DETAILED MODELING OF DROP EVAPORATION AND COMBUSTION

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Introduction

Drop combustion is a phenomenon comprising all main constituents of the combustion process, namely, fast exothermic chemical reactions complicated by diffusion of reactants and products, thermal energy deposition and spreading of heat in the medium, and convective flows. The classical theory implies that drop combustion is diffusion-cotrolled and therefore chemical kinetic aspects are out of the analysis. For problems dealing with combustion-generated pollutants and transient modes of combustion like ignition or extinction, it is necessary to consider the effects of finite-rate chemical kinetics. This paper deals with the mathematical model of drop ignition and combustion taking into account the realistic kinetics of fuel oxidation and pollutant (CO, NO, and soot) formation, transient heating, and multicomponent diffusion.

Formulation

The primary interest is combustion of a drop of a heavy primary hydrocarbon. For modeling the gasification and combustion of the drop, the following simplifying assumptions have been adopted: (i) the drop has a spherical shape; (ii) no internal diffusion of species and convection exists inside the drop; (iii) buoyancy effects in a gas phase are not con-

sidered, (iv) pressure is constant, and (v) concentration of fuel vapor at the drop surface is governed by the equilibrium relationship.

The governing equations of the model include the partial differential equations of energy conservation in the drop; gas-phase continuity and energy conservation equations; multicomponent diffusion equations for gas-phase species; and the real-gas equation of state for the gas phase. All relevant physical properties are considered as functions of pressure and temperature.

Boundary conditions comprise the symmetry condition in the drop center; temperature, heat and mass flux continuity conditions at the drop surface; equations for gaseous species concentrations at the drop surface; and the no-gradient conditions at the external boundary of the gas phase.

Initial conditions encounter homogeneous conditions inside the drop and inhomogeneous conditions in the gas phase that make a provision for a hot layer to induce drop ignition. The ambient temperature is taken equal to or higher than the drop temperature. Initial fuel vapor contents in the gas phase is taken zero.

Gas-phase oxidation of a heavy hydrocarbon fuel is modeled by means of the overall reaction mechanism containing 10 species (fuel, O_2, N_2, CO, CO_2, H_2, H_2O, NO, soot, and a generalized radical R). The kinetic mechanism has been preliminarily validated for premixed and nonpremixed counterflow flames.

Drop ignition was facilitated by adopting a time-variable activation energy of a rate-controlling gas-phase reaction of fuel decomposition. A characteristic time of the activation energy relaxation from very low values to the reaction-relevant value was typically less than 100 μs that was more than by the order of magnitude less than the drop lifetime.

A set of governing equations was integrated numerically with the use of the nonconservative implicit finite difference scheme and the movable, adapted, computational grid. The solution procedure included iterations at each time step. The important point of the algorithm is the linearization of the conditions at the drop surface. For ensuring rapid convergence of the iterations, the full Newton-type linearization of the interface conditions was required. The accuracy of the solution was controlled by checking the elementary balances of C and H atoms as well as the energy balance at each time step.

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Results
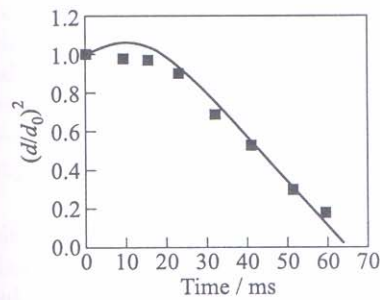
Figure 1 Comparison of the predicted $d^2(t)$-curve with experimental data [1] on evaporation of an unsupported n-tetradecane drop with $d_0 = 70 \pm 2$ μm in air at ambient temperature of $T_0 = 573$ °C

The mathematical model has been validated against available experimental data on evaporation and combustion and pollutant emission for hydrocarbon fuel drops.

Figure 1 shows the comparison of predicted and measured [1] surface regression curves for the n-tetradecane drop of initial diameter $d_0 = 70$ μm evaporating in air at ambient temperature of $T_0 = 573$ °C.

Curve in Fig. 2 shows the predicted dependence of the combustion constant, K, of n-heptane drops on the initial drop diameter. In the calculations, the combustion constant is determined as the slope of the $d^2(t)$-curve at the quasi-steady period of drop combustion, i.e.,
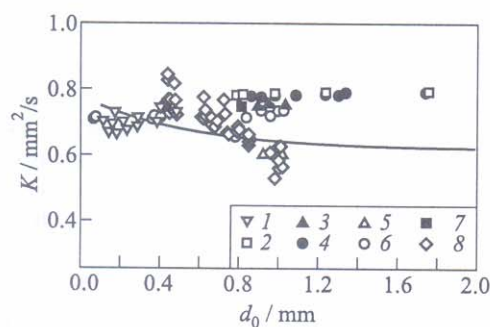
$$K = -\frac{d(d^2)}{dt}$$

