THEORY OF FLAME PROPAGATION IN A GAS AND DROP MIXTURE

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The equations of a reacting multiphase continuous medium [1] are used to investigate the problem of steady-state flame front propagation in a gas mixture with evaporating drops. A simple model for ignition of the liquid drops is proposed which is based on the application of the method of equally accessible surfaces [2] to the heat and mass exchange processes between the microflames surrounding the separate drops, the drops, and the carrying gas medium. The parameter distributions in the macroscopic flame front as well as the dependences of the flame propagation velocity in the gas suspension on a number of parameters governing the process under investigation are represented.

The flame front propagation velocity in a tetralin–air gas suspension has been determined experimentally in [3], and it has been detected that the drops evaporate completely prior to ignition for small diameters ($d_0 < 10\mu$) and the flame propagation velocity in the mixture is ~30 cm/sec, i.e., is close to the flame propagation velocity in a well-mixed mixture. The flame propagation in a gas suspension with coarser drops ($d_0 > 20\ \mu$) is accompanied by the formation of thin spherical microflames around the separate drops. The flame rate hence increases to values ~60 cm/sec.

An attempt at a qualitative explanation of such an increase in the flame front propagation velocity as the drop diameter increases is given by L. A. Klyachko in [4] on the basis of representations of the relay-race mechanism of the combustion of a suspension. It is considered that the flame is propagated because of the drop-by-drop ignition because of their being heated by heat waves from those ignited earlier but still not burned up (because of the coarseness of the drops).

If the time for one drop to burnup, τ, and the flame propagation velocity in a gas suspension, v_0, are such that $l \sim v_0\tau \gg l_1$, where l_1 is the spacing between drops, then a macroscopic flame front of thickness l is formed which includes a sufficiently large quantity of burning drops. In this case, the representations of the mechanics of continuous media are used to describe the structure of the flame front.

Williams [5, 6] proposed a theory of flame propagation in a gas suspension of evaporating fuel which is based on the equations of a two-phase continuous medium. All the heat of the chemical reaction is hence referred to the whole gas phase (which corresponds to a quasi-well-mixed mode according to the classification in [1]). Moreover, it is assumed that all the evaporating fuel is consumed in the chemical reaction, which is valid only for sufficiently coarse drops. Let us note that the Williams model yields a monotonely dropping dependence of the flame propagation velocity on the drop diameter. This model does not describe the passage of the drop combustion into the vapor phase mode with the formation of microflames and an increase in the combustion velocity for $d_0 \sim 20\ \mu$.

A theory of flame propagation taking account of the possible change in the mode from the quasi-well-mixed, i.e., with distributed heat liberation, to the vapor-phase diffusion mode with the formation of microflames around the separate drops is proposed herein.

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1. Fundamental Equations

The hydromechanics equations of a two-velocity, three-temperature continuous medium in the presence of chemical reactions have been obtained in [1] as applied to a gas mixture with drops. For plane one-dimensional stationary motion in the absence of external mass forces and external heat supply and neglecting longitudinal diffusion of the components and the radiation heat flux, they are

$$\begin{gathered}
\frac{dm_k}{dx} = -\nu_k J \quad (k = 11, 13, 14), \quad \frac{dm_{15}}{dx} = 0, \quad \frac{dm_2}{dx} = -\nu_2 J_f, \quad \frac{dnv_2}{dx} = 0 \\
m_1 \frac{dv_1}{dx} = -\alpha_1 \frac{dp}{dx} - f + \nu_2 J (v_2 - v_1), \quad m_2 v_2 \frac{dv_2}{dx} = -\alpha_2 \frac{dp}{dx} + f \\
\sum_k m_k \frac{d}{dx}\left(i_k + \frac{v_1^2}{2}\right) + m_2 \frac{d}{dx}\left(i_2 + \frac{v_2^2}{2}\right) = \frac{d}{dx} \lambda \frac{dT_1}{dx} + \\
JQ^\circ + \nu_2 J \frac{p - p_0}{\rho_2^\circ} + \nu_{11} J (c_{p1} - c_{p3})(T_1 - T_0) + \nu_2 J [c_2(T_2 - T_0) - \\
c_{p3}(T_1 - T_0) + \frac{v_2^2 - v_1^2}{2}\Big] \\
m_2 \frac{du_2}{dx} = -\nu_2 J (i_{12} - i_2) + q_{f2}, \quad \nu_2 J_f x_f = -q_{f1} - q_{f2} \\
\Big(m_1 = \sum_k m_k; \ k = 11, 13, 14, 15\Big)
\end{gathered} \tag{1.1}$$

