# COMBUSTION OF GAS MIXTURES WITH PARTICLES

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This paper discusses the motions of multiphase media, consisting of a homogeneous reaction mixture of gas with solid or liquid particles of fuel. Combustion of the particles takes place either in the condensed phase, or after preliminary vaporization; the vapors of the fuel burn in the volume of the gas or in the narrow front of the flame enveloping the particle.

A multivelocity and multitemperature model, with heterogeneous chemical reactions, is used to describe the motion of such media. The article gives expressions characterizing the force, thermal, and mass interaction between the phases. A study is made of the problem of the normal propagation of the flame front in the gas suspension for the case when the combustion of the particles takes place in the condensed phase. The values obtained for the rate of propagation of the flame front are given as a function of several parameters which determine the process under investigation (particle size, composition of the mixture, etc.).

An analysis of the experimental data permits the isolation of three limiting sets of conditions for combustion of the particles. In the first place, purely heterogeneous conditions, when the chemical reaction takes place directly within or on the surface of the particles (in the condensed phase) and, by the same token, the heat of the chemical reaction is evolved directly in the condensed phase. For example, particles of graphite or carbon, which contain no volatile substances, burn in this way. In the second place, quasihomogeneous conditions, when combustion and heat evolution take place over the whole volume of the gas phase after vaporization and mixing of the fuel vapors with an oxidizer. Sufficiently fine particles of an easily vaporized fuel burn in this fashion. In the third place, vapor-phase conditions, when combustion and direct heat evolution take place in thin layers of flames surrounding the particles. These layers of flame have a considerably higher temperature than the surrounding gas and the particles.

With regard to the combustion of a mixture with solid particles, the problem of the normal propagation of a flame front in a single-velocity and single-temperature approximation has been discussed by O. I. Leipununskii [1]. Papers [2, 3], for the case when the temperatures of the gas and the particles differ, discuss the combustion of a gas suspension under purely heterogeneous combustion conditions. Flame propagation in a gas suspension of an easily vaporizing fuel was studied experimentally by Burgoyne and Cohen [4]. They observed that, with an increase in the particle size, the quasi-homogeneous conditions go over into vapor-phase conditions. In such mixtures, for quasi-homogeneous conditions, the problem of the propagation of the flame front in its simplest form is investigated in the article of Williams [5].

To describe the above three sets of combustion conditions of a gas suspension, the concepts of the hydrodynamics of a multiphase medium with phase transformations have been used [6-8], while, for an examination of vapor-phase combustion conditions, use has also been made of a model of the combustion of an isolated particle, developed by Varshavskii [9] and by Spaulding.

1. Basic Assumptions. Let there be a mixture of a gas with suspended particles, in which a heterogeneous chemical reaction is taking place. In this case, the gas phase consists of a minimum of two components, the oxidizer and the reaction products. We assume that the basic assumption of the mechanics of a continuous medium holds, i.e., that the distances at which the flow parameters of the mixture vary substantially (outside of the breakaway surface) are much greater than the characteristic dimensions of the inclusions and of the special combustion zones (the diameter of the particles or drops, the diameter of the

flame around a particle), as well as the distances between them. This permits describing the above disperse mixture as a set of two or more continua, filling one and the same volume, at each point of which the parameters are determined for each phase, including the volumetric fractions, $\alpha_i$, entering into each phase.

As a first step in the simplification we shall assume: 1) the particles in an element of volume are, on the average, identical spheres moving at random; indirect collisions between the particles may be neglected;

2) the chemical combustion reaction obeys the simplest equation

$$\varkappa_{11}A + \varkappa_2 B = \varkappa_{13}C \tag{1.1}$$
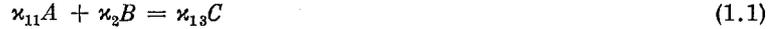
where A, B, C are the symbols of the chemical elements of the fuel, the oxidizer, and the reaction products, respectively, and $\varkappa_k$ (k = 11, 2, 13) are stoichiometric coefficients;

3) all the fuel entering the combustion zone in the form of vapors (into the carrier phase or into the flame) is burned completely, so that the presence of free fuel vapors in the gas can be disregarded;

4) in the case of vapor-phase combustion, the mass of substance contained within the flame layer is considerably less than the mass of a particle; therefore, the properties of this layer will be taken into account using the concept of a surface phase.

