

# Control of Single Droplet Combustion and Emission

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## Introduction

Chemical and physical processes accompanying combustion of a single fuel droplet are complex and interrelated. Chemical processes include oxidation reactions of fuel and its decomposition products, reactions of  $\text{NO}_x$  and soot formation, etc. Physical processes encounter transient molecular and convective heat and mass transfer and viscous dissipation in liquid and gas phases, phase transition, radiation, droplet thermal expansion, deformation and breakup, microexplosion of a multicomponent (solution or emulsion) droplet, etc. Particular issues are the flame ignition and extinction phenomena.

The ultimate objective of the research summarized in this paper is to compare combustion and pollutant-emission performances of pure-fuel and emulsified-fuel droplets. Based on general thermodynamic considerations, it is anticipated that addition of a volatile liquid component (e.g., water) to a heavy hydrocarbon fuel in emulsified form allows one to control droplet combustion by decreasing the amount of fuel vapor accumulated between the flame and the droplet surface and displacing the flame closer to the surface. As a consequence, more intense interphase fluxes can occur, affecting the droplet lifetime and pollutant emission.

Nowadays, no quantitative theory exists for combustion of an emulsified fuel droplet. Experimentally, ignition and combustion of such droplets has been studied elsewhere [1–7]. Recently [8], it has been demonstrated that the use of a specially prepared diesel fuel – water emulsion (Aquazole<sup>R</sup>) in heavy-duty diesel engines provided a significant decrease in soot and  $\text{NO}_x$  emission. The mathematical model described herein is aimed at better understanding of the encountered phenomena.

## Formulation

A pure-fuel droplet is a droplet of a heavy primary hydrocarbon. The emulsion droplet comprises the continuous phase (heavy primary hydrocarbon) and dispersed phase (volatile liquid component). At any time, component is uniformly distributed in the droplet in the form of microdroplets. Droplet heating results in internal evaporation of the additive and formation of additive vapor bubbles around microdroplets. Thus, in general, the emulsion droplet consists of three phases: I — fuel, II — dispersed liquid component, and III — component vapor bubbles. For modeling the gasification and combustion of the droplet, the following simplifying assumptions have been adopted: (1) the droplet has a spherical shape; (2) no internal diffusion of species and convection exists inside the droplet; (3) vapor bubbles are spherical and do not coagulate; (4) droplet history is continuous, i.e., no instabilities are considered leading to abrupt violation of droplet integrity (microexplosion); (5) buoyancy effects in a gas phase are not considered, (6) pressure is constant, (7) concentrations of fuel

and additive vapors at the droplet surface are governed by the equilibrium relationships for ideal binary solutions, (8) gas phase obeys the ideal-gas law. With no volatile liquid component, the emulsion droplet is equivalent to the pure-hydrocarbon fuel droplet.

The governing equations of the model include the partial differential equations of energy conservation for all three phases in the emulsion droplet with due regard for interphase heat fluxes and phase transition between phases II and III; gas-phase continuity and energy conservation equations; diffusion equations for gas-phase species; and the ideal-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 droplet center; temperature, heat and mass flux continuity conditions at the droplet surface; equation for gaseous species concentrations at the droplet surface; and the no-gradient conditions at the external boundary of the gas phase. Initial conditions encounter homogeneous conditions inside and outside the droplet. The ambient temperature is taken usually higher than the droplet temperature. Initial fuel and component vapor contents in the gas phase are taken zero. Gas-phase oxidation of a heavy hydrocarbon fuel is modeled by means of the overall reaction mechanism containing 10 species (fuel, O<sub>2</sub>, N<sub>2</sub>, CO, CO<sub>2</sub>, H<sub>2</sub>, H<sub>2</sub>O, NO, soot and a generalized radical R). The kinetic mechanism has been preliminarily validated for premixed and non-premixed counterflow flames.

Droplet 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 100 ns, that was more than by the order of magnitude less than the droplet lifetime.

A set of governing equations was integrated numerically with the use of the non-conservative 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 droplet interface. 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 at each time step and usually was as good as 0.1%. The mathematical model has been validated against available experimental data on evaporation and combustion and pollutant emission for pure-fuel droplets (*n*-heptane and *n*-tetradecane).

