
COMBUSTION
AND EXPLOSION

A Model of Laminar Flames in Droplet Suspensions

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Abstract—A mathematical model of steady laminar flame propagation through a suspension of liquid droplets was proposed, and numerical calculations within the framework of this model were performed. The model is constructed based on one-dimensional differential equations of the theory of laminar flames in homogeneous gaseous mixtures in conjunction with the theory of droplet burning in uniform monodisperse suspensions. The chemical process was described using a multistage kinetic scheme. A comparison of model predictions with the available experimental data demonstrated satisfactory agreement.

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INTRODUCTION

Suspension combustion is a complex physicochemical phenomenon widely used in practice, including in energetics and transport [1, 2]. Knowledge of the mechanism of this process and the capability of controlling it are expected to make it possible to enhance the efficiency of the combustion of liquid fuels and diminish the toxicity of the products. In contrast to the burning of an isolated droplet in an infinite oxidizing atmosphere [3–5], the character of droplet suspension combustion depends on the distance between droplets, sometimes rather strongly. For example, there are suspension combustion modes with local initiation and extinction of flames around droplets and with individual and collective flames, as well as other phenomena [6–8]. Figure 1 shows typical photos of the combustion of *n*-decane (Fig. 1a) and *n*-octane (Fig. 1b) under microgravity conditions [9]. Given that the interdroplet distance in a two-phase flow changes with time, a model of suspen-

sion combustion should describe the flow on a very small scale, at least comparable with the droplet size [10]. Clearly, such an approach is unacceptable in modeling the operation process in industrial energy-conversion installations.

Complex as it is, suspension combustion cannot be described exactly to date, a situation that calls for the development of approximate methods. One of the key issues of suspension combustion theory is the modeling of a laminar flame.

Previously, we proposed a simple method for calculating the propagation of laminar flames in two-phase media with monodisperse [11] and polydisperse [12] droplet size distributions within the framework of the *d*-squared law. When calculating the burning rate for a two-phase system, the authors of [13] employed a detailed chemical mechanism with empirical corrections for diffusional retardation of the reaction. In the present work, we attempted to solve the problem of

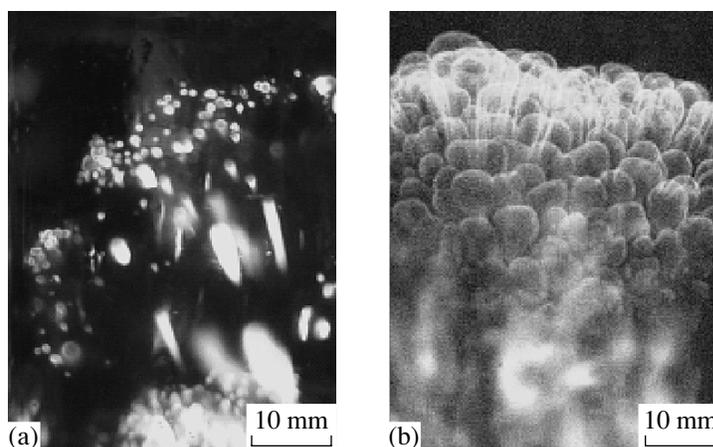


Fig. 1. Photos of flames in suspensions of (a) *n*-decane and (b) iso-octane under microgravity conditions [9].

laminar flame propagation by combining the theory of flame propagation in homogeneous mixtures with a nonempirical droplet burning theory [14, 15]. The chemical process was described within the framework of an overall kinetic scheme, but, as demonstrated below, there are no principle limitations on using nonempirical kinetic mechanisms.

1. MODEL

The proposed model of propagation of a steady laminar flame in a droplet suspension is based on one-dimensional differential equations of the theory of laminar flames in homogeneous gaseous mixtures and the theory of burning of fuel droplets in uniform monodisperse suspensions. Let us examine each species of the model separately.