The parameters referring to the gas (first phase), the drops (second phase), and the microflames around the drops (f = phase [1]) are everywhere provided with the subscripts 1, 2, and f, respectively. The gas phase components (oxidizer, fuel vapors, reaction products, and inert gas) are distinguished by using the secondary subscripts 1, 2, 3, 4, and 5, respectively. The subscript 0 corresponds to the unperturbed state of the system before the flame front. It is assumed that all the evaporating fuel is consumed in the chemical reaction, i.e., there are no free vapors.

A chemical reaction of the form $\varkappa_{11}A + \varkappa_2 B + \varkappa_{15} E = \varkappa_{13} C + \varkappa_{14} D + \nu_{15} E$ is considered, where A, B, C, D, and E are symbols for the oxidizer (A), fuel (B), two kinds of reaction products (C and D), and inert gas (E), respectively, and $\varkappa_k$ are stoichiometric coefficients. Moreover, $\nu_k = g_k \varkappa_k$, where g_k are the molecular weights of the chemical elements $m_k = \rho_k v_1$, $m_2 = \rho_2 v_2$ are the mass flow rates of the components, ρ_k, ρ_k° are the mean and true densities of the components, respectively, n is the number of drops per unit volume, α_1, α_2 are the volume phase concentrations, v_1, v_2 are the phase velocities, p is the mixture pressure, u_k and $i_k = u_k + p/\rho_k^\circ$ are the internal energy and enthalpy, T_1, T_2, and T_f are the gas, drop, and spherical microflame temperatures (f is the phase), J is the chemical reaction rate per unit volume, J_f is the reaction rate in the microflame fronts, f is the intensity of interaction between the phases because of friction, q_{f1} and q_{f2} is the heat exchange between phases, x_f is the heat flux from the f phase to the substance undergoing chemical conversion, and [1]

$$\begin{gathered}
\nu_2 x_f = \nu_{13} i_{13}(p, T_f) + \nu_{14} i_{14}(p, T_f) - \nu_2 i_{12}(p_s(T_2), T_2) - \\
- \nu_{11} i_{11}(p, T_f)
\end{gathered} \tag{1.2}$$

Let us assume that the first and second phase components satisfy the equations of state

$$\begin{gathered}
i_k = c_{pk}(T_1 - T_0) + h_k^\circ, \quad p_k = \rho_k^\circ R_k T_1 \quad (k = 11, 13, 14, 15) \\
i_2 = c_2(T_2 - T_0) + h_2^\circ + \frac{p - p_0}{\rho_2^\circ}, \quad \rho_2^\circ = \text{const}, \quad p = \sum_k p_k \\
i_{12} = c_2(T_2 - T_0) + \frac{p_s(T_2) - p_0}{\rho_{12}^\circ} + h_2^\circ + l_2(T_2), \quad p_s = \rho_{12}^\circ R_{12} T_2
\end{gathered}$$

Here $l_2(T_2)$ is the heat of vapor formation, p_s is the saturated vapor pressure, and h_k is the enthalpy of the components for $T = T_0$, $p = p_0$.