## Results

As an example of a heavy hydrocarbon fuel and volatile component, *n*-tetradecane and water were used. Fuel-water emulsion of this type simulates the performance of Aquazole<sup>R</sup> [8]. The main distinctive feature of the emulsion droplet gasification is the existence of a relatively long (up to 80% of the droplet lifetime) period of droplet expansion due to formation of steam bubbles in droplet interior. The predicted overheat of steam bubbles attains 100–150 K. Gasification of a single emulsion droplet of diameter *d* exhibits a fast stage of droplet surface regression after passing the maximum in the ‘*d*<sup>2</sup>– time’ curve. This stage can be conditionally treated as the microexplosion stage.

The predicted evolutions of temperature during ignition and combustion of pure *n*-tetradecane droplet and 90% *n*-tetradecane – 10% water emulsion droplet in air are shown in Figs. 1*a* and 1*b*, respectively, under essentially similar initial conditions in terms of the droplet size and temperature, and the same ambient conditions. In both cases, one can distinguish three stages in the droplet history: (1) ignition, (2) outward flame motion, and

(3) flame shrinking (shown by dashed curves). The ignition stage is quite similar for both cases. At the second stage, the emulsion droplet flame displaces to a considerably shorter distance from the droplet surface as compared to the pure-fuel droplet flame. Moreover, the maximum temperature in the emulsion droplet flame is considerably less due to the effect of water. At the third stage, flame shrinking is much more pronounced for the emulsion droplet.

These peculiarities are explained by the fact that addition of a volatile component (water) results in diminishing the fuel vapor partial pressure at the droplet surface and the amount of fuel vapor accumulated between the droplet surface and the flame. It is clearly demonstrated in Figs. 2a and 2b. As a result of this, and due to a more pronounced flame shrinking with the emulsion droplet, the amount of soot formed is significantly less for the emulsion droplet (see Figs. 3a and 3b). As it follows from Figs. 3a and 3b, the burning process of a droplet is accompanied with the formation of a spherical soot shell inside the flame. The shell initially forms close to the droplet surface. After some time, the shell maintains a relatively constant thickness. The mass fraction of soot in this shell structure rapidly increases as combustion proceeds until near the end of burning when the flame begins to shrink. The shrinking flame overtakes the soot shell, resulting in soot oxidation before flame extinguishing (as evident from Fig. 3b).

It is instructive to compare emission indices for combustion of pure-fuel and emulsion droplets. The emission index for the  $j$ th species is defined as the ratio of the total mass of this species in the gas phase,  $m_j$  to the initial mass of the droplet,  $m_{d0}$ , i.e.,

$$h_j = \frac{m_j}{m_{d0}} = \frac{4p \int_0^{\infty} r_j r^2 dr}{r_s m_{d0}}$$

where  $r_s$  is the instantaneous droplet radius,  $r_j$  is the partial density of the  $j$ th species in the gas phase. Figures 4a and 4b show the comparison of predicted emission indices of NO and soot.

Complex effects of volatile component loading ratio, ambient pressure and temperature, droplet size, the size of component microdroplets in the emulsion, and the droplet initial temperature on the droplet lifetime and gasification constants have been revealed. In a full paper, the results of the parametric computational studies will be discussed.