1.1. Model of a Laminar Flame in a Gas

Consider the problem of propagation of a steady planar laminar flame in a gaseous mixture within the range $-\infty < x < +\infty$, where x is the space coordinate. The structure of such a flame is described by the following system of nonlinear differential energy and diffusion equations:

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

$$\frac{\partial}{\partial x} \left(\rho D_j \frac{\partial Y_j}{\partial x} \right) - \rho_0 u_n \frac{\partial Y_j}{\partial x} + w_j = 0, \quad j = 1, 2, \dots, N, \quad (2)$$

where T is the temperature, Y_j is the mass fraction of the j th species, N is the number of species involved in the chemical reaction, u_n is the laminar flame velocity, ρ is the density (here and below, the subscript 0 denotes the initial mixture), c is the specific heat at constant pressure, λ is thermal conductivity, D_j binary diffusion coefficient for the j th species in the bath gas, Φ is the rate of heat release by chemical reactions, w_j is the overall rate of change of the concentration of the j th species involved in M stages of the chemical reaction

$$w_j = G_j \sum_{i=1}^M (v'_{ij} - v_{ij}) A_i T^{n_i} \times \exp(-E_i/R^0 T) \prod_{k=1}^N \left(\frac{\rho Y_k}{G_k} \right)^{v_{ik}}, \quad j = 1, 2, \dots, N. \quad (3)$$

Here, M is the number of chemical reactions; R^0 is the universal gas constant; G_j the molecular mass of the j th species; A_i , E_i , and n_i are, respectively, the preexponential factor, activation energy, and the exponent at temperature for the i th reaction; v_{ij} is the stoichiometric coefficient of the j th reactant of the i th reaction, and v'_{ij} is the stoichiometric coefficient for the j th product of the i th reaction.

To close the system of Eqs. (1) and (2), it is necessary to supplement it with a kinetic mechanism of the chemical reaction and an equation of state,

$$p = \rho R^0 T \sum_{j=1}^M \frac{Y_j}{G_j}, \quad (4)$$

where p is the pressure (constant). The boundary conditions for Eqs. (1) and (2) read as

$$\text{at } x \rightarrow -\infty, \quad T = T_0, \quad Y_j = Y_{j0}, \quad j = 1, 2, \dots, N; \quad (5)$$

$$\text{at } x \rightarrow \infty, \quad \frac{dT}{dx} = 0, \quad \frac{dY_j}{dx} = 0, \quad j = 1, 2, \dots, N. \quad (6)$$

Problem (1)–(6) can be solved numerically, for example, using the relaxation method implemented in the software package described in [16], so as to determine the flame velocity u_n and the profiles of the temperature T , concentrations Y_j , reaction rates w_j and heat release rate Φ along the x coordinate.

One important aspect of problem (1)–(6) is that, if the $T(x)$ dependence is monotonic, one can obtain the $\Phi(T)$ and $w_j(T)$ dependences. Such dependences can be presented in the form of tables or polynomials. Clearly, if the function $\Phi(T)$ is known, u_n can be approximately determined by solving Eq. (1) alone. Generally, based on the functions $\Phi(T)$ and $w_j(T)$, the repeated solution of the problem makes it possible to obtain the same value of u_n and the same $T(x)$ and $Y_j(x)$ profiles as in the case of directly solving problem (1)–(6), but without performing cumbersome calculations of w_j by formulas (3). The functions $\Phi(T)$ and $w_j(T)$ can be formally presented as

$$w_j = \int_{T_0}^{T_c} (w_{1j} - w_{2j}) P(T, \bar{T}) dT, \quad j = 1, 2, \dots, N, \quad (7)$$

$$\Phi = \sum_{j=1}^M \int_{T_0}^{T_c} H_j w_j P(T, \bar{T}) dT, \quad (8)$$

where T_c is adiabatic combustion temperature, H_j is the enthalpy of atomization or formation of the j th species of the mixture, w_{1j} and w_{2j} are, respectively, the overall rates of formation and consumption of the j th species in all the reactions occurring in the system (to make Y_j positive, the rate of consumption of the j th species should be specified as $w_{2j} = W_{2j} Y_j \rho_g / G_j$), and $P(T, \bar{T})$ is the probability density function (PDF) for flame temperature distribution, which can be defined as the probability of finding a local temperature within $T - T + dT$ at a mean temperature \bar{T} . For a laminar flame propagat-

