ON THE EFFECT OF HYDROCARBON ADDITIVE SUPPRESSING CHAIN REACTION DEVELOPMENT IN HYDROGEN–AIR MIXTURES

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Abstract: The inhibitory effect of small hydrocarbon additives on combustion and explosion of hydrogen–air mixtures has been proven by experimental data on detonation and combustion of fuel-rich compositions. The mechanism proposed in the works of domestic authors is related to the specific features of the course of branched chain reactions. Mathematical modeling of detonation of hydrogen–air mixtures with the addition of propylene confirmed the effect. However, in these works, detailed chemical kinetics was applied only to the hydrogen–air mixture. In the present work, detailed kinetics is applied to all components of the mixture. The solution was obtained for three model problems: self-ignition in a constant-volume reactor; laminar flame propagation; and gas ignition by a heated wire. The objects of the study were a stoichiometric mixture of hydrogen (29.6 %(vol.)) with air without additives and with 1% addition of propylene. Calculations have shown that besides propylene molecules, chemical reactions involve products of its decomposition and oxidation. Moreover, they are not only capable of adding atomic hydrogen causing chain termination but under certain conditions, they can generate it. A strong inhibition effect was obtained in a self-ignition problem (initial pressure 1 atm) at an initial temperature of 1000 K: the addition of propylene caused an increase in ignition delay by over 2 orders of magnitude. However, both with an increase and decrease in the initial temperature (the range from 800 to 1400 K was investigated), the inhibition effect almost completely disappears. There is no inhibition in calculations of the normal burning velocity (propylene addition reduces the burning velocity by only 11%) and the critical conditions for ignition by hot wire. Explanations of the obtained effects are given using the rates of the leading chemical reactions and physical features of the considered problems.

Keywords: hydrogen–air mixtures; propylene; inhibition; self-ignition; laminar flame; ignition by a heated surface

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Figure Captions

Figure 1 Temperature dependence of the ignition delay time of the stoichiometric H_2–air mixture without additive (*1*) and with the addition of 1% C_3H_6 (*2*). Experiments on ignition delays of the H_2–air mixture: squares — data from various authors given in [17]; and circles — [18]

Figure 2 Kinetic analysis diagram of formation/loss of atomic hydrogen indicating absolute rates of reactions. Ignition of a hydrogen–air mixture with a 1 percent addition of propylene at atmospheric pressure, $T_0 = 1000$ K. The bar to the right shows the formation of H and the bar to the left shows its decrease. Time point 26 ms; the temperature corresponding to this time is 1108 K

Figure 3 Time dependences of temperature and concentration of hydrogen atoms during self-ignition of a hydrogen–air mixture without addition of an inhibitor (*a*) and with a 1 percent addition of propylene (*b*) at an initial temperature of 1000 K

Figure 4 Time dependences of temperature and concentration of hydrogen atoms during self-ignition of a hydrogen–air mixture without addition of an inhibitor (*a*) and with a 1 percent addition of propylene (*b*) at an initial temperature of 850 K

Figure 5 Profiles of temperature (solid curves) and concentration of hydrogen atoms (dashed curves) in the front of the normal combustion wave of the stoichiometric mixture hydrogen–air at $p = 1$ atm: black curves — without addition of propylene; and grey curves — with a 1 percent addition of propylene

Figure 6 Relationship between the logarithm of the heat release rate and the temperature along the reaction zone of the normal combustion wave of a stoichiometric hydrogen–air mixture without additive (*1*) and with a 1 percent addition of propylene (*2*). Initial temperature 300 K and pressure 1 atm

Figure 7 Temperature profiles in a stoichiometric H_2–air mixture around a cylindrical heated body with a diameter of 1 cm and the surface temperature of 1000 K: *1* — the present authors' calculation; and *2* — experiment [22] (coordinate in the axial direction — 6 mm). Initial temperature 300 K and pressure 1 atm

Figure 8 Dependence of the ignition delay time τ_{ig} on the temperature of the heated wire for the H_2–air mixture without additive (*1*) and with 1 percent addition of propylene (*2*)

Figure 9 The relationship between the concentration of OH atoms and the temperature along the reaction zone of the normal combustion wave in a stoichiometric hydrogen–air mixture without additive (*1*) and with a 1 percent addition of propylene (*2*). Initial temperature 300 K and pressure 1 atm

Table Captions

Table 1 Ignition delay time of a stoichiometric hydrogen–air mixture with the 1 percent addition and without addition of propylene at different initial temperatures. Initial pressure 1 atm

Table 2 Results of calculations of ignition of a stoichiometric hydrogen–air mixture heated by wire with and without a 1 percent addition of propylene with detailed chemical kinetics. Temperature of incoming gas flow 300 K, pressure 1 atm, and wire diameter 1 mm

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