

IGNITION AND COMBUSTION OF HYDROCARBON FUEL DROPS

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Introduction

The classical theory of liquid drop vaporization, ignition, and combustion considers an isolated drop in unconfined ambience [1–4]. Within this presumption, notable progress in understanding relevant physical and chemical processes has been achieved recently [5–8]. However, in practice, these processes occur in presence of neighboring drops or confinement surfaces. The corresponding effects are usually referred to as ‘spray’ and ‘confinement’ effects. Spray effects manifest themselves in two-phase reactive flows [9–15]. In existing computational approaches, chemical reaction rates are determined based on considering gas-phase combustion with fuel drops treated as distributed source terms for fuel vapor. As a matter of fact, spray combustion is a complex combination of diffusion-controlled flames around individual drops, groups of drops, and gas-phase partially premixed flames. The objective of this study is to extend our knowledge on drop vaporization, ignition, and combustion with spray and confinement effects taken into account.

Formulation

For a spatially uniform and monodisperse drop suspension in air, an elementary cell in the form of hexahedron (in a plane, see Figs. 1a and 1b) or polyhedron with faces in the form of equilateral triangles (in space, see Fig. 1c) can be constructed around each drop.

The length of a polyhedron edge is equal to a half-distance between drops in suspension, R_c . Due to symmetry considerations, mass, momentum, and energy fluxes through the faces will be zero. Polyhedron volume, V_s , and surface area, S_c , are:

$$V_c = \frac{5\sqrt{2}}{3} R_c^3, \quad S_c = 5\sqrt{3} R_c^2$$

Thus, drop behavior in the suspension can be modeled by solving the governing conservation equations for a single drop with symmetry boundary conditions at the polyhedron faces. As shown in [16] based on three-dimensional (3D) simulation of laminar flow pattern around an evaporating drop, the polyhedron cell can be approximated with an elementary sphere. In this case, the 3D problem is reduced to one-dimensional formulation with zero-flux boundary conditions at the surface of the elementary sphere of radius, R , equal to

$$R = \left(\frac{5\sqrt{2}}{4\pi} \right)^{1/3} R_c \approx 0.826 R_c$$

The volume of the elementary sphere is $V = V_c$ and the surface area is $S/S_c \approx 0.99$. The error of such an approximation depends on the suspension density (loading ratio ζ — mass of dispersed liquid in the unit volume). At a given loading ration, the radius of the elementary sphere is equal to

