SIMULATION OF BREAKUP, EVAPORATION, AND SELF-IGNITION OF KEROSENE DROPLETS IN AIR

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Abstract: The known physical and mathematical models of aerodynamic droplet breakup and droplet evaporation are validated for the standard aviation kerosene and for its single-component physical surrogates (n-decane and n-dodecane). Also, kerosene single-component and 9-component chemical surrogates are selected and the known overall kinetic mechanisms are modified for modeling self-ignition and combustion of the vapors of these surrogates. The combination of the validated models, selected surrogates, and modified overall kinetic mechanisms is tested on the numerical solution of the multidimensional problem of kerosene spray self-ignition in a confined volume.

Keywords: aviation kerosene; droplet breakup; droplet evaporation; surrogate fuel; self-ignition; combustion; overall kinetic mechanism; computational fluid dynamics

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Figure Captions

Figure 1 Schematic of experimental setup [48] (*a*) and computational mesh (*b*)

Figure 2 Comparison of calculated and measured [48] spray penetration in air (*a*) and spray shape (*b*): *1* — $C_2 = 1$; *2* — 5; *3* — 10; *4* —20; *5* —30; *6* — $C_2 = 40$; and *7* — experiment

Figure 3 Schematic of experimental setup [52] (*a*) and computational mesh (*b*)

Figure 4 Comparison of calculated (*1*–*6*) and measured [52] (*7*) spray shapes: (*a*) $q = 2$; (*b*) 6; and (*c*) $q = 18$

Figure 5 Comparison of calculated (curves) and measured [56] (symbols) time histories of the squared droplet diameter of n-decane at $T_{g0} = 773$ K, $T_{l0} = 328$ K, $d_0 = 0.4$ mm, and two pressures: (*a*) $P = 0.1$ MPa and (*b*) $P = 0.5$ MPa

Figure 6 Comparison of calculated (*1*) and measured [56] (*2*) dependences of n-decane droplet evaporation constant on pressure

Figure 7 Calculated time histories of temperature and species volume fractions at self-ignition of the stoichiometric kerosene–air mixture at $T_0 = 760$ K and $P = 10$ atm: *1* — overall mechanism, 9-component surrogate; *2* — overall mechanism, single-component surrogate; and *3* — detailed kinetic mechanism [61]

Figure 8 Comparison of calculated (curves) and measured [64] (symbols) ignition delay times for stoichiometric mixtures of kerosene surrogates with air: *1* — overall mechanism, 9-component surrogate; *2* — overall mechanism, single-component surrogate; and *3* — detailed kinetic mechanism [61]

Figure 9 Comparison of calculated (curves) and measured [65] (symbols) ignition delay times for stoichiometric mixtures of kerozene surrogates with air: *1* — $P = 22$ atm; *2* — 32; *3* — $P = 50$ atm; solid curves — overall mechanism, 9-component surrogate; and dotted, dashed, and dash-dotted curves — overall mechanism, single-component surrogate
xx

Figure 10 Calculated time histories of pressure, temperature, and species mass fractions for self-ignition of the 9-component kerosene surrogate at a distance of 10 mm from the reflecting wall: (*a*) variant No. 1; and (*b*) variant No. 12

Figure 11 Comparison of calculated (*1*) and measured [63] (*2*) values of τ_{ign} reduced to a pressure of 20 atm

Figure 12 Comparison of calculated (curves) and measured (symbols) laminar flame velocities for kerosene–air mixtures of different composition at initial temperature $T_0 = 400$ K and pressure $P = 1.0$ atm: *1* — overall mechanism, 9-component surrogate; *2* — overall mechanism, single-component surrogate; *3* — [67]; *4* — [68]; *5* — [69]; *6* — [70]; *7* — [71]; and *8* — [72]

Figure 13 Schematic of experimental setup [72, 74] (a) and computational mesh (b)

Figure 14 Calculated (*1* — detailed kinetic mechanism; and *2* — overall kinetic mechanism) and measured [74] (*3* — broadband radiation; and *4* — OH) shapes of reaction zone at time 1.4 ms in variant No. 6 with a self-ignition delay of 0.5–0.7 ms

Table Captions

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