

MATHEMATICAL MODEL OF FLAME PROPAGATION IN DROP SUSPENSIONS

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A new model of laminar flame propagation in liquid drop suspensions was developed and validated against available experimental data. The model is based on the simple premixed flame theory and the theory of single drop combustion in a uniform monodispersed drop suspension and applies the formalism of delta-functions. Chemical energy release is modeled by the overall reaction mechanism of hydrocarbon oxidation containing 13 reactions and 10 species, including soot, NO_x, and CO.

1 Introduction

The complexity of combustion phenomena in liquid fuel sprays stimulates the development of approximate models [1]. One of the most important issues in the theory of spray combustion is adequate modeling of laminar flame propagation in fuel drop suspensions.

The mathematical model of laminar flame propagation in monodispersed drop suspensions was proposed in [2]. The model was based on the well-known quadratic law of drop surface regression with time. The effect of polydispersed drop distributions on the laminar flame velocity and structure was studied in [3]. In [4], for determining the laminar flame velocity in drop suspensions, the detailed reaction mechanism of gas-phase fuel oxidation with empirical correction factors accounting for diffusion-controlled drop combustion was applied. In this paper, a nonempirical model of single drop combustion in a monodisperse spray [5] was coupled with the premixed flame theory to develop a new

model of laminar flame propagation in drop suspensions. The chemical process was modeled by the overall reaction of fuel oxidation.

2 Model

Laminar flame propagation in drop suspension was simulated based on the equations governing premixed laminar flame propagation coupled with the model of drop combustion in the monodispersed spray.

2.1 Premixed combustion model

A simple model of premixed laminar flame propagation is based on the one-dimensional (1D) equations of thermal conductivity and diffusion in the region $-\infty < x < +\infty$, where x is the coordinate. The equations are written in the form:

$$\frac{\partial}{\partial x} \left(\lambda \frac{\partial T}{\partial x} \right) - c \rho_0 u_n \frac{\partial T}{\partial x} + \Phi = 0 \quad (1)$$

$$\frac{\partial}{\partial x} \left(\rho D_j \frac{\partial Y_j}{\partial x} \right) - \rho_0 u_n \frac{\partial Y_j}{\partial x} + w_j = 0 \quad (2)$$

where T is the temperature, Y_j is the mass fraction of the j th species, u_n is the laminar flame velocity, ρ is the density, c is the specific heat, λ is the thermal conductivity, D_j is the diffusion coefficient of the j th species, Φ is the rate of chemical energy release, w_j is the overall rate of j th species variation in i elementary reactions ($w_j = \sum_{ij} w_{ij}$, $w_{ij} = k_{ij} \Pi_j Y_j$, and k_{ij} is the reaction rate constant of an elementary reaction), and index 0 relates to the initial mixture.

In general, the set of Eqs. (1) and (2) has to be supplemented with either detailed or overall reaction mechanism of fuel oxidation and the equation of state, e.g.,

$$p = \rho R^0 T \sum_{j=1}^M \frac{Y_j}{G_j}$$

where p is the pressure, R^0 is the universal gas constant, and G_j is the molecular mass of the j th species. As a result of the numerical solution

of the problem, the laminar flame velocity u_n can be obtained. In addition, the corresponding reaction rates w_j and the overall energy release function Φ can be obtained as functions of coordinate x or temperature $T(x)$.

The procedure outlined above has an important implication. Once the functions $w_j(T)$ and $\Phi(T)$ are available, one can readily calculate the flame propagation velocity as well as the spatial distributions of temperature and species mass fractions in the reaction zone by solving Eqs. (1) and (2). For example, replacement of the reaction mechanism of fuel oxidation by the diffusion-controlled law of drop combustion makes it possible to derive functions $w_j(T)$ and $\Phi(T)$ for the problem of laminar flame propagation in fuel drop suspension. If one assumes that such a flame is governed by the same set of Eqs. (1) and (2), the flame structure and propagation velocity can be readily calculated [2]. There are several drawbacks of such an approach to model laminar flames in drop suspensions. It is applied to diffusion-controlled combustion modes of the fuel drop and does not take into account spatially nonuniform physical and chemical processes in the close vicinity to the drop. However, as is shown below, this approach can be generalized for the case of laminar and turbulent flame propagation in drop suspensions.