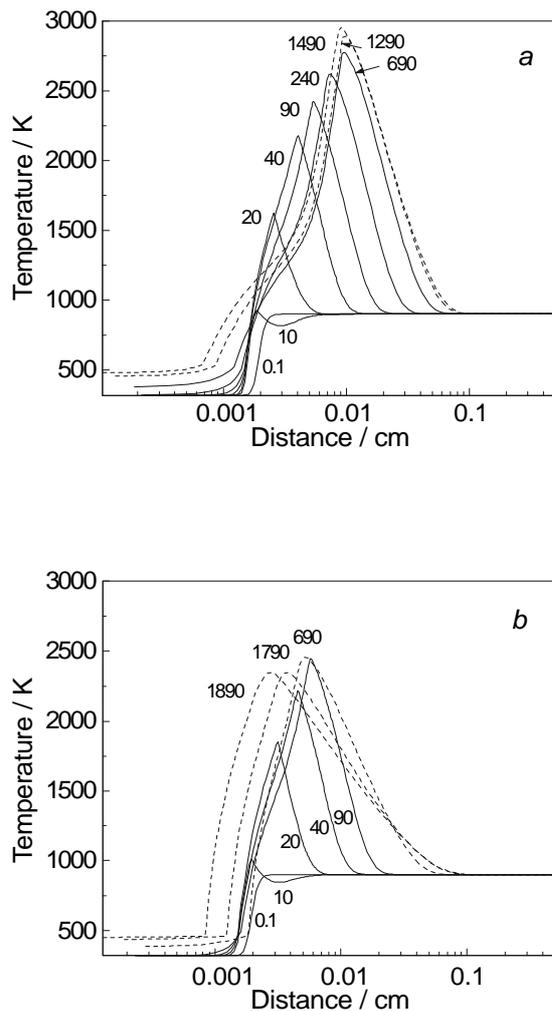
## Conclusion

The paper describes the mathematical model of pure-hydrocarbon fuel and emulsified-fuel droplet combustion and the results of its implementation. It has been shown that addition of a volatile liquid component to a hydrocarbon fuel allows one to control droplet combustion and emission performances.

