ON THE CRITERIA FOR DEFINING IGNITION DELAY TIME OF A HYDROGEN–OXYGEN MIXTURE AS APPLIED TO NUMERICAL SIMULATION

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Abstract: Using a recently developed reaction submechanism "JIHT-OHex(H_2)" aimed at describing the kinetics of the electronically excited OH^* radical, there were analyzed the features of the OH^* temporal evolution accompanying the autoignition of an argon-diluted (Ar mole fraction $\gamma_{Ar} = 0.97$) hydrogen–oxygen mixture over a wide range of initial conditions: temperature ($T_0 = 1000$–2000 K), pressure ($p_0 = 0.001$–50 atm), and equivalence ratio ($\phi = 0.1$–5). For these conditions, the present authors compared the ignition delays of hydrogen–oxygen mixtures determined by the maximum OH^* concentration and by other alternative criteria commonly used in numerical experiments that do not explicitly resolve the kinetics of chemiluminescent particles. It was found that at low pressures, the "JIHT-OHex(H_2)" submechanism predicts the OH^* concentration profiles without a pronounced maximum, in which case the discrepancy between the ignition delay values of the hydrogen–oxygen mixture determined by different methods can be significant. At normal and elevated pressures, the methods considered for defining the ignition delay of a hydrogen–oxygen mixture give close values of the induction time, with the best agreement with the position of the OH^* concentration peak being the time of maximum rate of temperature rise.

Keywords: hydrogen oxidation; hydroxyl radical; electronic excitation; ignition delay time; kinetic simulation; chemiluminescence

DOI: 10.30826/CE25180101 **EDN:** NWNIFB

Figure Captions

Figure 1 Calculated temporal [OH^*] profiles for hydrogen–oxygen mixture ($\phi = 1$ and $\gamma_{Ar} = 0.97$) at $p_0 = 1$ (*a*) and 0.01 atm (*b*): *1* — $T_0 = 1000$ K; *2* — 1100; *3* — 1200; and *4* — $T_0 = 1300$ K

Figure 2 The ignition delay times $\tau_{OH^*}^{max}$ (*1*), τ_{OH^*} (*2*), τ_{OH} (*3*), and τ_T (*4*) vs. initial temperature T_0 at $\phi = 1$, $\gamma_{Ar} = 0.97$, and $p_0 = 0.01$ atm

Figure 3 Two-parameter $\delta\tau_{OH^*}(T_0, \phi)$ dependence for hydrogen–oxygen mixture ($\gamma_{Ar} = 0.97$) at $p_0 = 1$ (*a*) and 0.1 atm (*b*)

Figure 4 The contours with $\delta\tau_{OH^*} = 2$ calculated for hydrogen–oxygen mixture ($\gamma_{Ar} = 0.97$) at different initial pressures p_0: *1* — 1 atm; *2* — 0,5; *3* — 0,1; *4* — 0,05; *5* — 0,01; and *6* — 0,001 atm

Figure 5 Comparison of the ignition delays determined based on different criteria for hydrogen–oxygen mixtures ($\gamma_{Ar} = 0.97$) at different equivalence ratios: (*a*) $\phi = 0.1$; (*b*) 1.0; and (*c*) 5.0; solid curves — $\tau_{OH^*}^{max}$; dotted curves — τ_T; dashed curves — τ_{OH}; and dash-dotted curves — τ_{OH^*}; *1* — $p_0 = 0.01$ atm; *2* — 0.1; *3* — 1; *4* — 10; and *5* — $p_0 = 50$ atm

Figure 6 Calculated temporal [OH^*] profiles at $\phi = 1.0$, $p_0 = 0.01$ atm, and different initial temperatures T_0: *1* — 1400 K; *2* — 1500; *3* — 1600; *4* — 1700; *5* — 1800; *6* — 1900; and *7* — 2000 K

Acknowledgments

The work was supported by the grant of the Russian Science Foundation (project No. 24-09-00152). The authors are grateful to their colleague B. I. Loukhovitski for his valuable advices, methodological guidance, and technical assistance.

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Received December 10, 2024
After revision January 21, 2025
Accepted January 22, 2025

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