2. Interaction between Phases

If a microflame front is introduced for a quasi-well-mixed combustion mode when there are no real microflames around the drops, as some mathematical surface on which the combustion occurs with a finite chemical reaction rate [7], then drop ignition can be considered as the passage of combustion on this surface from the kinetic into the diffusion domain.

Let each drop of diameter d be surrounded by a flame front surface of diameter d_f and a reduced film surface [2] of diameter d_1. Heat and mass exchange processes governed by heat conduction and diffusion occur between these surfaces. Let the partial vapor pressures on the drop surface and on the front surfaces be $p_s(T_2)$ and p_{2f}. Then the intensity of the mass exchange between the second and the f phase (J^{2f}), between the f phase and the first phase (J^{f1}), and between the first and the f phase (J^{1f}), can be represented as

$$\begin{aligned} J^{2f} &= \pi n d^2 \beta_{2f}\left(\frac{pg_2}{RT_2}\ln\frac{p}{p-p_s} - \rho_{2f}{}^\circ\right) \quad \left(\beta_{2f} = \frac{D_{12}}{d}\frac{2d_f}{d_f - d},\ \rho_{2f}{}^\circ = \frac{p_{2f}g_2}{RT_f}\right) \\ J^{f1} &= \pi n d^2 \beta_{f1}\rho_{2f}{}^\circ \left(\beta_{f1} = \frac{D_{12}}{d_f}\frac{2d_1}{d_1 - d_f}\right) \\ J^{1f} &= \pi n d_f{}^2 \beta_{1f}(\rho_{11}{}^\circ - \rho_{11f}{}^\circ)\left(\beta_{1f} = \frac{D_{11}}{d_f}\frac{2d_1}{d_1 - d_f},\ \rho_{11}{}^\circ = \frac{p_{11}g_{11}}{RT_1}\right) \end{aligned} \tag{2.1}$$

Here β_{2f}, β_{f1}, β_{1f} are the appropriate mass evolution coefficients, D_{12} and D_{11} are the diffusion coefficients of the vapor and oxidizer, respectively. The reaction rate on the front in the f phase is given as a function of the concentration of reagents on its surface. For a first-order reaction this rate can be given by the formula

$$\begin{gathered} \nu_2 J_f = nV_\delta k(\rho_{11f}{}^\circ)^{n_1}(\rho_{2f}{}^\circ)^{n_2}, \quad k = z\exp(-E/RT_f) \\ \left(\rho_{11f}{}^\circ = \frac{p_{11f}g_{11}}{RT_f},\ n_1 + n_2 = 1\right) \end{gathered} \tag{2.2}$$

Here V_δ is the characteristic volume of the chemical reaction, k is the chemical reaction rate constant, E is the activation energy, z is the pre-exponential factor, and n_i ($i = 1, 2$) is the order of the reaction in the oxidizer and the fuel, respectively. Let us write the four governing relationships

$$J^{2f} - J^{f1} = J_f,\quad \frac{J^{1f}}{\nu_{11}} = \frac{J_f}{\nu_2},\quad \frac{\rho_{11f}{}^\circ}{\nu_{11}} = \frac{\rho_{2f}{}^\circ}{\nu_2},\quad \nu_2 J = J^{2f} \tag{2.3}$$

The first of these relationships expresses the fact that the reaction rate (J_f) equals the difference between two fuel vapor streams, where the first is delivered to the microflame surface from the drop (J^{2f}) and the second is extracted from the microflames. The second relationship expresses the stoichiometry condition of the fluxes, the third [7] establishes the relationship between the oxidizer mass and the fuel vapor on the flame front, and the fourth is a consequence of the assumption that all the evaporating fuel is consumed in the chemical reaction. This assumption cannot be satisfied for sufficiently fine drops.