Mechanism of isooctane combustion

Reaction number	Reaction	h_{ij} , kcal/mol	A , l, mol, s	m	E , kcal/mol
1	$C_8H_{18} + 8.5O_2 = 8CO + 9H_2O$	696	$7.0 + 14^*$	0	50
2	$H_2 + H_2 + O_2 = H_2O + H_2O$	114	$7.0 + 13$	0	21
3	$CO + CO + O_2 = CO_2 + CO_2$	134	$8.5 + 12$	0	21
4	$CO + H_2O = CO_2 + H_2$	10	$1.0 + 12$	0	41.5
-4	$CO_2 + H_2 = CO + H_2O$	-10	$3.1 + 13$	0	49.1
5	$H_2O + M = R + R + M$	-118	$2.8 + 17$	-2	120
-5	$R + R + M = H_2O + M$	118	$9.5 + 12$	-1	0
6	$R + H_2 + O_2 = 3R + 0.5O_2$	118	$4.5 + 14$	0	16.4
7	$O_2 + N_2 + C_8H_{18} = NO + NO + C_8H_{18}$	43	$2.58 + 14$	0	50
8	$O_2 + N_2 = NO + NO$	-43	$1.7 + 17$	-0.5	136
-8	$NO + NO = O_2 + N_2$	43	$4.1 + 15$	-0.5	93.3
9	$C_8H_{18} + C_8H_{18} = 16C + 18H_2$	-2772	$6.4 + 14$	0	50
10	$C + C + O_2 = CO + CO$	394	$2.6 + 14$	0	0

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

ing in a homogeneous gaseous mixture, $T \equiv \bar{T}$, with the PDF given by the normalized delta function

$$\int_{T_0}^{T_c} P(T, \bar{T}) dT = \begin{cases} 1 & \text{at } T = \bar{T} \\ 0 & \text{at } T \neq \bar{T}. \end{cases}$$

Thus, if the function $w_j(T)$ is known, the value of u_n and the $T(x)$ and $Y_j(x)$ profiles can be calculated using the delta function formalism and relationship (8).

1.2. Model of the Burning of Droplets in a Uniform Monodisperse Suspension

In [11], we proposed a mathematical model for describing the burning of droplets in a uniform monodisperse suspension. In our opinion, this model can be applied to the problem of laminar flame propagation in suspensions. Note that very small droplets evaporate within a time interval shorter than the characteristic time of the chemical reaction in the laminar flame. According to the estimates obtained in [11], under normal conditions, such droplets have a diameter smaller than 7–10 μm . In the present work, we considered only droplets with a diameter larger than 20 μm . Upon finding themselves in a flame, such droplets burn in the diffusion-controlled regime.

The problem of ignition and burning of a droplet in the spherical symmetry approximation can be solved numerically by the method described in [14, 15]. The model proposed in [14, 15] makes use of time-dependent differential equations of conservation of mass and energy in the liquid and gas phases and postulates the variability of physical properties. The formulation of the problem makes an allowance for multicomponent

diffusion in a mixture containing fuel vapor, oxygen, nitrogen, and combustion products and the surface tension effect. The pressure was set to be constant, $p = p_0 = \text{const}$. Solving this problem makes it possible to determine the dependence of the droplet radius r_s on the time t , droplet lifetime, and the instantaneous radial distributions of the temperature T , density ρ , concentrations Y_j , reaction rates w_j , and heat release rate Φ . Since the model presented in [14, 15] considers a droplet in a suspension with equivalence ratio ψ , the solution to the problem was sought for within $0 < r < R$, where r is the radial coordinate originated at the center of the droplet, and R is the radius of the equivalent sphere around the droplet, i.e., the value of the r coordinate at which the ratio of the mass of the fuel to that of the air inside the sphere is equal to ψ :

$$R = r_{s0} \left(\frac{\rho_l}{\rho \psi \phi_{st}} \right)^{1/3}, \quad (9)$$

where r_{s0} is the initial droplet radius, ρ_l is the density of the liquid fuel, and ϕ_{st} is the stoichiometric fuel-to-oxidizer mass ratio (for hydrocarbon fuels, $\phi_{st} \approx 0.06$).