Further, everywhere in what follows parameters relating to the gas, the particles, and the flame around the particles, will be assigned the subscripts 1, 2, and $f$. The parameters of the first phase, i.e., the homogeneous mixture of gases (the carrier gas medium), relating to the oxidizer and to the reaction products, will have the subscripts 11 and 13. Correspondingly, the oxidizer will be called the first component, and the reaction products the third; the particles (the condensed phase) will be called the second phase (or the second component), and the flame around the particles will be called the $f$-phase.

At each point of the volume occupied by the mixture, we can introduce the macroscopic velocities and the mean densities of the components and phases, $v_i$, $\rho_i$ (i = 1, 11, 13, 2), and the volumetric contents of the phases $\alpha_i$ (i = 1, 2); here

$$\rho = \rho_1 + \rho_2, \ \rho_1 = \rho_{11} + \rho_{13}, \ \rho_{11} = \rho_{11}{}^\circ \alpha_1, \ \rho_{13} = \rho_{13}{}^\circ \alpha_1, \ \rho_2 = \rho{}^\circ_2 \alpha_2$$
$$\alpha_i \geqslant 0, \ \alpha_1 + \alpha_2 = 1, \ \alpha_2 = {}^1\!/_2 \pi n d^3 \tag{1.2}$$

Here $\rho$ is the density of the mixture; $\rho_i^\circ$ (i = 1, 11, 2, 13) is the true density of the substance of the i-th component or phase; n is the number of particles or drops (in the given case, spherical with a diameter d) in unit volume of the mixture. The mean mass velocity of the first phase, $v_1$, is determined in terms of the velocities of the components

$$\rho_1 v_1 = \rho_{11} v_{11} + \rho_{13} v_{13} \tag{1.3}$$

The relative motion of the components in the gas mixture, which constitutes the gas phase, is determined by diffusion processes (in contrast to the relative motion of the gas and the disperse condensed phases). Therefore, we can determined the diffusion rates of the first and third components $w_{11}$ and $w_{13}$

$$v_{11} = v_1 + w_{11}, \quad v_{13} = v_1 + w_{13} \qquad (\rho_{11}w_{11} + \rho_{13}w_{13} = 0) \tag{1.4}$$

which are described using Fick's law

$$c_{11}w_{11} = - D_{13}\nabla c_{11} \qquad (c_i = \rho_i / \rho_1, \ i = 11, 13) \tag{1.5}$$

where $D_{13}$ is the coefficient of binary diffusion; $c_i$ are the mass concentrations of the components in the first phase.

Following [6-8], we have the following equations for the masses and the momentums (with the exception of the external mass forces) of each phase, as well the equation for the constancy of the number of particles (in the case where there are not processes involving pulverization or adhesion of the particles)

$$\frac{\partial \rho_{11}}{\partial t} + \nabla \rho_{11}(v_1 + w_{11}) = - J_{11}, \qquad \frac{\partial \rho_{13}}{\partial t} + \nabla \rho_{13}(v_1 + w_{13}) = J_{13}$$
$$\frac{\partial \rho_2'}{\partial t} + \nabla \rho_2 v_2 = - J_2, \qquad \frac{\partial n}{\partial t} + \nabla n v_2 = 0$$
$$\rho_1 \frac{d_1 v_1}{dt} = \nabla^m \sigma_1{}^m - r_{12} + J_2(v_2' - v_1), \qquad \rho_2 \frac{d_2 v_2}{dt} = \nabla^m \sigma_2{}^m + r_{12} - J_2(v_2' - v_2)$$
$$\left(\frac{d_i}{dt} = \frac{\partial}{\partial t} + v_i \nabla = \frac{\partial}{\partial t} + v_i{}^m \nabla^m\right) \tag{1.6}$$

Here and in what follows, summation is carried out only for the superscripts, referred to the coordinate axes; $J_j$ ($j = 11, 13, 2$) is the rate of change of the mass of the corresponding component in unit volume of the mixture, calculated for a heterogeneous chemical reaction; $r_{12}$ is the force of the interaction between the phases, referred to unit volume of the mixture; $\sigma_i$ ($i = 1, 2$) is the tensor of the surface forces of the corresponding phase; $v_2'$ characterizes the momentum of the mass undergoing conversion as a result of the chemical reaction.