The intensity of the heat exchange between the f phase and the first and second phases, referred to unit mixture volume, is represented as

$$\begin{gathered} g_{f1} = \pi n d_f{}^2 h_{f1}(T_{f1} - T_1),\ q_{f2} = \pi n d^2 (T_f - T_1) h_{2f} \\ \left(h_{f1} = \frac{\lambda_f}{d_f}\frac{2d_1}{d_1 - d_f},\ h_{f2} = \frac{\lambda_f}{d}\frac{2d_f}{d_f - d},\ \lambda_f = \lambda_1(T_f)\right) \end{gathered} \tag{2.4}$$

Here h_{f1} and h_{f2} are the appropriate mass evolution coefficients. Substituting (2.4) into the last equation in (1.1), we obtain an equation to determine the stationary flame front temperature

$$T_f = \frac{J_f x_f}{\pi n d_f{}^2 h_{f1} + \pi n d^2 h_{f2}} + T_{f0}\left(T_{f0} = \frac{d_f{}^2 h_{f1} T_1 + d^2 h_{f2} T_2}{d_f{}^2 h_{f1} + d^2 h_{f2}}\right) \tag{2.5}$$

Using (2.1), and the first and third relationships in (2.3), we obtain

$$\begin{aligned} J_{2f} &= \frac{\pi n d^2 \beta_{2f}(\pi n d_f{}^2 \beta_{f1} + nV_\delta(\nu_{11}/\nu_2)^{n_1}k)\, pg_2 \ln p/(p - p_s)}{RT_2(\pi n d^2 \beta_{2f} + \pi n d_f{}^2 \beta_{f1} + nV_\delta(\nu_{11}/\nu_2)^{n_1}k)} \\ J_f &= \frac{\pi n d^2 \beta_{2f} nV_\delta(\nu_{11}/\nu_2)^{n_1}k\,(pg_2/RT_2)\ln p/(p - p_s)}{\nu_2(\pi n d^2 \beta_{2f} + \pi n d_f{}^2 \beta_{f1} + nV_\delta(\nu_{11}/\nu_2)^{n_1}k)} \end{aligned} \tag{2.6}$$

In the case of the kinetic and diffusion modes, we obtain from (2.6), respectively,

$$J^{2f} = \pi n d^2 \beta_{21} \frac{p g_2}{R T_2} \ln \frac{p}{p - p_s}, \quad \frac{J_f}{J^{2f}} \ll 1 \quad \left(\beta_{21} = \frac{D_{12}}{d} \frac{2 d_1}{d_1 - d}\right)$$

$$J^{2f} = \pi n d^2 \beta_{2f} \frac{p g_2}{R T_2} \ln \frac{p}{p - p_s}, \quad \frac{J_f}{J^{2f}} = 1 \tag{2.7}$$

Using (2.6), we obtain a quadratic equation for the mass evolution coefficient from the second equation in (2.3)

$$a \beta_{2f}^2 - b \beta_{2f} + c = 0$$

$$a = \frac{p g_2}{\nu_2 R T_2} \ln \frac{p}{p - p_s} \left[n V_\delta (\nu_{11}/\nu_2)^{n_1} k + \frac{D_{11} \pi n d^2}{D_{12}} \right] - \pi n d^2 \beta_{21} \rho_{11}^{\circ} \frac{D_{11}}{D_{12}}$$

$$b = \frac{p g_2}{\nu_2 R T_2} \ln \frac{p}{p - p_s} \pi n d^2 \beta_{21} \left[2 n V_\delta \left(\frac{\nu_{11}}{\nu_2}\right)^{n_1} k + \pi n d^2 \beta_{21} \frac{D_{11}}{D_{12}} \right] + \pi n d^2 \beta_{21} n V_\delta \left(\frac{\nu_{11}}{\nu_2}\right)^{n_1} k \rho_{11}^{\circ} \frac{D_{11}}{D_{12}} \tag{2.8}$$

$$c = n V_\delta \left(\frac{\nu_{11}}{\nu_2}\right)^{n_1} k (\pi n d^2 \beta_{21})^2 \left(\frac{p g_2}{\nu_2 R T_2} \ln \frac{p}{p - p_s} + \rho_{11}^{\circ} \frac{D_{11}}{D_{12}} \right)$$

An analytical investigation of the ignition condition [the approximate solution of the transcendental equation (2.5) taking into account (2.6) and (2.8)] can be carried out analogously to [2], where heterogeneous ignition of a solid surface has been investigated. In particular, it can be shown that for high values of the activation energy and the heat of chemical reaction, the lower temperature mode is purely kinetic ($J_f \ll J^{2f}$) and the upper is purely diffusion ($J_f = J^{2f}$).