The relationships for the source terms w_j and Φ in Eqs. (1) and (2) can be formally represented via a probability density function (PDF) as

$$\Phi = \sum_{j=1}^M \int_{T_0}^{T_c} H_j W_j(T) P(T, \bar{T}) dT \quad (3)$$

$$w_j = \sum_{j=1}^M \int_{T_0}^{T_c} \left[W_{1j}(T) - W_{2j}(T) \frac{Y_j \rho_g}{G_j} \right] P(T, \bar{T}) dT \quad (4)$$

where H_j is the heat of atomization or the enthalpy of the j th species in the mixture, W_j is the rate of variation of the j th species in all chemical reactions, and $P(T, \bar{T})$ is the two-parameter PDF of the local temperature T at a given mean temperature \bar{T} . By definition, the PDF is the probability of finding the local temperature T in the range from T_0 to T_c at a given mean temperature \bar{T} . The PDF is normalized as

$$\int_{T_0}^{T_c} P(T, \bar{T}) dT = 1$$

In the laminar premixed flame, T is equivalent to \bar{T} and the PDF should be taken in the form of delta-function, i.e.,

$$P(T, \bar{T}) = \begin{cases} 1 & \text{at } T = \bar{T} \\ 0 & \text{at } T \neq \bar{T} \end{cases} \quad (5)$$

where T_0 is the initial mixture temperature and T_c is the combustion temperature. In the turbulent premixed flame, the PDF has a complex shape, which can be either presumed or determined from a PDF transport equation. Note that the turbulent premixed flame can be also modeled by Eqs. (1) and (2) with proper modifications for transport coefficients λ and D_j . To apply the approach for modeling laminar flame propagation in drop suspensions, the PDF of Eq. (5) can be also applied. As for the function $W_j(T)$, it can be obtained from the detailed model of drop combustion reported elsewhere [5].

2.2 Drop combustion model

The governing equations of the drop combustion model [5] 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 ideal-gas equation of state for the gas phase. All relevant physical processes are considered as functions of pressure and temperature. Note that fine fuel drops with the initial diameter of up to 7–10 μm evaporate faster than ignite in the flame [2]. Therefore, only relatively large fuel drops with the initial diameter exceeding 20 μm were considered in this study. The drop combustion model makes it possible to determine time histories and spatial distributions of temperature, density, species mass fractions, etc. in the region $r_s \leq r \leq R$, where r is the radial coordinate, r_s is the drop radius, and R is the “stoichiometric” radius, i.e., the radius of the sphere around a drop containing the amount of air corresponding to the overall fuel–air ratio φ in the drop suspension [5]:

$$R = r_{s0} \left(\frac{\rho_l}{\rho_g \Phi \varphi_{st}} \right)^{1/3}$$

where r_{s0} is the initial drop radius, ρ_l is the liquid density, and φ_{st} is the stoichiometric fuel–air ratio.

When the solution for drop combustion is available, it is possible to determine the mean gas temperature and the mean values of W_j in the region $r_s(t_k) \leq r \leq R(t_k)$ at any time t_k using the following formulae:

$$\begin{aligned}\langle c \rangle &= \int_{V_s}^V c \, dV \\ \langle cT \rangle &= \int_{V_s}^V cT \, dV \\ \langle T \rangle &= \frac{\langle cT \rangle}{\langle c \rangle} \\ \langle W_j \rangle &= \int_{V_s}^V \tilde{W}_j \, dV\end{aligned}$$

where symbol $\langle \rangle$ denotes the mean value, V_s and V are the volumes of the spheres of radius r_s and R , and

$$\tilde{W}_j = G_j \sum_{k=1}^N (v'_{j,k} - v_{j,k}) A_k T^{n_k} \exp\left(-\frac{E_k}{R^0 T}\right) \prod_{i=1}^M \left(\frac{Y_i \rho}{G_i}\right)^{v_{i,k}} \quad (6)$$

In Eq. (6), N is the number of elementary stages in the chemical mechanism, A_k , E_k , and n_k are the preexponential factor, activation energy, and the temperature exponent in the Arrhenius expression for the k th reaction, $v_{j,k}$ is the stoichiometric coefficient of the j th species serving as a reactant in the k th reaction, and $v'_{j,k}$ is the stoichiometric coefficient of the j th species serving as a product of the k th reaction.