Symbols in Fig. 2 represent experimental data [2–8] obtained both under microgravity conditions (for relatively large drops with $d_0 > 0.4$–0.5 mm) and normal gravity conditions (for relatively small drops $d_0 <$ 0.4–0.5 mm). In some experimental studies (e.g., [7]) the combustion constant was defined as $K = d_0^2/t_d$, where t_d is the drop burning time. Clearly, the model correlates fairly well with the measurements for drops of relatively small initial size. For drops of large initial diameter, the combustion constant is somewhat underpredicted. Note that for such drops, the contribution of convective heat and mass transfer becomes significant, while the model does not include these effects.

For n-decane drops, the model provides satisfactory agreement with low-gravity experimental data [9] for the evolution of drop (Fig. 3 a) and flame (Fig. 3 b) diameter.

Figure 2 Comparison of predicted (curve) and measured (symbols) dependencies of n-heptane combustion constant K on the initial drop diameter. Experimental data: 1 — [2], 2, 3 — [3], 4 — [4], 5 — [5], 6 — [6], 7 — [7], and 8 — [8]
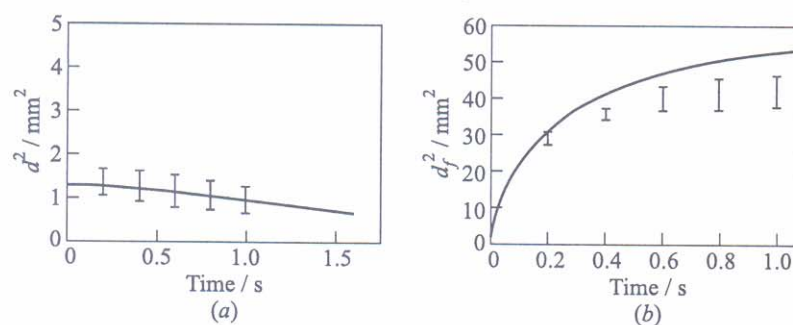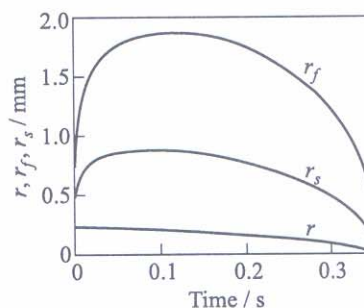

Figure 3 Comparison of predicted (curves) and measured (error bars) dependencies of drop (a) and flame (b) diameter for burning n-decane drop under low-gravity conditions. Experimental data [9]

In the above examples, the maximum gas temperature attained during the drop lifetime varies from 1800 to 2200 K, with higher temperature values related to initially larger drops.

The predicted dynamics and structure of the drop flame exhibits several important features. The first one is the existence of a soot shell located between the flame and the drop surface. The second is that

the flame, after drop ignition, moves outwards from the drop, but at later stages it changes the direction of motion (flame "shrinks"). These both features were observed experimentally [5, 9–12], and reviewed in the recent paper [13].

Figure 4 shows the predicted histories of the drop radius r, flame radius r_f (determined as the radial position of temperature maximum), and soot shell radius r_s (determined as the radial position of maximum soot concentration). When considering Fig. 4, one can distinguish three stages in the drop history: (*i*) ignition, (*ii*) outward flame motion, and (*iii*) flame "shrinking." The

Figure 4 Predicted histories of drop radius, r, flame radius, r_f, and soot shell radius, r_s, during ignition and combustion of n-heptane drop of initial diameter 0.48 mm in air at ambient pressure of 1 atm and temperature of 300 K

burning process of a drop is accompanied with the formation of a spherical soot shell inside the flame. The mass fraction of soot in this shell structure remains nearly constant as combustion proceeds until near the end of burning when the flame begins to "shrink." The "shrinking" flame approaches the soot shell, resulting in soot oxidation before flame extinguishing. This understanding of soot formation mechanism at drop combustion provides the measures to control soot emission, for example, by applying water-in-oil emulsions [14].

Concluding Remarks

The paper describes the mathematical model of fuel drop combustion and the results of its implementation. The model has been validated against available experimental data for combustion of hydrocarbon fuel drops under low-gravity and normal-gravity atmospheric conditions. Analysis of drop combustion dynamics indicates that the drop burning process is accompanied with the formation of a spherical soot shell

between the drop surface and the flame. Due to different kinetic laws of flame and soot-shell evolution, a part of soot is burned in the flame at the late, "shrinking" stage of flame motion. This understanding of soot formation mechanism provides the prerequisites to control soot emission.

Acknowledgments

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