

VALIDATION OF DETAILED KINETIC MECHANISMS FOR NUMERICAL SIMULATION OF PROPENE AUTOIGNITION AND PYROLYSIS IN SHOCK WAVES

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Abstract: The possibility of using detailed kinetic mechanisms (DKMs) for numerical simulation of autoignition and pyrolysis of propene behind reflected shock waves has been explored. Four DKMs presented in the literature have been considered. Calculated values of ignition delay τ have been compared with those measured for propene–argon–oxygen mixtures with equivalence ratio ϕ ranging from 0.5 to 2.0 at temperatures of 1000 to 1760 K and pressures of 2 to 40 bar. In the numerical simulations of pyrolysis, time profiles of H-atom concentration have been computed for propene–argon mixtures with initial propene concentration varied between 2 and 30 ppm at pressures of 0.3 to 4.7 bar. In summary, sufficiently accurate prediction of the values of τ has been achieved but the DKMs employed have failed to provide even an adequate description of experimental data on C_3H_6 pyrolysis. An analysis has shown that a better simulation of propene pyrolysis requires the use of refined values of the pressure-dependent rate constants for decomposition of C_3H_6 and the αC_3H_5 radical.

Keywords: propene; ignition delay; pyrolysis; shock waves; numerical simulation; detailed kinetic mechanism

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Figure Captions

Figure 1 Temperature dependences of ignition delay at $\phi = 0.5$ for 2.25% C_3H_6 + air (a) and 0.45% C_3H_6 + 4% O_2 + 95.5%Ar (b): signs — experimental data [24] at $P_{50} = 2$ (1), 2.3 (2), 10 (3), and 40 bar (4); and curves — calculations using the DKMs ChemPhysMech 2.0 (5), JetSurF 2.0 (6), Aramco 3.0 (7), and OXYMECH 2.0 (8)

Figure 2 Temperature dependences of ignition delay at $\phi = 1$ for 0.89% C_3H_6 + 4% O_2 + 95.11%Ar (a) and 2.67% C_3H_6 + 12% O_2 + 85.33%Ar (b) at $P_{50} = 2$ (1), 10 (2), and 40 bar (3): signs — experimental data [24]; and curves — calculations using the DKMs ChemPhysMech 2.0 (4), JetSurF 2.0 (5), Aramco 3.0 (6), and OXYMECH 2.0 (7)

Figure 3 Temperature dependences of ignition delay at $\phi = 1$ for 0.89% C_3H_6 + 4% O_2 + 95.11%Ar (1) and 1.6% C_3H_6 + 7.2% O_2 + 91.2%Ar (2) at $P_{50} = 4.4$ bar (a) and 4.46% C_3H_6 + air at $P_{50} = 10$ (3) and 40 bar (4) (b): signs — experimental data [24]; and curves — calculations using the DKMs ChemPhysMech 2.0 (5), JetSurF 2.0 (6), Aramco 3.0 (7), and OXYMECH 2.0 (8)

Figure 4 Temperature dependences of ignition delay at $\phi = 2$ for 1.78% C_3H_6 + 4% O_2 + 94.22%Ar (a) and 8.54% C_3H_6 + air (b): signs — experimental data [24] at $P_{50} = 2$ (1), 10 (2), 40 (3), and 45.4 bar (4); and curves — calculations using the DKMs ChemPhysMech 2.0 (5), JetSurF 2.0 (6), Aramco 3.0 (7), and OXYMECH 2.0 (8)

Figure 5 Noisy curves represent time profiles of H-atom concentration measured during propene pyrolysis in argon for mixtures with 0.5 ppm C_3H_6 (a), 3.8 ppm of C_3H_6 (b), and 21 ppm of C_3H_6 (c). Experimental conditions (1): (a) $P_{50} = 2.0$ bar, $T_{50} = 1714$ K [25]; (b) $P_{50} = 0.357$ bar, $T_{50} = 1590$ K [26]; and (c) $P_{50} = 4.85$ bar, $T_{50} = 1470$ K [26]. Smooth curves are calculated using the DKMs: 2 — ChemPhysMech 2.0; 3 — JetSurF 2.0; 4 — Aramco 3.0; and 5 — OXYMECH 2.0

Figure 6 Sensitivity analysis for H-atom concentration profile under the experimental conditions of Fig. 5b: 1 — $CH_3 + H + M = CH_4 + M$; 2 — $CH_4 + H = CH_3 + H_2$; 3 — $C_2H_2 + CH_3 = PC_3H_4 + H$; 4 — $AC_3H_5 = C_2H_2 + CH_3$; 5 — $AC_3H_5 = AC_3H_4 + H$; 6 — $AC_3H_5 + H + M = C_3H_6 + M$; 7 — $TC_3H_5 = C_2H_2 + CH_3$; 8 — $C_3H_6 = C_2H_2 + CH_4$; 9 — $C_3H_6 = C_2H_3 + CH_3$; 10 — $C_3H_6 + H = AC_3H_5 + H_2$; 11 — $C_3H_6 + H = C_2H_4 + CH_3$; 12 — $n^*C_3H_7 = C_3H_6 + H$; and 13 — $n^*C_3H_7 = C_2H_4 + CH_3$

Table Caption

Experimental conditions and techniques used to measure ignition delay for propene autoignition by various research groups presented in [24]

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