For the purely kinetic mode, the characteristic volume of the reaction zone is the whole volume arriving at the gas phase; hence.

$$n V_\delta = \alpha_1 \tag{2.9}$$

For the purely diffusion mode the chemical reaction intrinsically proceeds so rapidly that the macroscopic evaporation rate is generally independent of the chemical kinetics and the variations V_δ exert practically no influence on the process.

If, other conditions being equal, the initial drop diameter d_0 diminishes, then the ignition condition can be reached for higher temperatures of the surrounding medium. Since the temperature of the ambient medium cannot be greater than the equilibrium temperature behind the macroscopic flame front, T_e, then the ignition condition cannot be achieved for some $d = d_*$, and, therefore, drop deflagration will not occur during the flame propagation.

The friction between the phases is taken equal to

$$f = n \frac{\pi d^2}{4} C_d \frac{m_1}{\alpha_1 v_1} \frac{(v_1 - v_2)^2}{2} \quad \left(C_d = \frac{24}{N_{Re}} \right) \tag{2.10}$$

The diameter of the reduced film d_1 is determined by the relations

$$N_{Nu} = \frac{2 d_1}{d_1 - d}, \quad N_{Nu} = 2 + 0.6 N_{Re}^{1/2} N_{Pr}^{1/3} \tag{2.11}$$

Equations (1.1), (1.2), and (1.3) in conjunction with (2.4), (2.6), (2.8), (2.10) which describe the interphasal interaction, are used for the numerical solution of the steady-state flame front propagation problem. Assigning the boundary conditions, determining the equilibrium parameters behind the flame front [in the state (e)], and investigating the singularity corresponding to the state of the medium in front of the flame front [the state (0)] are analogous to the case of thermal flame propagation in purely heterogeneous particle combustion [8]. Exactly as in [8], it can be shown that in the case of excess oxidizer the microflame temperature T_f tends to some temperature T_{fe}, where $T_{fe} > T_{1e}$, during total burn-up of the drops. In the case of a stoichiometric mixture, the microflame and the gas temperatures during total burn-up succeed in being equalized.

The problem reduces to seeking the eigenvalue which is the flame propagation velocity v_0 in this case.

A dimensionless form of (1.1)-(1.3) and the relations (2.4), (2.6), (2.8), and (2.10) are used for the computations. Obtaining the dimensionless equations is analogous to [1].

3. Results of the Computations

The combustion of tetralin drops in air is examined. It is assumed that the chemical reaction[9]

$$C_{10}H_{12} + 13\ O_2 = 10\ CO_2 + 6\ H_2O$$

proceeds with the following thermodynamic data [10, 11]: $p_0 = 1$ atm. gage, $T_0 = 298°K$, $\gamma_{10} = 1.4$, $\rho_{10}° = 0.118 \cdot 10^{-2}$ g/cm³, $\rho_2° = 0.969$ g/cm³, $c_{p1} = 0.915$ J/g · deg, $c_2 = 1.64$ J/g · deg, $c_{p3} = 0.84$ J/g · deg, $c_{p4} = 1.86$ J/g · deg, $c_{p5} = 1.1$ J/g · deg, $\lambda_{110} = 5.89 \cdot 10^{-5}$ cal/cm · sec · deg, $\lambda_{130} = 3.28 \cdot 10^{-5}$ cal/cm · sec · deg, $\lambda_{140} = 1.15 \cdot 10^{-5}$ cal/cm · sec · deg, $\lambda_{150} = 6.6 \cdot 10^{-5}$ cal/cm · sec · deg, $D_{110} = 0.186$ cm²/sec, $D_{120} = 0.054$ cm²/sec, $\mu_{110} = 202 \cdot 10^{-6}$ g/cm · sec, $\mu_{130} = 146 \cdot 10^{-6}$ g/cm · sec, $\mu_{140} = 182 \cdot 10^{-6}$ g/cm · sec, $h_3 = -94.052 \cdot 10^{-3}$ cal/mole, $h_{14} = 57.798 \cdot 10^3$ cal/mole.