$$R \approx R_0 \left(\frac{r_l}{h} \right)^{1/3}$$

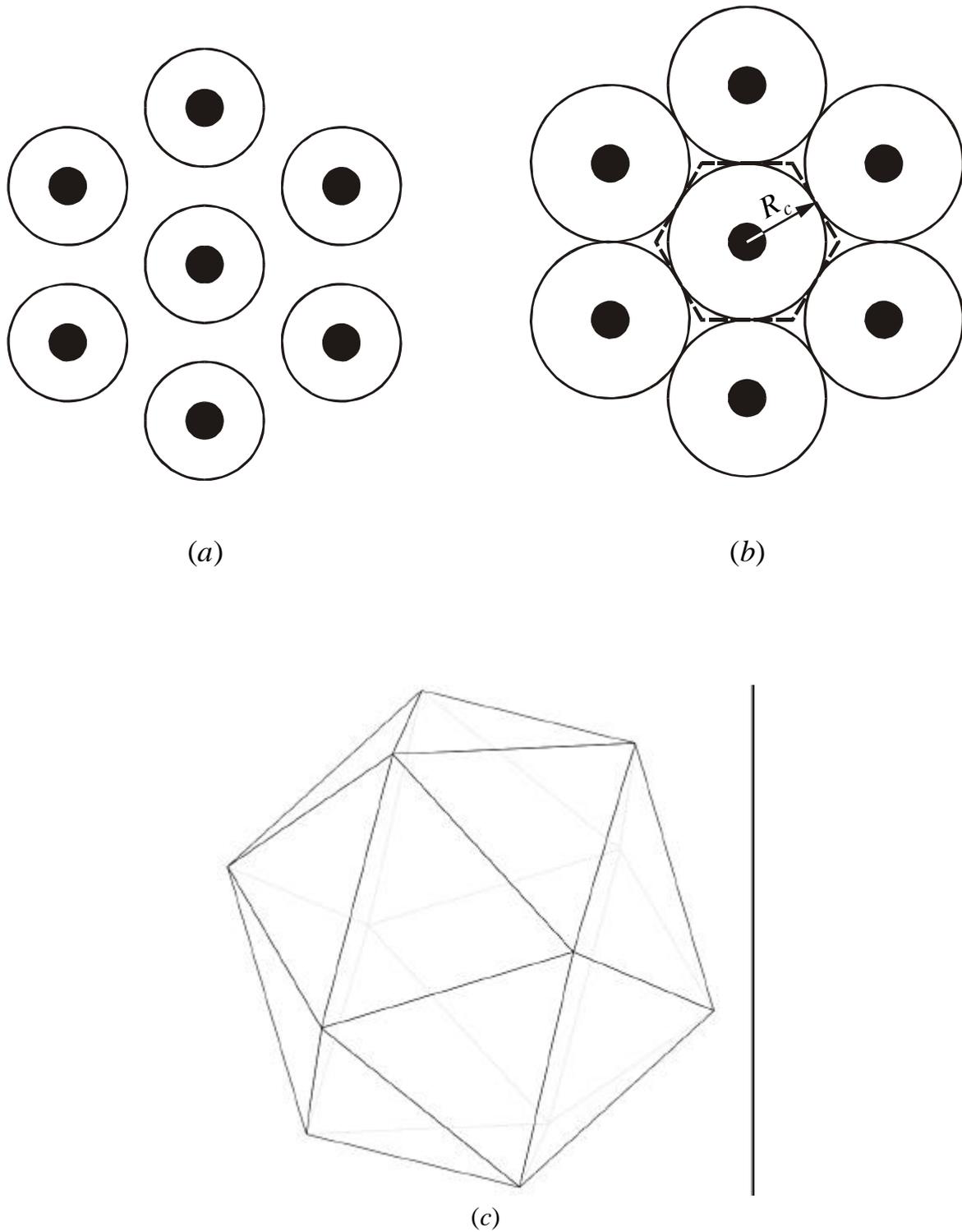


Figure 1: Elementary cell for the uniform monodisperse drop suspension. Black circles denote drops. Circumferences around drops characterize the spread of diffusion fluxes from individual drops. (a) Spray effects are absent; (b) spray effects manifest themselves. Dashed line bounds the elementary cell with zero mass and energy fluxes through its surface; R_c is the characteristic cell size (half-distance between drops); (c) three-dimensional elementary cell in the form of regular polyhedron with 20 faces

where R_0 is the initial drop radius and r_l is the liquid density. In terms of the equivalence ratio $\Phi = h / (f_{st} r_g)$, the radius of the elementary sphere is equal to

$$R \approx R_0 \left(\frac{r_l}{r_g \Phi f_{st}} \right)^{1/3}$$

where r_g is the initial gas density and f_{st} is the stoichiometric fuel–air ratio. At normal atmospheric conditions, for stoichiometric mixtures of liquid hydrocarbon fuels $r_g = 1.19 \text{ kg/m}^3$, $r_l = 700\text{--}800 \text{ kg/m}^3$, $f_{st} \approx 0.06$ and $\Phi = 1$, therefore $h = h_{st} \approx 0.07\text{--}0.08 \text{ kg/m}^3$, $R_c / R_0 \approx 25\text{--}27$ and $R / R_0 \approx 21\text{--}22$. At elevated pressure, for example at the end of compression stroke in a Diesel engine, ($r_g \approx 30 \text{ kg/m}^3$) $R_c / R_0 \approx 9$ and $R / R_0 \approx 8$.