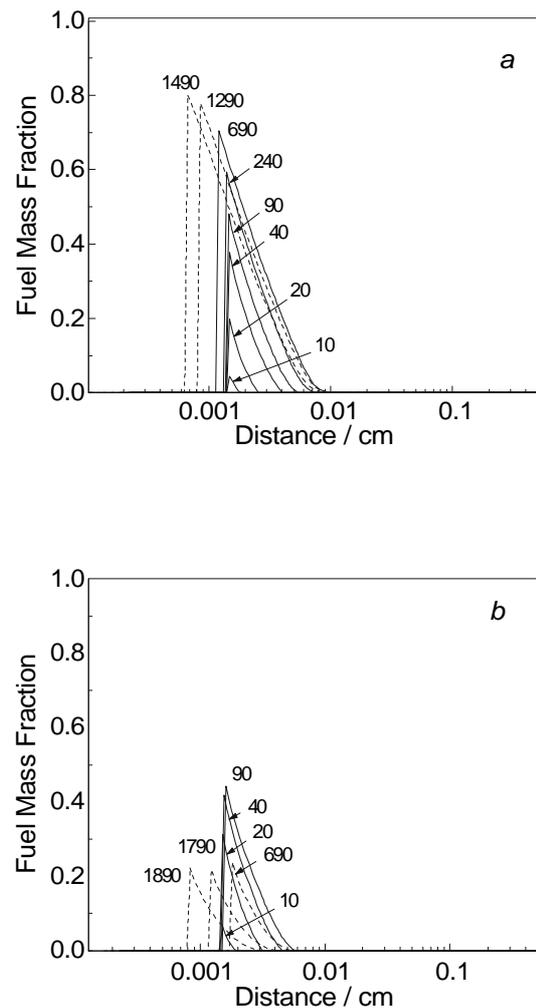
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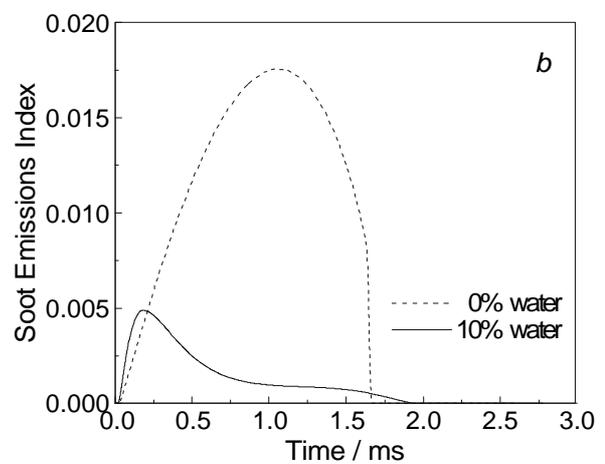
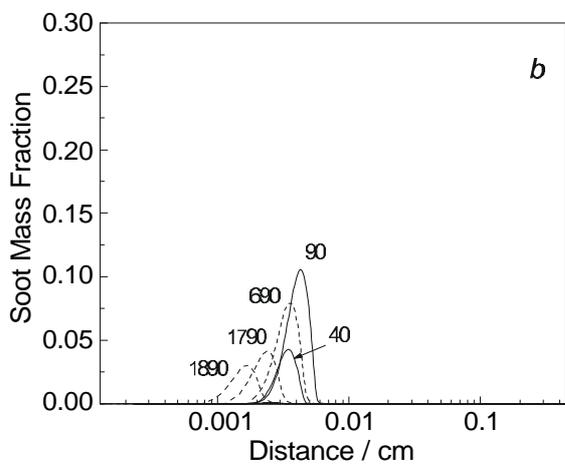
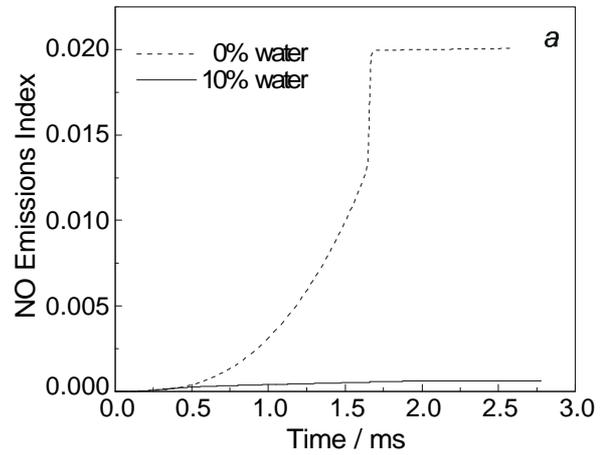
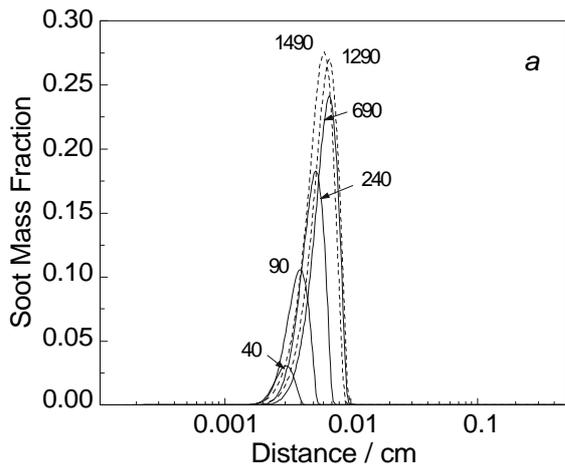
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**Fig. 1** Predicted evolution of temperature profiles in and around the burning droplet of initial diameter 30  $\mu\text{m}$  at  $p = 5$  bar. Dashed curves show the profiles at the flame shrinking stage. Numbers denote time in  $\text{ms}$ : (a)  $n$ -tetradecane, (b) 90%  $n$ -tetradecane – 10% water emulsion



**Fig. 2** Predicted evolution of fuel concentration profiles around the burning of initial diameter 30  $\mu\text{m}$  at  $p = 5$  bar. Dashed curves show the profiles at the flame shrinking stage. Numbers denote time in  $\text{ms}$ : (a)  $n$ -tetradecane, (b) 90%  $n$ -tetradecane – 10% water emulsion



**Fig. 3** Predicted evolution of soot concentration profiles around the burning droplet of initial diameter  $30 \mu\text{m}$  at  $p = 5$  bar. Dashed curves show the profiles at the flame shrinking stage. Numbers denote time in **ms**: (a) *n*-tetradecane, (b) 90% *n*-tetradecane – 10% water emulsion

**Fig. 4** Predicted histories of emission indices for the burning *n*-tetradecane (dashed curves) and 90% *n*-tetradecane – 10% water emulsion (solid curves) droplets of initial diameter  $30 \mu\text{m}$  at  $p = 5$  bar: (a) NO, (b) soot