The dependence of the thermodynamic coefficients [c_p, λ, D, μ on the gas temperature and $l_2(T_2)$ and $p_s(T)$] was taken in conformity with [10, 11]. The corresponding kinetic constants were taken equal to $E = 2.5 \cdot 10^4$ cal/mole, $z = 3.2 \cdot 10^7$ sec^{-1}, which is in the range of the data recommended in [7, 9]. Moreover, it was assumed that the reaction has a zero order in the oxygen ($n_1 = 0$), which is valid for oxidizer excesses Figures 1 and 2 present results of a numerical integration mapping the flame front structure ($v_0 = 53.1$ cm/sec) in a gas suspension with the initial composition $M_{20} = 0.052$ (oxidizer excess, stoichiometric composition for $M_{20} = 0.065$), and the initial drop diameter $d_0 = 38$ μ.

It follows from the graphs presented that initial heating of the drops (Fig. 1) first occurs in some domain because of heat exchange with the gas, which is heated in turn because of heat evolution from a higher temperature zone. A gradual increase in the temperature T_f occurs which at this time is between the temperature of the gas and the drops. In this domain the reaction rate is small, whereupon a quasi-well-mixed mode is realized because all the combustion occurs in the gas phase. Ignition of the drops occurs later. The microflame temperature T_f hence increases by a jump, reaching the maximum value. Further drop combustion occurs in the diffusion domain, where $J_f/J = 1$ (pure diffusion mode). The drop temperature hence reaches the boiling point and does not change henceforth. As the drops and oxidizer burn (curve M_2 in Fig. 2) the reaction rate and the combustion rate tend to zero in the microflame fronts J_f. The gas temperature hence tends to the equilibrium value T_e and the temperature T_f does not succeed in being equalized to the gas temperature until the time of complete burn up of the drops.

An increase in the gas velocity v_1 (Fig. 2) occurs because of thermal expansion, where the velocity of the burned-up mixture motion v_{1e} is almost an order of magnitude greater than the velocity of front motion relative to the cold mixture v_0 in this case. The particle velocity v_2 varies only under the effect of friction. The particles are entrained in the gas motion after the relative motion has become sufficiently high, where this process is magnified as the drops burn.

The relative velocity of the drop and gas motion during flame propagation results in more intensive heat and mass exchange, which affects the value of the velocity v_0 substantially. Thus, not taking account of two-velocity effects in a computation by the one-velocity approximation ($v_1 = v_2$) and with the friction law $C_d = 24/N_{Re}$ for the mixture $M_{20} = 0.052$, $d_0 = 34$ μ will result in a reduction in the flame velocity to $v_0 = 40$ cm/sec, as compared to $v_0 = 58$ cm/sec.