To ignite a fuel drop, a provision for a hot spherical layer of air was made in the initial distribution of gas temperature. The temperature of the hot layer was taken equal to 1500 K. The temperature of air outside the hot layer was taken equal to 293 K, so that initially $\langle T \rangle \approx 293$ K. The overall fuel–air ratio φ was taken equal to 1.0, i.e., only the stoichiometric drop suspension was considered. The pressure was taken constant and equal to 1 atm.

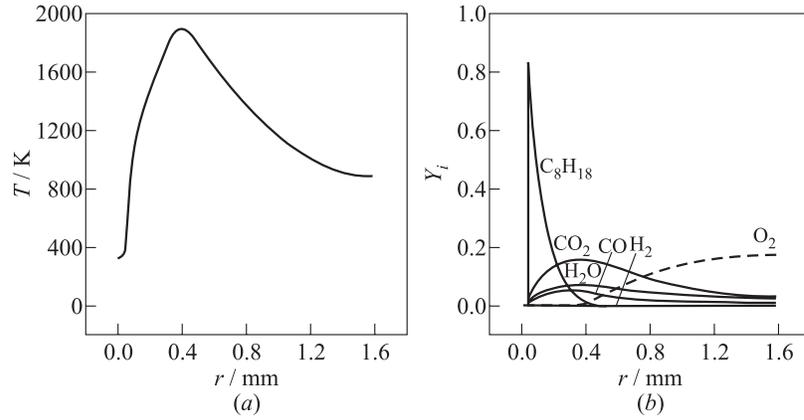


Figure 1 Predicted radial distributions of gas temperature T (a) and species mass fractions (b) in the vicinity of *iso*-octane drop of initial diameter $100 \mu\text{m}$ at time instant 4 ms after ignition; $\varphi = 1$, $\langle T \rangle = 1044$ K, $T_0 = 293$ K, and $p = 1$ atm

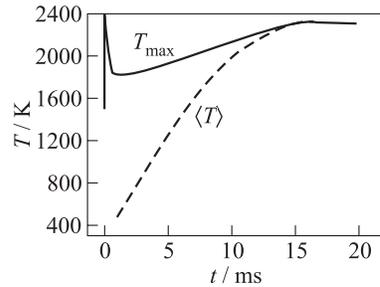


Figure 2 Predicted time histories of the maximal T_{max} and mean $\langle T \rangle$ temperatures at *iso*-octane drop combustion in air. Initial drop diameter is $100 \mu\text{m}$; $\varphi = 1$, $T_0 = 293$ K, and $p = 1$ atm.

As an example, Fig. 1 shows the results of calculations of *iso*-octane drop combustion in air in terms of spatial distributions of gas temperature T and species mass fractions 4 ms after ignition, when $\langle T \rangle = 1044$ K. The flame front corresponding to the maximal temperature locates at a distance of 0.04–0.05 cm from the drop center. Figure 2 shows the corresponding predicted time histories of the maximal gas temperature T_{max} and mean temperature $\langle T \rangle$ during drop combustion. At the end of combustion, $T_{\text{max}} = \langle T \rangle$.

