KINETIC MODELING OF THE INFLUENCE OF REACTIONS OCCURRING ON THE SURFACE OF Pt-CATALYST ON METHANE OXIDATION UNDER CONDITIONS OF MATRIX CONVERSION

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Abstract: One of the ways to expand the combustion limits of rich hydrocarbon mixtures is the catalytic activation of the initial mixture. The combination of precatalytic activation and heat recuperation from the outgoing conversion products can make it possible to create compact converters of hydrocarbon gases to synthesis gas with high performance. In this work, kinetic modeling of the matrix conversion of methane in the presence of Pt catalyst was carried out. The air-to-fuel equivalence ratio α for the studied methane–air mixture was about 0.25. The computational model consisted of two consecutive plug flow reactors (PFR). The first rector considered the kinetics of heterogeneous processes using Honeycomb monolith — a subtype of PFR that allows calculating the microkinetics of catalytic processes. In the second reactor, gas-phase matrix conversion processes were considered. The correspondence of the calculated and experimental results was shown. The pathway of catalytic formation of CO_2 under conditions of matrix conversion of rich methane-containing mixtures has been established.

Keywords: oxidation kinetics; numerical modeling; detailed kinetic mechanism

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Figure Captions

Figure 1 Comparison of experimental (signs) and calculated (lines) dependences of the indicators of partial oxidation of methane on temperature [8]: *1* — selectivity of CO formation; *2* — oxygen conversion; and *3* — methane conversion. The CH_4/O_2 ratio is 2.5; the inlet flow rate is 10 m/s; initial temperature is 600 K; and pressure is 1.3 bar

Figure 2 The model of the matrix conversion of methane in the presence of Pt-catalyst

Figure 3 The concentration of the components of the reacting mixture vs. the length of the matrix: (*a*) calculation No. 8; (*b*) calculation No. 9 (excluding the kinetics of heterogeneous reactions); *1* — O_2; *2* — CH_4; *3* — H_2O; *4* — CO_2; *5* — H_2; *6* — CO; *7* — temperature; *8* — conversion of CH_4; and *9* — conversion of O_2. Temperature profile (curve *7*, Fig. 3*a*) is the same for both calculations

Table Captions

Table 1 Calculation conditions

Table 2 The properties of Pt-catalyst used in the calculations

Table 3 Results of calculations of the kinetics of partial oxidation of methane in the presence of Pt-catalyst. The concentrations and conversion of reactants correspond to the syngas at the outlet of the Honeycomb monolith. Conditions: methane–air mixture; $\alpha = 0.25$; $P = 1$ bar; and mixture consumption is 150 ml/s. The contribution of gas-phase and heterogeneous processes in the Honeycomb monolith was varied by changing the code parameter (a multiplier taking values from 0 to 1) which determines the contribution of individual reactions at the ith point of the reaction space

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