C_5-C_7 hydrocarbons chemical transformations includes isomerization reactions (1), paraffin cracking with the formation of olefins reactions (2), reactions of hydrogen transfer in olefins with the formation of aromatic hydrocarbons and n-paraffins (3.1), as well as diolefins (3.2), which, when interacting with olefins by diene synthesis (4), form cycloolefins. Hydrogen transfer in cycloolefins (3.3) also leads to the formation of aromatic hydrocarbons and naphthenes. In addition, the formation of naphthenes is facilitated by the alkylation reactions of olefins (5) with the formation of naphthenes with side methyl and ethyl groups, which undergo dealkylation reactions (6) with the formation of olefins and naphthenes without side chains.

4. Conclusion

1. The processing of pure n-pentane, n-hexane, n-heptane has been carried out, using a laboratory catalytic unit and the ZSM-5 structural type zeolite catalyst in the temperature range of 375-425°C with a step of 25°C, at a constant pressure of 0.35 MPa and a weight hour space velocity of 2 h^{-1}.
2. The hydrocarbon composition has been determined by gas chromatography for all obtained products. It was found that with an increase in the process temperature in the obtained products during the processing of C_5-C_7 hydrocarbons, the content of aromatic compounds,

represented to the greatest extent by toluene and xylenes, significantly increases. Also, with an increase in the process temperature in the composition of the obtained products, the content of isoparaffins and naphthenes decreases. A decrease in the content of naphthenes occurs due to a change in equilibrium in the reactions of hydrogen transfer towards the formation of products. The total content of n-paraffins in the products practically does not depend on the temperature of the process, however, as the temperature rises, the content of heavy C_{9+} n-paraffins in the products increases and the content of C_6-C_8 n-paraffins decreases.

3. Based on the analysis of the obtained products composition as well as theoretical ideas about the mechanism of occurring chemical transformations, a list of theoretically possible reactions has been formed. The complete list consists of 865 theoretically possible reactions. According to the results of thermodynamic analysis, it was found that under the process implementation conditions the 777 reactions are thermodynamically possible.
4. According to the results of thermodynamic analysis, the most probable types of occurring chemical transformations and the most stable isomers of the compounds have been established.
5. Based on the obtained results, a formalized scheme of chemical transformations of C_5-C_7 hydrocarbons on a zeolite catalyst has been developed. The created scheme includes 8 types of chemical reactions.

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List of symbols

SGC – stable gas condensate;
LNG – liquefied natural gas;
O – olefin;
H – naphthene;
A – aromatic hydrocarbon;
P – n-paraffin.

References

1. Sziklai BR, Kóczy LÁ, Csercsik D. The impact of Nord Stream 2 on the European gas market bargaining positions. Energy Policy, 2020; 144.
2. Zhiznin SZ, Timokhov VM. Economic and geopolitical aspects of the nord Stream 2 GAS pipeline. Balt Reg, 2019; 11(3): 25-42.
3. Zolfagharifard E. Nord stream: The world's largest gas pipeline. Engineer, 2010; 4.
4. Ozawa M, Chyong CK, Lin K, Reilly T, Humphrey C, Wood-Donnelly C. The power of siberia: A eurasian pipeline policy 'good' for whom? In Search of Good Energy Policy; 2019. p. 305-335.
5. Dastan SA. Negotiation of a cross-border natural gas pipeline: An analytical contribution to the discussions on Turkish Stream. Energy Policy, 2018; 120: 749-760.
6. Putin VV. Message from the president to the federal assembly April 21, 2021. Representative power – 21st century: legislation, commentary, problems, 2021; 186(3): 1-11.
7. Wan KW. Sakhalin-2 LNG steps on the gas. Pet. Econ., 2011; 78(9).
8. Yamal LNG: Meeting the challenges of natural gas liquefaction in the arctic. IGT International Liquefied Natural Gas Conference Proceedings; 2019.
9. Murphy J. Gazprom plays LNG catch-up. Pet. Econ., 2019; 86(9): 68-69.
10. Altynov A, Bogdanov I, Korotkova E, Kirgina M. Development of Gasoline Blending Recipes Based on the Product Obtained by Processing of Stable Gas Condensate on Zeolite Catalyst. Pet. Coal. 2021; 63(1): 91-95.
11. Hoelderich W, Gallei E. Industrial application of zeolite catalysts in petrochemical processes. Ger Chem. Eng., 1985; 8(6): 337-345.
12. Serrano DP, Melero JA, Morales G, Iglesias J, Pizarro P. Progress in the design of zeolite catalysts for biomass conversion into biofuels and bio-based chemicals. Catal. Rev. Sci. Eng., 2018; 60(1): 1-70.

13. Liao M, Ning X, Chen J, Zheng J, Li W, Li R. Mesoporous ZSM-5 catalysts for the synthesis of clean jet-fuels by 1-hexene oligomerization. Fuel, 2021; 304.
14. Bellussi G, Mizia F, Calemma V, Pollesel P, Millini R. Oligomerization of olefins from Light Cracking Naphtha over zeolite-based catalyst for the production of high-quality diesel fuel. Microporous Mesoporous Mater, 2012; 164: 127-134.
15. Li J, Gao H, Yao W, Xiang Y, Zhang Y, Wang G, et al. Preparation of mesoporous ZSM-5 zeolite and its performance in FCC gasoline hydrofining. Pet. Process Petrochem, 2020; 51(8): 37-42.
16. Alotibi MF, Alshammari BA, Alotaibi MH, Alotaibi FM, Alshihri S, Navarro RM, et al. ZSM-5 Zeolite Based Additive in FCC Process: A Review on Modifications for Improving Propylene Production. Catal. Surv. Asia, 2020; 24(1).
17. Gusev AA, Psarras AC, Triantafyllidis KS, Lappas AA, Diddams PA. Effect of steam deactivation severity of ZSM-5 additives on LPG olefins production in the FCC process. Molecules, 2017; 22(10).
18. Altynov AA, Bogdanov IA, Belinskaya NS, Popok EV, Kirgina MV. Production of automobile gasolines with stable gas condensate and of zeoforming process products as mixture components. Oil and Gas Business, 2019; 2: 217-242.
19. EN 14517:2004 "Liquid petroleum products – Determination of hydrocarbon types and oxygenates in petrol – Multidimensional gas chromatography method".
20. Ochterski JW. Thermochemistry in Gaussian. Gaussian, Inc., 2000. 19 p.
21. Belinskaya N, Altynov A, Bogdanov I, Popok E, Kirgina M, Simakov DSA. Production of gasoline using stable gas condensate and zeoforming process products as blending components. Energy Fuels. 2019; 33 (5): 4202-4210.

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