Table 1 Overall reaction mechanism of *iso*-octane oxidation

No.	Reaction	h_{ij} , kcal/mole	A , l , mole, s	m	E , kcal/mole
1	$C_8H_{18} + 8.5O_2 = 8CO + 9H_2O$	696	$7.0 \cdot 10^{14}$ *)	0	50
2	$H_2 + H_2 + O_2 = H_2O + H_2O$	114	$7.0 \cdot 10^{13}$	0	21
3	$CO + CO + O_2 = CO_2 + CO_2$	134	$8.5 \cdot 10^{12}$	0	21
4	$CO + H_2O = CO_2 + H_2$	10	$1.0 \cdot 10^{12}$	0	41.5
-4**	$CO_2 + H_2 = CO + H_2O$	-10	$3.1 \cdot 10^{13}$	0	49.1
5	$H_2O + M = R + R + M$	-118	$2.8 \cdot 10^{17}$	-2	120
-5	$R + R + M = H_2O + M$	118	$9.5 \cdot 10^{12}$	-1	0
6	$R + H_2 + O_2 = 3R + 0.5O_2$	118	$4.5 \cdot 10^{14}$	0	16.4
7	$O_2 + N_2 + C_8H_{18} = NO + NO$ $+ C_8H_{18}$	43	$2.58 \cdot 10^{14}$	0	50
8	$O_2 + N_2 = NO + NO$	-43	$1.7 \cdot 10^{17}$	-0.5	136
-8	$NO + NO = O_2 + N_2$	43	$4.1 \cdot 10^{15}$	-0.5	93.3
9	$C_8H_{18} + C_8H_{18} = 8C + 18H_2$	-2772	$6.4 \cdot 10^{14}$	0	50
10	$C + C + O_2 = CO + CO$	394	$2.6 \cdot 10^{14}$	0	0

*) $w_1 = k_1[C_8H_{18}][O_2]$.

***) Minus sign denotes reverse reactions.

For calculating the rates of chemical reactions, the overall reaction mechanism of gas-phase *iso*-octane oxidation [6] containing 13 reactions and 10 species (C_8H_{18} , O_2 , H_2O , CO , H_2 , CO_2 , N_2 , NO , radical $R = HO_{1/2}$, and soot C) was used. The formation of pollutants (soot and NO_x) is out of the scope of the present study. The mechanism is presented in Table 1.

2.3 Suspension combustion model

To calculate laminar flame structure and propagation in drop suspensions, the look-up tables of $\langle W_j \rangle$ were generated for the discrete values of $\langle T \rangle$ using the drop combustion model described above. The values of $\langle T \rangle$ and $\langle W \rangle$ were attributed to the values of T and W_j entering Eqs. (1) and (2), i.e.,

$$W_j(T) = \langle W_j \rangle(\langle T \rangle)$$

The source terms defined by Eqs. (3) and (4) can thus be readily calculated based on the drop combustion model.

A special algorithm was developed to process automatically the results of calculations of individual drop combustion and obtain the look-up tables of mean reaction rates for solving Eqs. (1) and (2). Equations (1) and (2) were integrated using a code of [7]. Note that in this formulation, the model of laminar flame propagation in drop suspension does not contain any fitting parameter.

3 Results

The suspension combustion model was validated against the experimental data of [8] for laminar flame propagation in the stoichiometric *iso*-octane (*iso*-C₈H₁₈) drop suspensions in air at normal atmospheric conditions. The look-up tables with mean reaction rates were first obtained based on the solution of the drop combustion problem for individual *iso*-octane drops of initial diameter 60, 100, and 150 μm . The overall reaction mechanism of Table 1 was applied.

As a result of solution of Eqs. (1) and (2), the values of laminar flame propagation velocity u_n and spatial distributions of temperature and species mass fractions were obtained.

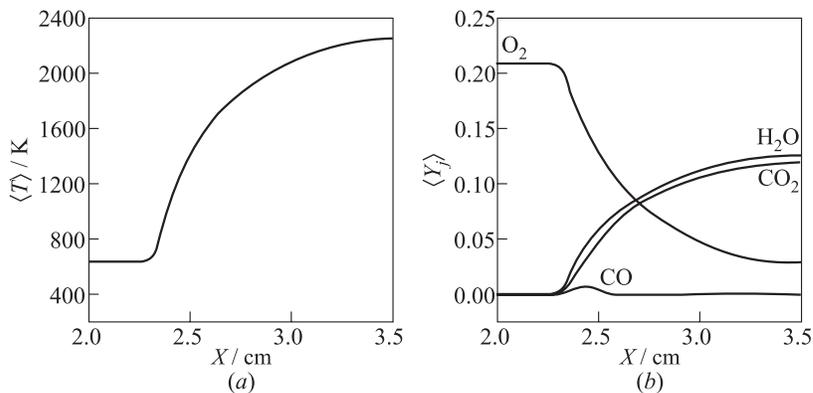


Figure 3 Predicted spatial distributions of temperature $\langle T \rangle$ (a) and molar fractions of main species (b) in the laminar flame propagating in *iso*-octane drop suspension in air. Initial drop diameter is 100 μm ; $\varphi = 1$, $T_0 = 293$ K, and $p = 1$ atm