1.3. A Model of Laminar Flame in a Suspension

Calculating the characteristics of the burning of a droplet as a function of time makes it possible to determine the mean temperature \bar{T} of the gas around the droplet from the mean thermal enthalpy \bar{h} and mean specific heat \bar{c} :

$$\bar{T} = \frac{\bar{h}}{\bar{c}}, \quad (10)$$

where

$$\bar{c} = \frac{3}{R^3} \int_{r_s}^R c r^2 dr, \quad \bar{h} = \frac{3}{R^3} \int_{r_s}^R c T r^2 dr.$$

The mean rates of formation and consumption of the j th species, \bar{w}_j , and the mean heat release rate $\bar{\Phi}$ can be calculated in the same manner:

$$\bar{w}_j = \frac{3}{R^3} \int_{r_s}^R w_j r^2 dr, \quad (11)$$

$$\bar{\Phi} = \frac{3}{R^3} \int_{r_s}^R \Phi r^2 dr. \quad (12)$$

Given that there is an unequivocal relationship between the mean rates given by (11) and (12) and the mean temperature defined by (10), the problem of laminar flame propagation in a suspension can be reduced to equations (1)–(6) under the assumption that $w_j = w_j(T) = \bar{w}_j(\bar{T})$ and $\Phi = \Phi(T) = \bar{\Phi}(\bar{T})$. In this formulation, problem (1)–(6) is solved for the mean gas temperature and mean concentrations of the gas-phase species \bar{Y}_j in the interdroplet space, i.e., in (1)–(6), $T = \bar{T}$ and $Y_j = \bar{Y}_j$, while expressions (7) and (8) are replaced by (11) and (12), respectively.

Let us briefly discuss the validity of such a model of laminar flame propagation in suspensions.

First, as can be seen, Eqs. (1)–(6) contain the density of the gas rather than that of the suspension. This is acceptable only when the mass fraction of liquid droplets in the reaction mixture is small. Given that the mass fraction of fuel in stoichiometric air–liquid hydrocarbon mixtures is about 6.0–6.5%, it stands to reason that the proposed approach is applicable to lean and stoichiometric air–hydrocarbon suspensions.

Second, the proposed model is based on the assumption that the heat conduction mechanism plays the predominant role in flame propagation while the contribution from radiative energy transfer is negligibly small. This approximation is evidently acceptable only for finely dispersed suspensions [2].

Third, the model does not explicitly treat dynamic and thermal relaxation processes in the two-phase mixture, more specifically, the entrainment of droplets into the flow, their collisions, coagulation, deformations and drop dispersion, as well as the energy consumption on the heating and ignition of droplets. Since laminar flames are characterized by moderate values of the bulk gas velocity (below 3–5 m/s), the effect of a number of processes, such as the dispersion, deformation, and coagulation of droplets can probably be disregarded [17]. As to the energy consumption on the heating and ignition of droplets, these are indirectly allowed for in

calculating the mean heat-release rate near the droplet. That the velocities of the gas and droplets may differ is an important factor that may be responsible for a number of experimentally observed, but so far inexplicable phenomena. For example, for nonvolatile fuel suspensions, the lean combustion limit expands with increasing droplet size [18]. Another example is the observation that, under certain conditions, the flame velocity in a suspension exceeds that in a homogeneous mixture with the same equivalence ratio [19].

2. CALCULATION RESULTS AND COMPARISON WITH EXPERIMENTAL DATA

The speed and structure of laminar flames in stoichiometric ($\psi = 1$) isooctane (C_8H_{18})–air suspensions were calculated at $p = 0.1$ MPa and $T_0 = 293$ K, conditions typical of the experiments performed in [20]. The diameters of the initial droplets, $d_{s0} = 2r_{s0}$, were 60, 100, and 150 μm .

Preliminarily, we calculated the burning characteristics of isooctane droplets according to the method described in [14, 15] and determined the $\bar{\Phi}(\bar{T})$ and $\bar{w}_j(\bar{T})$ dependences (using Eqs. (10)–(12)). The calculations were based on a multistage kinetic scheme of octane oxidation [21] (table) composed of 13 reactions ($M = 13$) involving 10 species ($N = 10$): C_8H_{18} , O_2 , H_2O , CO , H_2 , CO_2 , N_2 , NO , generalized radical R, and soot So. To ignite the droplet, we increased the gas temperature within a narrow spherical layer adjacent to the gas–liquid interface to 1500 K, with the temperature outside being 293 K. The radius of the equivalent sphere around the droplet was calculated by formula (9) at $\psi = 1$. Note that the method described in [14, 15] makes it possible to calculate the burning characteristics of suspension droplets at an arbitrary degree of preliminary evaporation of liquid fuel, $0 \leq E_v < 100\%$, which is defined as the ratio of the fuel vapor mass to the total fuel mass in the suspension at the initial instant of time. At $E_v \neq 0$, for the sake of definiteness, we assumed that the fuel vapor distribution inside the sphere is uniform.

