THERMODYNAMIC ANALYSIS OF THE CATALYTIC ACTIVITY OF ALUMINUM OXIDE (Al_2O_3) AND PYRITE (FeS_2)

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In this work, the kinetics of anthracene hydrogenation in the presence of a mixture of pyrite and aluminum oxide in a 1:1 ratio at a hydrogen pressure of 3 MPa and temperatures of 648 K, 673 K, 698 K. were studied by equilibrium kinetic analysis. It was found that an increase in the temperature of the hydrogenation reaction leads to an increase in the degree of conversion of anthracene, equilibrium constants, and a decrease in Gibbs energies. Chromatographic analysis of anthracene hydrogenation products showed the presence of 9,10-dihydroanthracene (DHA), 1,2,3,4-tetrahydroanthracene (THA), methylnaphthalene (MN), naphthalene (H) and other unidentified compounds.

The use of equilibrium kinetic analysis makes it possible to establish the relationship between direct and reverse reactions for a better understanding of the catalytic properties of a mixture of aluminum oxide and pyrite during the hydrogenation of anthracene, as well as to establish the dependence of the reaction rate on time and temperature. Anthracene hydrogenation was carried out in a CJF-0.05 reactor with a capacity of 0.05 liters, equipped with a stirrer, temperature and pressure sensors. Anthracene hydrogenation was carried out at temperatures of 648 K, 673 K, 698 K, with an initial hydrogen pressure of 3 MPa and a heating rate of 10 °C/min in the presence of a mixture (1:1) of pyrite and aluminum oxide. It was found that the process of anthracene hydrogenation in the presence of a mixture of FeS_2 and Al_2O_3 is limited from the kinetic to the diffusion region as the temperature increases, which is confirmed by the activation energies of the forward (39.4 kJ/mol) and reverse reactions (13.04 kJ/mol). An increase in the rate constants of the direct hydrogenation reaction of anthracene with increasing temperature is probably due to an increase in the number of effective collisions of reagent molecules at the active centers of the catalyst, which reduces the likelihood of a dehydrogenation reaction.

Thus, there is reason to believe that the mixture of pyrite and aluminum oxide used in the reaction acts catalytically in both directions of the reaction, which, on the one hand, ensures its implementation in the selected temperature range and, on the other hand, explains its moderate total rate. In addition, it was found that the Gibbs energy decreases with increasing temperature, which makes the process of direct reaction (hydrogenation) more thermodynamically advantageous.Values of enthalpy (ΔH = 67.5 kJ/mol) and entropy (ΔS = 61.2 J/(mol·K)) The reactions calculated using the Gibbs-Helmholtz equation indicate the endothermic nature of the process. A positive value of entropy also implies an increase in disorder in the system, which may be due to a partial loss of aromaticity of anthracene during hydrogenation.

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