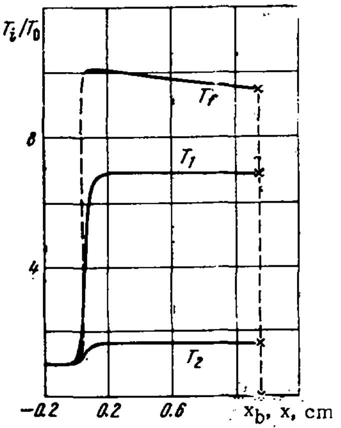

Fig. 1

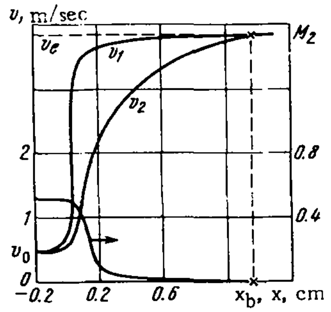

Fig. 2

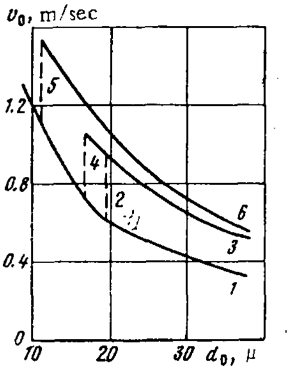

Fig. 3

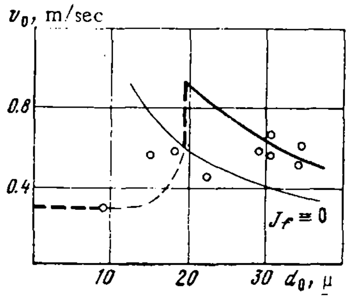

Fig. 4

If it is artifically assumed that $J_f \equiv 0$ for a mixture in which drop ignition occurs, then the velocity values v_0 obtained will be significantly lower than the values given by theories taking ignition into account. Thus, for the mixture $M_{20} = 0.0507$, $d_0 = 29$ μ under the condition $J_f \equiv 0$ we have $v_0 = 45$ cm/sec, while we have $v_0 = 65$cm/sec,taking account of ignition and combustion in the microflames.

Let us note that the Williams theory [5], which does not take account of the possibility of diffusion microflame formation and corresponds to the case $J_f \equiv 0$ mentioned, yields $v_0 = 50$ cm/sec for a mixture with the same parameters. The slight discrepancy between the velocities obtained for $J_f \equiv 0$ ($v_0 = 45$ cm/sec) and that given by the Williams theory ($v_0 = 50$ cm/sec) is explained by the additional simplifications in the latter. Namely, it is assumed in [5] that all the heat transmitted to the drops over the whole extent of the flame front goes into their evaporation, and the evaporation rate is not zero. It is hence not taken into account automatically that a large part of the heat goes into heating the drop in some domain (see Fig. 1) and the evaporation rate is almost zero. Moreover, the temperature dependence of the thermodynamic coefficients, including the coefficient of heat conduction, is not taken into account in the computations in [5].

The increase in the flame propagation velocity v_0 as the mixture combustion mode changes is explained by the jump diminution in the burning time of a fixed fuel mass in the presence of diffusion microflames, sincethe quantity of heat transmitted to the drops and going into evaporating them is hence increased.

The dependence of the flame propagation velocity v_0 on the initial particle diameter d_0 is represented in Fig. 3 for a fixed fresh mixture composition ($M_{20} = 0.052$) with different kinetic constants. Curve 1 corresponds to the dependence $v_0(d_0)$ for $J_f \equiv 0$(a quasi-well-mixed mode for $J^{2f} = \nu_2 J$, $\rho_{12} = 0$). Its position is independent of the kinetic constants z and E, and it yields a monotone drop in the flame velocity as the particle diameter increases. A change in the mixture combustion mode from quasi-well-mixed to diffusion occurs for $d_0 \simeq 20$ μ. The velocity v_0 hence increases in a jump (the dashed line 2). As d_0 increases further, the flame propagation velocity drops (curve 3), which is explained by the increase in the burning time of a fixed fuel mass.