The mathematical statement of the problem is based on the following simplifying assumptions: (1) the drop has a spherical shape, (2) no internal diffusion of species and convection exists inside the drop, (3) buoyancy effects in a gas phase are not considered, (4) pressure is constant, and (5) 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 processes 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; and the no-gradient conditions at the spherical elementary cell surface. As the model implies constant pressure, the radius of the elementary sphere is dependent of time, i.e., $R = R(t)$. The expansion/shrinking of the sphere is found from the solution by allowing the external boundary of the sphere to move with the gas at a radial distance of $r = R$.

Initial conditions encounter homogeneous conditions inside and outside the drop. To facilitate drop ignition, a provision for a thin hot layer is made in the gas phase. The ambient temperature is taken equal or higher than the drop temperature. Initial fuel vapor content in the gas phase is taken zero (in case of no prevaporization).

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.). The kinetic mechanism has been preliminarily validated for propagating premixed flames, nonpremixed counterflow flames, fuel drop autoignition and diffusion flames [17–21].

Results and Discussions

Numerical solution of mass, momentum, and energy conservation equations for a hydrocarbon drop within the elementary sphere resulted in several important findings. Below these findings are discussed on examples of drop vaporization, autoignition, and combustion.

Drop Vaporization

Analysis of drop vaporization in dense drop suspensions indicates [16] that drop lifetime increases considerably as compared to the isolated drop in an unconfined atmosphere. Figure 2 shows the

calculated time histories of the squared drop diameter depending on \ddot{O} . Three important findings are worth mentioning: (1) drops evaporate slower, (2) the deviations from the classical d^2 -law increase as \ddot{O} increases, and (3) at a certain \ddot{O} drops evaporate only partly. The latter finding is due to a considerable screening effect of neighboring drops in the cloud resulting in vapor saturation conditions in the interdrop space. Slower vaporization of individual drops has been observed in experiments with linear drop arrays [22].

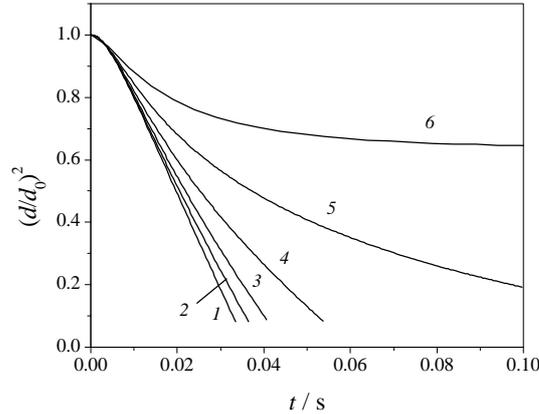


Figure 2: Predicted time histories of normalized surface of an *n*-heptane drop evaporating in air as a function of \ddot{O} [16]. Initial parameters: drop diameter $d_0 = 70 \text{ }\mu\text{m}$, drop temperature $T_{l0} = 293.15 \text{ K}$, gas temperature $T_{g0} = 573.15 \text{ K}$, and pressure $p = 0.1 \text{ MPa}$. 1 — $\Phi = 0$ (isolated drop), 2 — 1.06, 3 — 2.12, 4 — 4.25, 5 — 8.5, and 6 — 17.0

Drop Autoignition

For analyzing spray effects on hydrocarbon drop autoignition, it is instructive to introduce a fuel index as the ratio of fuel mass in the gas phase to the initial mass of fuel drop:

$$I(Fu) = \frac{6}{\rho d_0^3 r_l} \int_{R_s}^R 4\rho r^2 Y(t, r) dr \quad (1)$$

where Y is the fuel vapor concentration, R_s is the instantaneous drop radius, and Fu stands for fuel. There are two fuel indices: $I(Fu_d)$ — for the fuel vapor originating from the drop due to its vaporization at time $t > 0$, and $I(Fu_g)$ — for the fuel vapor existing in the gas phase at $t = 0$ due to drop prevaporization.