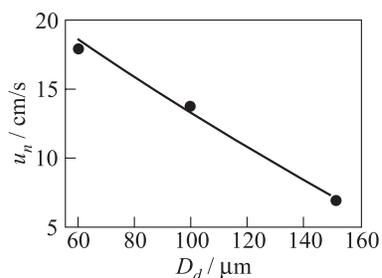


Figure 4 Comparison of predicted (line) and measured (symbols, [8]) laminar flame velocities in *iso*-octane drop suspensions in air as a function of initial drop diameter; $\varphi = 1$, $T_0 = 293$ K, and $p = 1$ atm

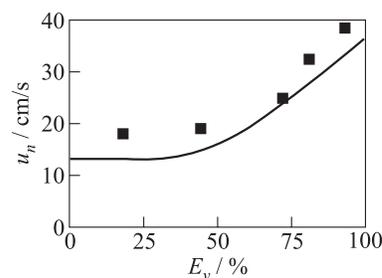


Figure 5 Predicted (curve) and measured (symbols, [8]) laminar flame velocities in *iso*-octane drop suspensions in air depending on the prevaporization degree, E_v . $\varphi = 1$, $T_0 = 293$ K, $p = 1$ atm. Drop diameter at $E_v = 0$ is $100 \mu\text{m}$

Figure 3 shows the predicted spatial distributions of temperature $\langle T \rangle$ and mean molar fractions of main species $\langle Y_j \rangle$ in the reaction zone of the laminar flame propagating in the suspension of *iso*-octane drops of initial diameter $100 \mu\text{m}$. The drop suspension flame was about 1 cm thick, which was much thicker than the laminar premixed flame.

Figure 4 shows the comparison of predicted and measured values of u_n as a function of initial drop diameter. A good qualitative and quantitative agreement between the results is worth mentioning. The predicted value of laminar flame velocity in the premixed stoichiometric *iso*-octane–air mixture at normal atmospheric conditions was $u_n = 36.4$ cm/s. It is seen from Fig. 4 that the values of u_n in drop suspensions are considerably lower than in the homogeneous mixture of the same stoichiometric composition. This is evidently caused by smaller mean reaction rates of fuel oxidation in the vicinity of drops.

Figure 5 shows the comparison of predicted and measured laminar flame velocities in *iso*-octane drop suspensions depending on the fuel prevaporization degree E_v . Clearly, the partial preliminary vaporization of fuel drops results in the growth of the laminar flame velocity. In the limit $E_v = 100\%$, the suspension flame velocity approaches the value relevant to the premixed laminar flame velocity. A reasonable

qualitative and quantitative agreement with the experimental data [8] allows one to treat the model as satisfactory.

Concluding Remarks

A new model of laminar flame propagation in liquid drop suspensions was developed. The model combined a 1D premixed flame theory and the theory of single drop combustion and applied the formalism of PDFs. Chemical energy release was modeled by the overall reaction mechanism of hydrocarbon oxidation containing 13 reactions and 10 species, including soot, NO_x, and CO. The model was validated against available experimental data for monodispersed *iso*-octane drop suspensions of different initial size and prevaporization degree. The model can be readily generalized for polydispersed drop suspensions and for turbulent flames. The future work will be concentrated on modeling transient turbulent flames in polydispersed drop suspensions — a problem closely related to deflagration-to-detonation transition in liquid fuel sprays.

Acknowledgments

This work was partly supported by the International Science and Technology Center (project No. 2740) and Russian Foundation for Basic Research (grants 05-08-18200a, 05-08-50115a, and 05-08-33411a).

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