Modeling of drop ignition and combustion in dense suspensions

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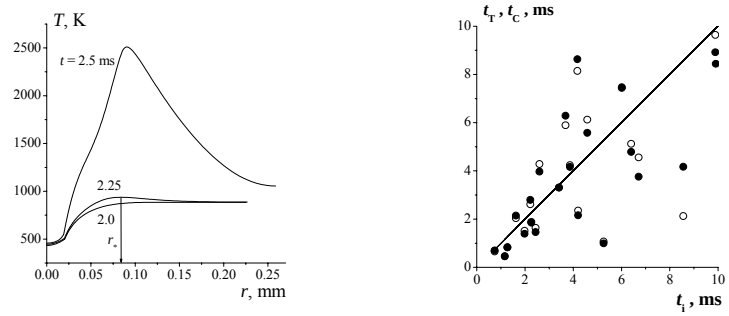
The classical theory of liquid drop vaporization, ignition, and combustion considers an isolated drop in unconfined ambience. Within this presumption, notable progress in understanding relevant physical and chemical processes has been achieved recently. However, in practice, these processes occur in presence of neighboring drops. The corresponding effects are usually referred to as 'spray' effects. Spray effects manifest themselves in two-phase reactive flows. In existing computational approaches, chemical reaction rates are determined based on considering homogeneous gas-phase autoignition and combustion with fuel drops treated only as source terms for fuel vapor. As a matter of fact, spray autoignition and combustion are complex combinations of localized ignition events in inhomogeneous mixture and diffusion-controlled flames around individual drops, groups of drops, and gas-phase partially premixed flames. The objective of this study was to develop detailed and simple models of drop vaporization, ignition, and combustion with spray effects taken into account.

The model was based on the "suspension elementary cell" concept [1] and comprised partial differential equations of energy conservation in a drop; gas-phase continuity and energy equations; multicomponent diffusion equations for gas-phase species, and the real-gas equation of state. Boundary conditions comprised the symmetry condition in the drop center; temperature, heat and mass flux continuity conditions at the drop surface; and zero gradient conditions at the spherical elementary cell surface. The model was used for making two sets of comparative calculations, namely, drop autoignition and combustion and drop vaporization without chemical reactions. The calculations were performed in the wide ranges of initial drop diameter ($d_0 = 20$–150 μm), suspension equivalence ratio ($\Phi = 0.1$–2.0), pressure ($p = 2$–8 MPa), and temperature ($T_0 = 800$–900 K). The fuels considered were *n*-decane and *n*-tetradecane.

In the course of drop-autoignition calculations, the temperature profiles in the drop vicinity (*i*) before autoignition, (*ii*) at the instant of autoignition, and (*iii*) at completion of localized autoignition, were purposefully monitored as shown in Fig. 1*a*. In the example of Fig. 1*a*, the instant (*i*) corresponds to $t = 2.0$ ms, instant (*ii*) — to 2.25 ms, and instant (*iii*) — to 2.5 ms.

Such an approach allowed determining the ignition delay time t_i (≈ 2.25 ms in Fig. 1*a*) and the location of the autoignition site in terms of the distance from the drop center r_i (≈ 0.085 mm in Fig. 1*a*). For further generalization of these data, the concept of normalized autoignition radius $r_* = 2r_i / d_0$ ($r_* \approx 4.25$ in Fig. 1*a*) was introduced. One of the main findings of these calculations was the fact that the normalized autoignition radius appeared to be nearly insensitive to the governing parameters within the ranges investigated. It was found that $r_* \approx 4 - 5$. Thus, the drop ignition calculations made it possible to collect the database on t_i and r_* depending on the various governing parameters of the problem.



(*a*) (*b*)

Fig. 1: Predicted temperature evolution at autoignition of *n*-decane drops in air at $d_0 = 40$ μm, $T_0 = 900$ K, $p = 2$ MPa, and $\Phi = 1.0$ (*a*) and correlation between t_i, t_T, and t_C (*b*).

Thereafter, a series of drop-vaporization calculations was made with the same values of governing parameters but with deactivated chemical reactions. The main objective of these calculations was monitoring of the local gas-phase equivalence ratio φ and normalized temperature $\theta_* = (T/T_0)_*$ at the normalized autoignition radius r_* obtained from the drop-autoignition calculations. More specifically, we were interested in the values of $\theta_* = (T/T_0)_*$ and $\varphi_* = \varphi(r_*)$ at $t = t_i$. Such an analysis was performed for numerous computational cases. It has been found that θ_* varied within the range from 0.83 to 1.0 with the mean value on the level of $\theta_* = 0.9$, whereas φ_* varied within the range from 0.25 to 2.0 with the mean value of $\varphi_* \approx 0.6$.

Statistical analysis of the data revealed a correlation between drop-autoignition and drop-vaporization calculations. Figure 1*b* shows the correlation between t_i and the predicted values of t_T and t_C, where t_T and t_C are the ignition delays obtained using the $\theta_* = 0.9$ and $\varphi_* \approx 0.6$ criteria in drop-vaporization calculations, respectively. It follows from Fig. 1*b* that there definitely exists an approximate universal correlation between the values of t_i, t_T, and t_C. Based on this finding, the following criteria of drop autoignition were suggested: ignition occurs when $\theta_* = 0.9$ and/or $\varphi_* \approx 0.6$ is reached at $r_* \approx 4$. One important implication has to be taken into account. Ignition delay t_i is known to decrease with decreasing the initial drop diameter down to the ignition delay in the homogeneous mixture $t_{i,h}$, whereas the values of t_T and t_C tend to zero. This deficiency can be readily overcome by introducing a constraint $t_T, t_C \geq t_{i,h}$.

The new ignition criteria were coupled with a simple drop vaporization model taking into account spray effects and were implemented into the 3D control-volume based CFD code, AVL FIRE. The new model was proved to be capable of adequately simulating drop vaporization, ignition and diffusion-controlled combustion, as well as combined diffusion-controlled and homogeneous combustion in dense suspensions.

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[1] Frolov, S. M., Basevich, V. Ya., Belyaev, A. A., Posvianskii, V. S., & Smetanyuk V. A. "Modeling of drop vaporization and combustion with regard for spray effects," Combustion and Atmospheric Pollution. Edited by G. Roy, S. Frolov, and A. Starik, Moscow, Torus Press, pp. 207–213, 2003.