

EFFECT OF TRANSITION FROM LOW-TEMPERATURE TO HIGH-TEMPERATURE MECHANISMS OF METHANE AND HYDROGEN OXIDATION ON IGNITION OF GAS MIXTURES CONTAINING THEM

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Abstract: The features of ignition of methane, hydrogen, and gas mixtures containing them in the temperature range $800 < T < 1000$ K, associated with a change in the mechanisms of their oxidation and a change in the role of processes involving hydrogen peroxide H_2O_2 and hydroperoxide radicals $HO_2^\bullet$, are considered. The possibility of a sharp change in the kinetic parameters of the ignition process in this range and the manifestation of such unusual effects as inhibition of methane ignition by hydrogen additives and promotion of hydrogen ignition by carbon monoxide additives is shown. The possibility of sharp changes in the main parameters characterizing the ignition of methane and hydrogen-containing gas mixtures requires consideration when analyzing the safety of their use and determining the knock resistance of gas engine fuels.

Keywords: methane; hydrogen; gas engine fuel; ignition delay time; hydrogen peroxide

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Figure Captions

Figure 1 The dependence of the activation energy of the ignition delay of alkanes C_1 – C_4 on the number of atoms N_c in their molecule. Filled and empty symbols represent two different series of experiments

Figure 2 The temperature dependence of the radical removal rate in the forward W_f (1) and reverse W_r (2) reactions (1) during oxidation of a stoichiometric $CH_4 + O_2$ mixture at $P = 1$ atm. Calculation is based on mechanism [17]

Figure 3 Isomerization of ethyl peroxide radical $CH_3CH_2OO^\bullet$ with subsequent decomposition to ethylene and radical $HO_2^\bullet$

Figure 4 (a) Calculated ($P_0 = 15$ atm) and (b) experimental ($P_0 = 3.0$ – 3.2 atm) temperature dependences of the ignition delay of stoichiometric CH_4 – H_2 –air mixtures at different concentrations of H_2 : 1 – 0%; 2 – 2%; 3 – 2.5%; 4 – 5%; 5 – 10%; 6 – 20%; 7 – 30%; 8 – 40%; and 9 – 50%

Figure 5 The temperature dependence of the characteristic decomposition time of hydrogen peroxide t_d and the characteristic ignition delay time of hydrogen t_i as well as the rate of reaction (4) W_H . Calculation is based on mechanism [17]

Figure 6 The calculated temperature dependence of the concentration of $H^\bullet$ atoms during ignition of a stoichiometric hydrogen–air mixture at the moment of preexplosive heating of the mixture when its temperature exceeds the initial value by 100 K: 1 – real concentration of $H^\bullet$ atoms $[H]_t$; and 2 – concentration of $H^\bullet$ atoms $[H]_{t+10}$ with a 10-fold increased rate of constant of reaction (3)

Figure 7 The effect of pressure (1 – 1 atm; 2 – 3; and 3 – 15 atm) on the temperature dependence of the ignition delay time of stoichiometric CH_4 – H_2 –air mixtures at a hydrogen concentration in the fuel of 80%

Figure 8 The calculated dependence of the ignition delay time of the syngas on the CO concentration for the conditions of a constant volume reactor, $T = 800$ K, $P = 1$ atm, $\varphi = 1.0$

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