Figure 2 shows typical calculated radial profiles of the temperature T and mass concentrations Y_j near an isooctane droplet with an initial diameter of 100 μm at instant of time of 4 ms (when $\bar{T} = 1044$ K). As can be seen, the maximum flame temperature (~ 1900 K) is observed at $r \approx 0.4$ mm, a point at which the concentrations of C_8H_{18} and O_2 drop to zero. Figure 3 shows how the maximum temperature T_{max} and mean temperature \bar{T} near the same droplet change with time. At the end of the combustion process, the temperatures T_{max} and \bar{T} coincide.

The $\bar{\Phi}(\bar{T})$ and $\bar{w}_j(\bar{T})$ dependences were tabulated and used for solving Eqs. (1) and (2) employing a linear

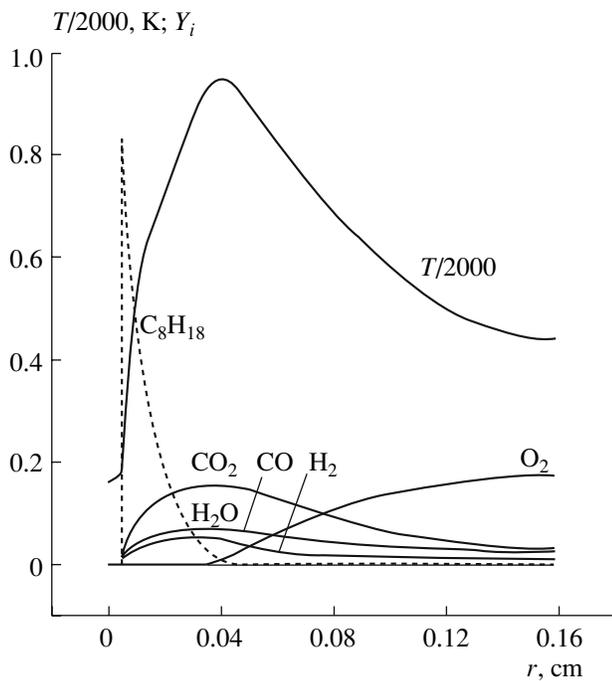


Fig. 2. Calculated radial profiles of the temperature T and concentrations of the main species of the reaction mixture (in mass fractions) across the reaction zone of an isooctane droplet with an initial diameter of $100 \mu\text{m}$ at 4 ms after ignition ($\bar{T} = 1044 \text{ K}$). The fuel excess coefficient, $\phi = 1$; initial temperature, 293 K; pressure, 1 atm.

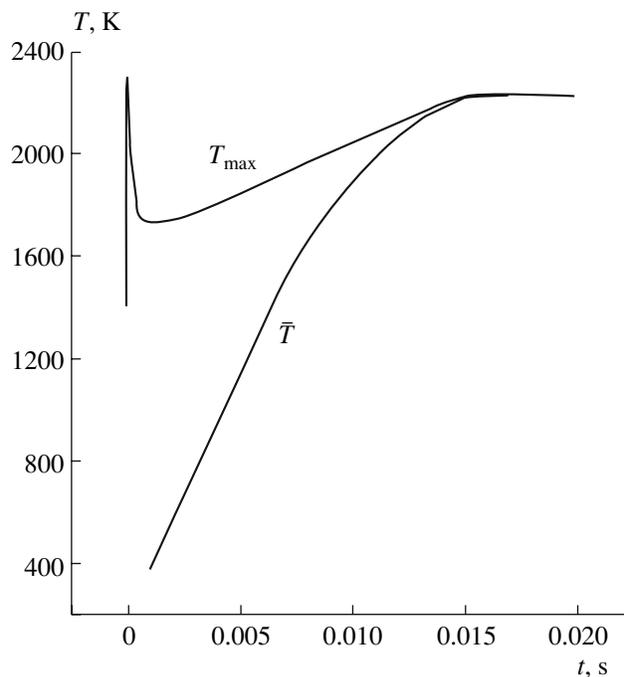


Fig. 3. Time dependences of the maximum T_{max} and mean \bar{T} temperature near an isooctane droplet with an initial diameter of $100 \mu\text{m}$ burning in air. The fuel excess coefficient, $\phi = 1$; initial temperature, 293 K; pressure, 1 atm.