Figures 3a and 3b show the time histories of fuel index $I(Fu_d)$ in a stoichiometric spray for small *n*-heptane drops from 2 to 8 μm in initial diameter with no prevaporization (a) and with $I(Fu_g) = 0.25$. At the conditions adopted ($T_{g0} = 1500 \text{ K}$, and $p = 3 \text{ MPa}$), drops of initial diameter 2 μm evaporate in approximately 5.8 μs , however chemical reaction is almost absent during a period of 0.1 μs . The same is valid for drops 4, 6, and 8 μm in diameter. Combustion is considerably accelerated if at the beginning of the process the gas phase contains some amount of prevaporized fuel. Note that the total initial equivalence ratio was always kept constant and equal

to 1, i.e., in cases with $Fu_g > 0$, the radius of the elementary sphere R was correspondingly changed.

It follows from Fig. 3b that during ignition delay period, fuel vapor accumulates around the drop and after ignition it is rapidly consumed. Clearly, at $Fu_g > 0$, the rate of $I(Fu_d)$ decay can change drastically starting from a certain time. For example, at $t = 60 \text{ ns}$ drops of initial diameter 6 nm exhibit fast decrease of fuel vapor concentration (see Fig. 3b) caused by ignition of initially prevaporized fuel. After ignition, the rate of fuel vapor depletion decreases due to transition to diffusion controlled drop combustion. At $t = 100 \text{ ns}$, only 2.5% of fuel vapor remains unburned. In case of drops of initial diameter 8 nm , 4.6% of fuel vapor remains unburned at $t = 100 \text{ ns}$. Drops of initial diameter 4 nm ignite with ignition delay of approximately 80 ns (strong cooling due to evaporation manifests itself), but completely burn out before 100 ns . Drops of initial diameter 2 nm do not ignite during 100 ns . Thus, the ignition delay and fuel burning time in the spray are complex functions of the initial drop diameter and are strongly affected by the amount of prevaporized fuel.

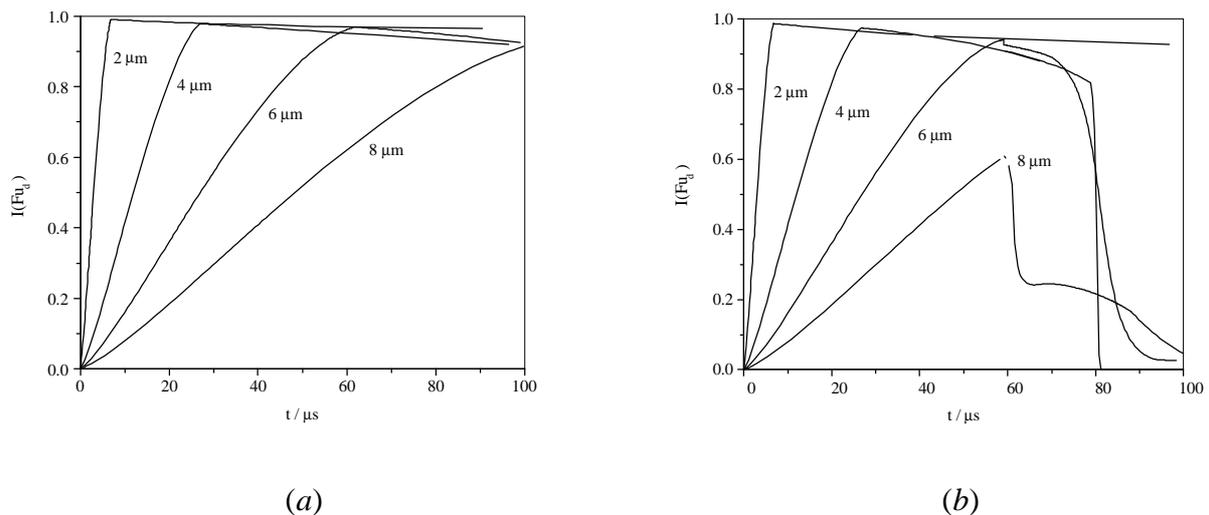


Figure 3: Predicted time histories of fuel index $I(Fu_d)$ in a stoichiometric spray of small n -heptane drops with $d_0 = 2, 4, 6,$ and 8 nm at initial air pressure and temperature of 3 MPa and 1500 K , respectively. (a) $Fu_g = 0$, and (b) $Fu_g = 0.25$

Drop Combustion

Similar to vaporization, volumetric combustion in dense drop suspensions is very sensitive to the drop loading ratio. The lifetime of burning drops also increases with \ddot{O} . Moreover, temperature and flame dynamics in the interdrop space behave very different from that typical for the isolated drop other conditions being equal. Figure 4 shows the calculated time histories of the flame (maximum) temperature T_{\max} as well as dimensionless flame and drop radii, R_f/R_0 and R_s/R_0 , respectively, for the isolated drop (solid curves) and drop in suspension (dashed curves) of similar initial radius R_0 .

