SPECIFIC FEATURES OF NUMERICAL SIMULATION OF LEAN HYDROGEN–AIR MIXTURE IGNITION

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Abstract: Numerical simulation of ignition delays τ and laminar burning velocity S_L of hydrogen–air mixtures near the lower concentration limit has been carried out. The mixtures with hydrogen concentration varying from 6% to 14% in the temperature range from 800 to 2000 K at an initial pressure of 1 and 6 atm have been investigated. Analysis of various detailed kinetic mechanisms (DKMs) presented in literature showed that the obtained calculated values of τ and S_L are quite close. At the same time, the temperature dependences of the delay τ and the amount of heat release behave differently when the initial pressure increases. It is shown that an increase in the H_2 initial concentration near the lower concentration limit leads to an insignificant decrease in τ. It is concluded that any of considered DKMs can be applied to predict various technological situations dealing with hydrogen fire and explosion safety near the lower concentration limit.

Keywords: lean hydrogen–air mixtures; self-ignition; ignition delay; laminar burning velocity; computer modeling; chemical kinetics; detailed kinetic mechanism

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Figure Captions

Figure 1 Temperature (*1*) and OH* emission (*2*) during self-ignition of 10% H_2–air mixture at 1 atm for a variety of initial temperature: (*a*) $T_0 = 800$ K; (*b*) 1000; (*c*) 1400; and (*d*) $T_0 = 2000$ K [3]. Hereafter, references in captions mean DKMs used for calculations

Figure 2 Ignition delay times for 6% H_2 – air: *1*, *2*, and *3* — DKMs [3], [28], and [29], respectively, at $P_0 = 1$ (black lines) and 6 atm (grey lines)

Figure 3 Ignition delay times (*a*) and heat release (*b*) for 6% (*1*) and 14% H_2–air (*2*) at $P_0 = 1$ (black lines) and 6 atm (grey lines) [3]

Figure 4 Hydrogen–air laminar burning velocity vs. H_2 concentration: *1*, *2*, and *3* — DKMs [3], [28], and [29], respectively. Initial conditions: $P_0 = 1$ atm and $T_0 = 298$ K

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