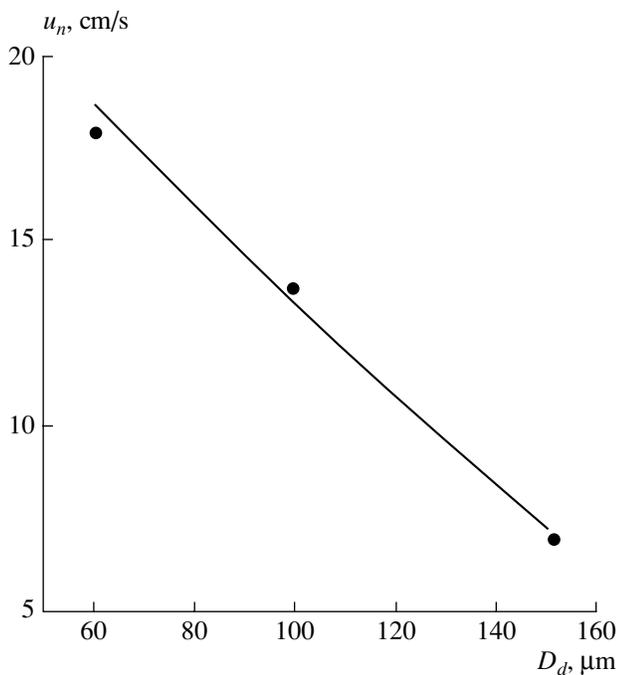


Fig. 4. Comparison of the calculated (curve) dependence of the laminar flame velocity on the isooctane droplet diameter with the experimental data from [20]. The fuel excess coefficient, $\phi = 1$; initial temperature, 293 K; pressure, 1 atm.

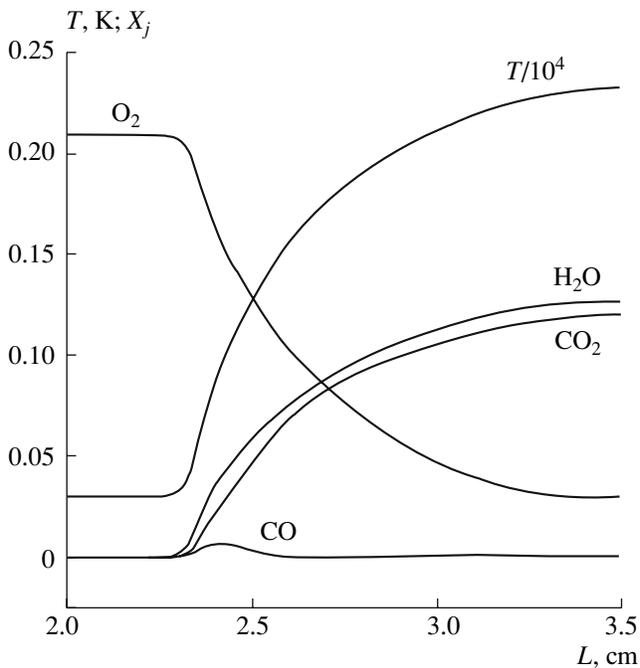


Fig. 5. Calculated radial profiles of the mean temperature \bar{T} and concentrations of the main species of the reaction mixture (in volume fractions) across a flame in a suspension of isooctane droplets with an initial diameter of $100 \mu\text{m}$. The fuel excess coefficient, $\phi = 1$; initial temperature, 293 K; pressure, 1 atm.