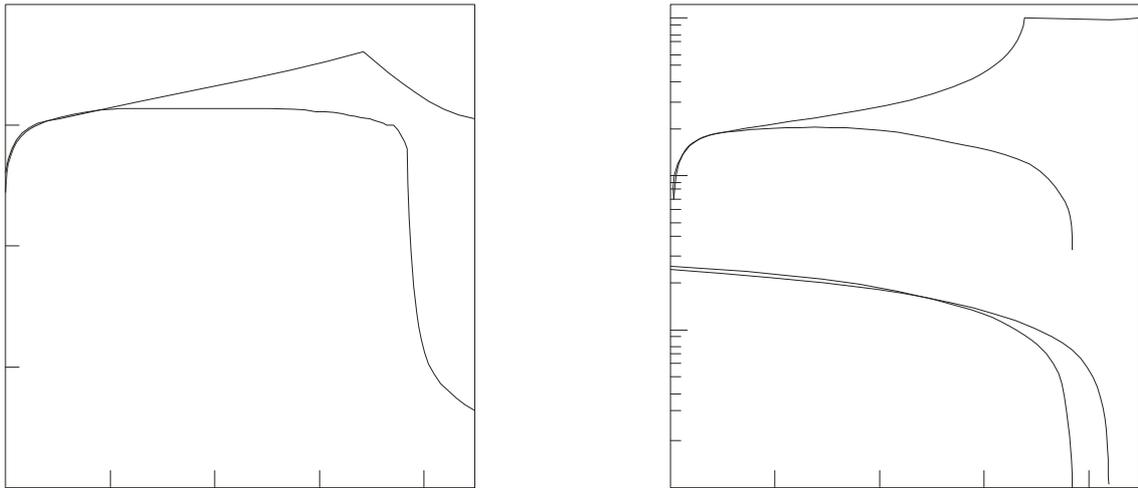


Figure 4 Comparison of flame temperature (*a*) and dimensionless flame and drop radii, R_f/R_0 and R_d/R_0 , histories for the isolated drop (solid curve) and drop in suspension (dashed curve, $\ddot{O} = 1.1$). Fuel: *n*-heptane, Oxidizer: air, Initial pressure and temperature: 0.1 MPa and 300 K; $R_0 = 0.25$ mm

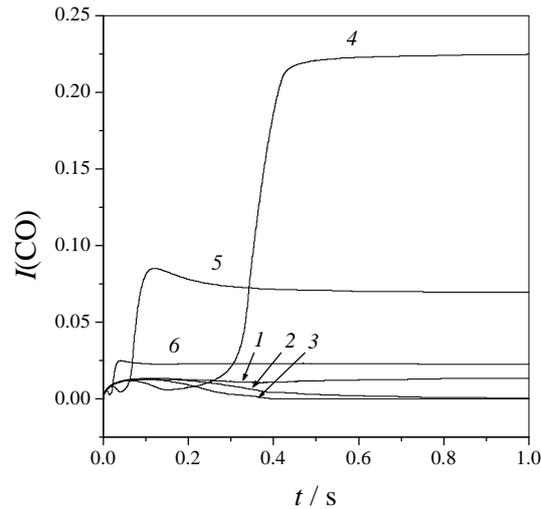
The suspension density in this case is characterized by the equivalence ratio $\Phi = 1.1$. The flame temperature for the drop in suspension is considerably higher than that for the isolated drop, in particular at the end of combustion. For the isolated drop, the flame stabilizes at a distance of about $8R_0$, whereas for the drop in suspension the flame spreads towards the edge of the elementary sphere consuming all available oxygen. In fuel-rich suspensions, only a part of fuel is burned and the remaining fuel is vaporized and accumulated in the interdrop space together with the combustion products. As the temperature in the interdrop space is high, fuel vapor can partly decompose to more reactive intermediate species.

