MODELLING OF THE VACUUM GASOIL HYDROCRACKING PROCESS

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At present, the Russian oil refining industry is experiencing a growing demand for processes related to the processing of high-boiling petroleum fractions. Hydrocracking is the most common type of cracking, including the processing of high boiling petroleum fractions, such as fuel oil, vacuum gas oil, jet fuel and diesel fuel. Increasing the efficiency of the hydrocracking process by mathematical modeling is an urgent task [1].

One of the initial stages in the development of a mathematical model of any oil refining process is the thermodynamic analysis of the ongoing reactions [2]. Thermodynamic analysis of reactions under process conditions of the process makes it possible to evaluate the probability of their occurrence, their reversibility or irreversibility.

On the basis of thermodynamic analysis, a formalized scheme for the transformation of hydrocarbons in the process is prepared.

In addition, the calculated thermal effects of the reactions are used in the thermal balance of the process, and the values of the Gibbs energy of the reactions are used to calculate the inverse reaction constants in the case of reversible reactions [3].

The purpose of this work is to calculate the thermodynamic parameters of the reactions of the vacuum gas oil hydrocracking process.

Using the quantum-chemical methods and the Gaussian software package, the basic thermodynamic characteristics of the molecules of the reagents participating in the hydrogenation of aromatic compounds, such as enthalpy, Gibbs energy and entropy, were calculated. Further, the thermodynamic parameters of the hydrogenation reactions of aromatic compounds occurring in the process of hydrocracking of vacuum gas oil were calculated, namely the change in the enthalpy, entropy, and Gibbs free energy.

The conditions for carrying out the process of hydrocracking in industry, taken in the calculations are following: temperature is 633 K and pressure is 158 atm.

The results of the calculations are presented in Table 1.

Table 1. Hydrogenation reactions of aromatic compounds and basic thermodynamic characteristics

№	Reaction	ΔH, kJ/mol	ΔS, J/mol•K	ΔG, kJ/mol
1	Benzene + 3 • H_2 = Cyclohexane	–248.03	–291.18	–63.71
2	Toluene + 3 • H_2 = Methylcyclohexane	–246.63	–296.62	–58.87
3	Ethylbenzene + 3 • H_2 = Ethylcyclohexane	–242.24	–282.98	–63.11
4	O–xylene + 3 • H_2 = 1,2-dimethylcyclohexane	–240.14	–288.08	–57.79
5	M–xylene + 3 • H_2 = 1,3-dimethylcyclohexane	–244.47	–310.99	–47.61
6	P–xylene + 3 • H_2 = 1,4-dimethylcyclohexane	–245.25	–319.24	–43.17

As a result of calculations of the thermodynamic characteristics of the vacuum gas oil hydrocracking process, it was found that all reactions take place under the given industrial process conditions (T=633 K and P=158 atm) and are reversible, since the change in Gibbs energy during the reaction is less than zero.

Reference

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METHOD OF OBTAINING HIGH-MOLECULAR INULIN

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It is known that inulin is a fructose polysaccharide (polyfructosan), is a product of photosynthesis of some plants and is a mixture of structurally similar polymorphs containing about 35 fructose fragments with variable specific rotation $[\alpha]_D$ from –32 to –40. A high molecular weight inulin polymer, which is isolated by recrystallization from water, can have $[\alpha]_D$=–40 [1]. Inulin is a good dietary product and a therapeutic and prophylactic drug for people with diabetes mellitus. the absorption of fructose is much less dependent on the hormone of the insulin pancreas than for glucose. Moderate intake of fructose does not cause significant changes in blood sugar levels [2].

We have found that crude inulin, obtained by precipitation with alcohol or after a single crystallization, contains impurities such as pectin, protein and amino acid residues, organic acids, phenolic compounds and oxidation products. Impurities are detected by paper chromatography with appropriate diagnostic reagents or in the UV light of a fluorescent lamp.

It is possible to note the shortcomings of these methods [4, 5]. The use of acetic acid lead to precipitate colloids is not justifiable from a medical point of view because of the toxicity of the metal ion. The use of ultrafiltration to purify inulin requires the presence of special filters and membranes that are not readily available for industrial use. In addition, purification of extracts from Jerusalem artichoke by ultrafiltration and filtration on membranes does not make it possible to release extracts containing inulin from high molecular weight natural polymers of proteins and pectins. Extraction with 25% alcohol will result in a partial loss of inulin, which is poorly soluble in alcohol solutions and will not be completely extracted under these conditions. Acidification of an inulin solution may result in loss of inulin. For example, 0.2 N. a solution of sulfuric acid causes hydrolysis of inulin for 10–15 minutes at 70 °C .

To produce high molecular weight inulin, juice from the raw material was extracted and the substances were extracted from the mash and from the raw material with hot water at 80 °C for 60 minutes. As a raw material, crushed tubers of Jerusalem artichoke were used. Juice was squeezed out of crushed Jerusalem artichoke tubers using a juicer. Additional water extracts were obtained from the mash. The extracts were carried out with heating for 60 minutes at 80 °C. The juice was diluted with hot water (95 °C) 1 : 1, and separately, the hot aqueous extracts were treated with calcium carbonate (chalk) at 80–85 °C for 60 minutes and filtered hot through the coarse layer. This made it possible to destroy the inulin-pectin complex, to coagulate proteins, to get rid of water-soluble pectins, in part from organic acids, proteins, without destroying inulin, where the pH is kept close to neutral. The filtrate of the aqueous solution of the juice was evaporated in vacuo. Crystallization of inulin was carried out at 4 °C in a refrigerator for 5 days. To the evaporated aqueous extracts, alcohol 1 : 1 was added. The precipitated precipitates of crude inulin are gray. Further purification of inulin was carried out. To this end, the inulin solution was passed through a column with an anion exchanger in the OH form. The column is washed with water at 45 °C to a volume equal to the original solution taken. Anionite allows the removal of organic acids, phenolic acids and other acidic compounds, as well as anions of organic and inorganic salts; Further, alumina was added to the eluate and heated with constant stirring for 30 minutes at 75 °C and the coarse layer was filtered and the precipitate from the filter was washed with hot water. This allows to remove impurities that are sorbed on aluminum oxide (phenols, polyphenols, products of their oxidation). 96% alcohol 1 : 3 was added to the resulting solution and inulin in the refrigerator crys-