The pre-exponential factor z and the activation energy E which govern the chemical kinetics substantially influence just the value of the critical diameter at which mixture combustion occurs with drop ignition and have practically no influence on the dependence $v_0(d_0)$ in the vapor phase mode. The curve 1–2–3 in Fig. 3 corresponds to the above-mentioned values of z and E ($z = 3.2 \cdot 10^7$ sec^{-1}, $E = 2.5 \cdot 10^4$ cal/mole), the curve 1–4–3 corresponds to the same value of E but with an elevated value of z ($z = 4.5 \cdot 10^7$ sec^{-1}, $E = 2.5 \cdot 10^5$ cal/mole), and curve 1–5–6 corresponds to a diminished value of E ($z = 3.2 \cdot 10^7$ sec^{-1}, $E = 2 \cdot 10^4$ cal/mole). The influence of the activation energy E is naturally more essential than the influence of z. A change in the activation energy strongly affects the change in the reaction rate constant; hence, its diminution results in a noticeable diminution in the lag in drop ignition, which increases the value of the velocity v_0 somewhat in the vapor phase mode.

As has already been remarked, for sufficiently small drop diameters (for tetralin–air mixtures $d_0 < 10$ μ), the flame propagation in the gas suspension occurs exactly as in a well-mixed gas mixture because the drops succeed, in practice, in being evaporated prior to the beginning of the combustion reaction. Hence, the Zel'dovich–Frank-Kamenetskii formula [9] can be used for v_0 for small d_0

$$v_0^2 = \frac{2\lambda_e z}{\rho_{1k} c_p (T_e - T_0)^2} \frac{T_0}{T_e} \left(\frac{RT_e^2}{E}\right)^2 \exp(-E/RT_e) \tag{3.1}$$

On the basis of the experimental results [3] for a tetralin–air mixture and the computational results herein and (3.1), we determined z and E (the inverse problem of combustion theory) in such a way that the theoretical results best corresponded to experiment. The constants were selected so that for small diameters ($d_0 < 10\ \mu$) the values given by (3.1) agreed with experiment and a change in the combustion mode occurred for $d_0 \approx 20\ \mu$ in the computations using the present theory. The values obtained for the kinetic constants were then determined uniquely. The following values $z = 3.2 \cdot 10^7\ \mathrm{sec}^{-1}$, $E = 2.5 \cdot 10^4$ cal/mole were obtained as a result of such processing.

The results of comparing the theoretical values obtained for the flame propagation velocity v_0 with the experimental data in [3] are represented in Fig. 4. The circles denote the experimental points obtained as a result of processing the data in [3], which reduced to determining the dependence $v_0(d_0)$ for a fixed M_{20} from the available set of experimental values of $v_0\ (d_0, M_{20})$, by numerically determining the derivatives $\partial v_0/\partial M_{20}$, $\partial v_0/\partial d_0$ at separate points and subsequent linear interpolation. The horizontal dashed line (in Fig. 4) corresponds to the velocity given by (3.1) in the domain of small diameters. A quasi-well-mixed mode is apparently realized for the drop diameters $10\ \mu < d_0 < 20\ \mu$, when both evaporation and diffusion and chemical kinetics influence the combustion velocity which occurs without the formation of microflames.

In order to describe flame propagation in a mixture in this domain as contrasted to the $J_f \equiv 0$ mode considered herein, the presence of free fuel vapors in the gas phase ($\rho_{12} > 0$ and $J^2 f > \nu_2 J$) must be taken into account. The dependence $v_0\ (d_0)$ in the domain $10\ \mu < d_0 < 20\ \mu$ is shown provisionally in Fig. 4 by the fine dashed curve. For high activation energies and high heats of chemical reaction this transition region apparently includes a small range of drop diameters so that the change in flame propagation mode from the well-mixed to the diffusion occurs sufficiently rarely. The velocity jumps for the mode change given by the experimental points in Fig. 4, which are not quite definite enough, are explained by a certain smoothing during processing of the experiment. However, the fact of the increase in velocity as the mode changes is established experimentally and is described qualitatively by the theory. Agreement between the experimental and theoretical results in the large diameter domain is satisfactory.

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