ON THE INFLUENCE OF PRESSURE AND HETEROGENEOUS PROCESSES ON PYROLYSIS AND OXIDATIVE CRACKING OF LIGHT ALKANES

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Abstract: The results of experimental studies and kinetic modeling of pyrolysis and oxycracking of light alkanes (ethane and propane) in the temperature range of 773–1023 K and at pressures of 1 to 3 atm in a plug-flow reactor allow one to conclude that pressure does not significantly affect the thermal processes of their transformation but significantly affects the oxidative processes. In laboratory-scale reactors, the influence of heterogeneous processes on the kinetics of pyrolysis of light alkanes is negligible which makes it possible to use modern homogeneous mechanisms for their quantitative description. To quantitatively describe oxidative processes involving light alkanes in laboratory-scale reactors, homogeneous mechanisms should be supplemented with heterogeneous stages on the reactor surface.

Keywords: natural gas; ethane; propane; ethylene; pyrolysis; partial oxidation; oxidative cracking; kinetic modeling

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Figure Captions

Figure 1 Dependences of the concentrations of ethane ((*a*) $[C_2H_6]_0 = 3.3\,\%$(mol.) and (*b*) $[C_2H_6]_0 = 6.1–6.4\,\%$(mol.)) and propane ((*c*) $[C_3H_8]_0 = 2.3–2.4\,\%$(mol.) and (*d*) $[C_3H_8]_0 = 5.0–5.7\,\%$(mol.)) on the pyrolysis temperature at different pressures: *1* — $p = 1$ atm; *2* — 2; *3* — 3; and *4* — $p = 15$ atm. The residence time in the hot zone of the reactor is $t = 2$ s. The diluent gas is nitrogen. Signs — experimental data; and curves — results of numerical simulation

Figure 2 Temperature dependence of the formation of the main pyrolysis products of ethane ($[C_2H_6]_0 = 6.4\,\%$(mol.)) (*a*) and propane ($[C_3H_8]_0 = 5.38\ \%$(mol.)) (*b*). The residence time in the hot zone of the reactor is $t = 2$ s. The diluent gas is nitrogen. Signs — experimental data; curves — results of numerical simulation: *1* — H_2, $p = 1$ atm; *2* — H_2, $p = 3$ atm; *3* — H_2, $p = 15$ atm; *4* — C_2H_4 (C_3H_6), $p = 1$ atm; *5* — C_2H_4 (C_3H_6), $p = 3$ atm; and *6* — C_2H_4 (C_3H_6), $p = 15$ atm

Figure 3 Temperature dependences of the concentrations of the reagents and main products of partial oxidation of ethane at the reactor outlet at a pressure of 1 (*a*) and 2 atm (*b*). Signs — experimental data. Curves *1*, *2*, and *3* — results of numerical simulations including the reactions on the reactor surface (mechanisms [10] and [11]) and neglecting them (mechanism [10]), respectively. The composition of the mixture at the reactor inlet is $C_2H_6/O_2/N_2 = 0.0503/0.0248/0.9249$. The accommodation coefficients are $\gamma_1 = 2.8 \cdot 10^{-3}$, $\gamma_2 = 3.9 \cdot 10^{-4}$, and $\gamma_3 = 3.5 \cdot 10^{-7}$ (*a*), and $\gamma_1 = 2.7 \cdot 10^{-3}$, $\gamma_2 = 1.9 \cdot 10^{-4}$, and $\gamma_3 = 8.8 \cdot 10^{-8}$ (*b*) for HO_2 radicals, H_2O_2, and CO molecules, respectively

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