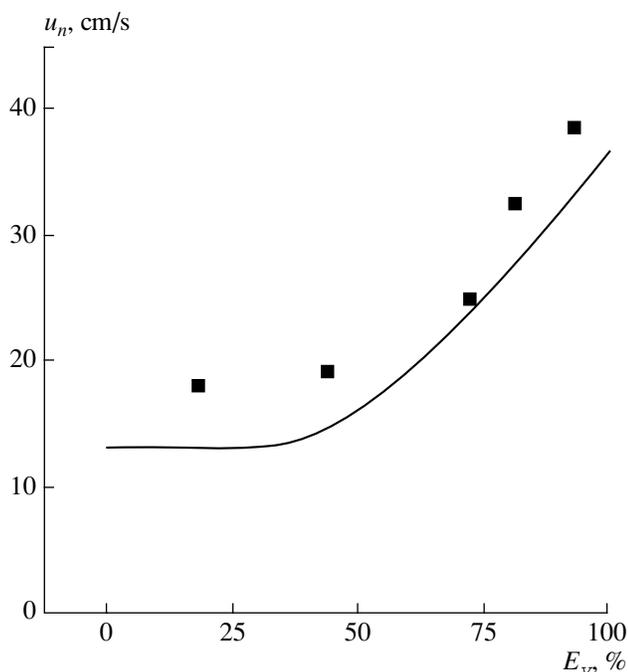


Fig. 6. Comparison of the calculated (curve) dependence of the laminar flame velocity on the degree of preliminary evaporation of isooctane droplets with the experimental data from [20]. The fuel excess coefficient, $\phi = 1$; initial temperature, 293 K; pressure, 1 atm.

interpolation. As a result, we obtained the laminar flame velocity and the profiles of the temperature and concentrations of all species along the x coordinate. As can be seen from Fig. 4, the calculated (curve) and measured ([20], points) u_n values for monodisperse isooctane suspensions with various initial droplet diameters are in close agreement. Figure 5 displays the calculated profiles of the temperature and mole fractions of the basic species across a laminar flame in suspension of isooctane droplets with an initial diameter of 100 μm . The thickness of this flame (~ 1 cm) is substantially larger than that of a laminar flame in a homogeneous gaseous mixture of the same composition (~ 0.15 cm). Note also that the calculated value of u_n for this flame (~ 14 cm/s) is considerably lower than that for a laminar flame in a gaseous mixture of identical composition ($u_n = 36.4$ cm/s).

Figure 6 compares the calculated (curve) and measured ([20], points) dependences of the laminar flame velocity in a suspension of isooctane droplets 100 μm in diameter on the degree of preliminary evaporation of the droplets. As can be seen, at $E_v < 50\%$, the laminar flame velocity is virtually independent of E_v . At $E_v > 75\%$, the speed of the laminar flame in the suspension increases with E_v , attaining the value characteristic of the homogeneous mixture at $E_v \rightarrow 100\%$. Recall that, at $E_v \neq 0$, calculations were performed only for droplets smaller than 20 μm in diameter. As seen in Fig. 6, the

calculation results compare favorably with the experimental data from [20].

CONCLUSIONS

A new model of a steady laminar flame in suspensions was proposed. The model, based on one-dimensional differential equations of the theory of laminar flames in homogeneous gaseous mixtures in conjunction with the theory of droplet burning in uniform monodisperse suspensions, contains no adjustable parameters. The key postulate underlying the model is the assumption that there is an unequivocal relationship between the instantaneous mean temperature and the instantaneous mean rates of the reactions occurring in the interdroplet space of the suspension during its combustion. The model makes it possible to calculate the speed and structure of a laminar flame propagating through a monodisperse suspension of fuel droplets. We performed calculations of the speed and structure of a laminar flame in a suspension of isooctane droplets in air at normal initial conditions and various degrees of preliminary evaporation of the liquid. The calculations were based on multistage scheme of isooctane oxidation, composed of 13 reactions involving 10 species. The calculation results were compared to the known experimental data. It was demonstrated that the model predictions are in satisfactory qualitative and quantitative agreement with the experimental data regarding the dependences of the laminar flame velocity on the initial droplet size and the degree of preliminary evaporation of the liquid.

The model is planned to be extended to cover polydisperse suspensions and turbulent flames. For describing turbulent flames, we are going to use presumed probability density functions instead of delta functions.

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