Emission indices of pollutants depend considerably on suspension density. Figure 5 shows the predicted emission indices of CO (*a*), NO (*b*), and soot (*c*). The emission indices are defined by Eq. (1) with Y treated as the concentration of the corresponding species in the gas phase.

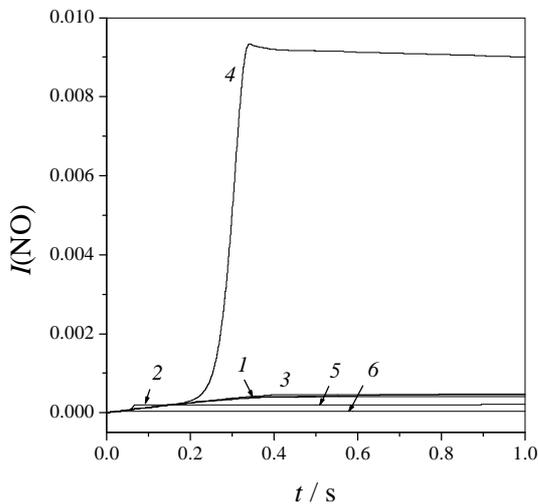
It follows from Fig. 5 that the near-stoichiometric suspensions exhibit maximal emission indices. As could be expected, fuel-rich suspensions exhibit higher emission indices of CO and soot, but lower emission indices of NO than the fuel-lean mixtures.

Concluding Remarks

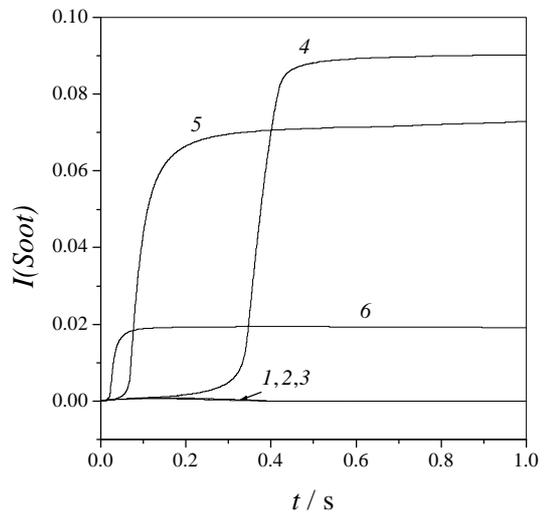
Based on the detailed simulation of drop behavior in a uniform monodisperse suspension, it has been shown that (1) drops in suspension vaporize slower than isolated drops, (2) quasistationary d^2 -law is, in general, not valid for drops in suspension, (3) at suspension densities exceeding a certain limiting value, drops vaporize only partly or virtually do not vaporize, (4) drop autoignition delay depends on the drop diameter and suspension density and is strongly affected by the amount of prevaporized fuel, (5) individual drop flame structure and parameters depend on suspension density, (6) individual drop flame exists within a limited range of suspension densities, and (7) emission indices of pollutants (CO, NO, and soot) depend considerably on suspension density. Results of



(a)



(b)



(c)

Figure 5: Predicted time histories of emission indices of CO (a), NO (b), and soot (c) for burning drops in suspension depending on \ddot{O} . Initial parameters: $d_0 = 500 \text{ \mu m}$, $T_{l0} = T_{g0} = 293.15 \text{ \textcircled{E}}$, and $p = 0.1 \text{ MPa}$. 1 — $\Phi = 0$ (isolated drop), 2 — 0.32, 3 — 0.55, 4 — 1.1, 5 — 5.3, and 6 — $\Phi = 18.5$

calculations have been compared with available experimental data. The analysis reported herein is also applicable for approximate description of local phenomena in nonuniform polydisperse drop suspensions. It is intended to use the results for improved ignition and combustion modeling in two-phase reactive flows.

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