APPLICATION OF FOUR-COMPONENT KEROSENE SURROGATE FOR MODELING IGNITION AND COMBUSTION OF AVIATION FUEL VAPORS IN MIXTURES WITH AIR

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Abstract: A reduced kinetic mechanism describing the ignition and combustion of four-component surrogate of kerosene, comprising n-decane, iso-octane, iso-cetane, and toluene is proposed. The mechanism consists of 68 species and 248 reactions and includes the submechanisms of n-decane (42 species), iso-octane (8 species), iso-cetane (7 species), and toluene (11 species) oxidation. The mechanism is validated against experimental data on the ignition delay time, laminar flame speed, and changes in concentrations of main species in wide ranges of temperature (T_0 = 450–1400 K), pressure (P_0 = 1–50 атм), and fuel-to-oxidizer equivalence ratio (ϕ = 0.25–1.7). The kinetic mechanism provides a reasonable agreement with the experimental data.

Keywords: kerosene surrogate; oxidation; combustion; ignition; reaction mechanism

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Figure Captions

Figure 1 Ignition delay time as a function of initial temperature at $P = 20$ atm and $\varphi = 1$. Signs — experimental data for Jet-A (filled) and JP-8 jet fuels (empty): *1* — [13]; *2* — [14]; *3* — [15]; *4* — [16]; *5* — [17]; and *6* — [18]. Lines — predictions with the reaction mechanism of the present work for the individual components of the surrogate composition: *7* — n-$C_{10}H_{22}$; *8* — i-$C_{16}H_{34}$; *9* — i-C_8H_{18}; and *10* — C_7H_8

Figure 2 Ignition delay time as a function of initial temperature at $\varphi = 1$ and different pressures. Signs — experimental data for Jet-A (filled) and JP-8 jet fuels (empty): *1* — [20], 3 atm; *2* — [16], 5 atm; *3* — [20], 6 atm; *4* — [15], 8 atm; *5* — [15], 10 atm; *6* — [17], 10 atm; *7* — [16], 10 atm; *8* и *9* — [13], 30 atm; *10* — [15], 40 atm; *11* — [18], 4 atm; and *12* — [13], 50 atm. Lines — predictions with the reaction mechanism of the present work for surrogate S4

Figure 3 Ignition delay time as a function of initial temperature at $\varphi = 0.5$ and different pressures. Signs — experimental data for Jet-A (filled) and JP-8 jet fuels (empty): *1* — [21], 1 atm; *2* — [20], 3 atm; *3* — [6], 7,7 atm; *4* — [17], 10 atm; *5* — [17], 20 atm; *6* — [13], 20 atm; *7* — [15], 20 atm; *8* — [18], 20 atm; and *9* — [16], 20 atm

Figure 4 Ignition delay time as a function of initial temperature at $P = 20$ atm and $\varphi = 0.25$, 0.5, and 1. Signs — experimental data for Jet-A (filled) and JP-8 jet fuels (empty): *1–3* — [15]; *4* and *5* — [16]; and *6* — [14]

Figure 5 Laminar burning velocities as a function of fuel-to-air equivalence ratio of kerosene–air mixture at $T_0 = 450$ (filled signs) and 470 K (empty signs) and $P_0 = 1$ atm. Signs — experimental data for the Jet A/air mixture: *1* — [23]; *2* — [24]; and *3* — [22]. Solid and dashed lines — predictions with the reaction mechanism of the present work for the n-$C_{10}H_{22}$/i-C_8H_{18}/i-$C_{16}H_{34}$/C_7H_8 = 60/10/10/20 surrogate at $T_0 = 450$ and 470 K, respectively

Figure 6 Experimental [25] (*1*) and predicted temperature profiles: *2* — $T_{\min}$; *3* — $T_{\max}$; *4* — T_{S4}; and *5* — T_{SDoute}

Figure 7 Comparison of the results of calculations based on the kerosene70 reaction mechanism with experimental data [25] (empty signs) using surrogate models S4 (n-$C_{10}H_{22}$/i-C_8H_{18}/i-$C_{16}H_{34}$/C_7H_8=60/10/10/20) (black filled signs) and SDoute (n-$C_{10}H_{22}$/C_7H_8 = 90/10) (grey filled signs); $T_{\mathrm{mix}} = 473$ K, $P = 1$ atm, and $\phi = 1.7$

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