INFLUENCE OF THE CHOICE OF KINETIC MECHANISM ON PREDICTED PRESSURE RISE IN NUMERICAL SIMULATIONS OF PREMIXED HYDROGEN–AIR IGNITION AND COMBUSTION

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Abstract: Numerical simulations of ignition delay and pressure rise during autoignition have been performed for lean (6% H_2), stoichiometric (29.6% H_2), and rich (75% H_2) hydrogen–air mixtures at initial pressures of 1 and 6 bar in the temperature range from 850 to 1700 K. Pressure rise for lean and rich mixtures is found to be virtually independent of the choice of a detailed kinetic mechanism (DKM), whereas a dependence of this kind is predicted for the stoichiometric mixture. The time to reach thermodynamic equilibrium (TE), measured in the units of induction period, decreases with increasing initial temperature, whereas the approach to TE accelerates with pressure rise. For the stoichiometric mixture, TE is reached faster than for the lean and rich ones. It is demonstrated that the dynamics of pressure rise determined by the chemical kinetics after the induction period varies with the choice of a DKM and is independent of ignition delay. This observation may be of importance for processes at relatively high temperatures.

Keywords: hydrogen–air mixture; dynamics of pressure rise; autoignition; ignition delay; numerical simulation; chemical kinetics; detailed kinetic mechanism

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Figure Captions

Figure 1 Pressure rise at $\tau_{\max}$ (*1*, *3*, and *5*), and $2\tau_{\max}$ (*2*, *4*, and *6*) based on DKMs of [25] (*1* and *2*), [8] (*3* and *4*), and [13] (*5* and *6*) for 6% H_2 in air (*a*), stoichiometric H_2–air mixture (*b*), and 75% H_2 in air (*c*) at $P_0 = 1$ (left column) and 6 bar (right column). Signs — pressure at thermodynamic equilibrium

Figure 2 Pressure (black curves) and OH^* (grey curves) histories calculated by using DKMs of [25] (*1*), [8] (*2*), and [13] (*3*) for stoichiometric H_2–air mixture at $P_0 = 1$ bar and $T_0 = 1100$ K

Table Captions

Table 1 Values of $\tau_{\max}$ (in seconds) for 6% of hydrogen in air vs. temperature calculated by using DKMs from [8, 13, 25] at $P_0 = 1$ and 6 bar

Table 2 Values of $\tau_{\max}$ (in seconds) for stoichiometric hydrogen–air mixture vs. temperature calculated by using DKMs from [5, 18, 19] at $P_0 = 1$ and 6 bar

Table 3 Values of $\tau_{\max}$ (in seconds) for 75% of hydrogen in air vs. temperature calculated by using DKMs from [5, 18, 19] at $P_0 = 1$ and 6 bar

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