From assumptions 2) and 3) it follows that

$$\frac{J_{11}}{v_{11}} = \frac{J_2}{v_2} = \frac{J_{13}}{v_{13}} = J, \qquad v_{13} = v_{11} + v_2$$
$$(v_{11} = g_{11}\varkappa_{11}, \ v_2 = g_2\varkappa_2, \ v_{13} = g_{13}\varkappa_{13}) \tag{1.7}$$

For disperse systems with sufficiently small volumetric contents of the suspended phase, $\alpha_2$, taking account of the effect of the viscosity of the carrier medium only in processes involving phase interaction, it can be assumed that

$$\sigma_1{}^{mn} = p_1\delta^{mn}, \qquad \sigma_2{}^{mn} = 0 \tag{1.8}$$

The force of the interaction between phases, $r_{12}$, can be represented in the form

$$\mathbf{r}_{12} = -\alpha_2\nabla p + \mathbf{f} \tag{1.9}$$

where the first term is connected with the action of the pressure field of the carrier phase on the inclusions (the Archimedes force), while the second is, in fact, the force of friction between the phases.

Assuming that the velocity of the gas at the surface of a particle is equal to the velocity of the latter, which, in turn, moves as a solid body, it can be taken that

$$\mathbf{v}_2' = \mathbf{v}_2 \tag{1.10}$$

From (1.6), (1.2), and from the condition of the incompressibility of the material of the particles ($\rho_2^\circ = \text{const}$), there follow the relationships:

$$\frac{\partial\rho_1}{\partial t} + \nabla\rho_1\mathbf{v}_1 = v_2 J, \qquad \frac{\alpha_1}{\rho_1^\circ}\frac{d_1\rho_1^\bullet}{dt} = v_2 J\left(\frac{1}{\rho_1^\circ} - \frac{1}{\rho_2^\circ}\right) - \nabla\left(\alpha_1\mathbf{v}_1 + \alpha_2\mathbf{v}_2\right) \tag{1.11}$$

2. Energy of the Mixture. Heat Flux Equations. We adopt the following definition of the total energy, E, of <u>unit mass of the mixture</u>:

$$\rho E = \rho_1\left(u_1 + \frac{v_1^2}{2}\right) + \rho_2\left(u_2 + \frac{v_2^2}{2}\right) + nu_f{}^* \tag{2.1}$$

where $u_i$ ($i = 1, 2$) is the internal energy of the corresponding phase; $u_f{}^*$ is the internal energy of the flame layers around the particles, arriving at one single particle. For the internal energy of the first phase we adopt the condition of additivity with respect to the mass of the components entering into it

$$\rho_1 u_1 = \rho_{11}u_{11} + \rho_{13}u_{13} \tag{2.2}$$

In a fixed element of volume dV, the total energy of the mixture varies as a result of the influx of mass and of external action, i.e.,

$$\frac{\partial\rho E}{\partial t} = -\nabla\left[\rho_{11}(\mathbf{v}_1 + \mathbf{w}_{11})\left(u_{11} + \frac{v_1^2}{2}\right) + \rho_{13}(\mathbf{v}_1 + \mathbf{w}_{13})\left(u_{13} + \frac{v_1^2}{2}\right) + \rho_2\mathbf{v}_2\left(u_2 + \frac{v_2^2}{2}\right) + n\mathbf{v}_2 u_f{}^*\right] + \rho\frac{dE}{dt} \tag{2.3}$$

where dE/dt is a quantity which, by definition, is the change in the total energy of the mixture arriving at unit mass of the medium in the fixed volume as the result of external action. From (2.3), (2.1), (1.7), and (1.6) there follows a generalization of the concept of the substantive derivative of the total energy of the mixture

$$\rho\frac{dE}{dt} = \rho_1\frac{d_1}{dt}\left(u_1 + \frac{v_1^2}{2}\right) + \rho_2\frac{d_2}{dt}\left(u_2 + \frac{v_2^2}{2}\right) + n\frac{d_2 u_f{}^*}{dt} + J_2\left(u_1 - u_2 + \frac{v_1^2 - v_2^2}{2}\right)$$

$$+ \nabla\left[\rho_{11}\mathbf{w}_{11}(u_{11} - u_{13})\right] = \rho_{11}\frac{d_1}{dt}\left(u_{11} + \frac{v_1^2}{2}\right) + \rho_{13}\frac{d_1}{dt}\left(u_{13} + \frac{v_1^2}{2}\right)$$

$$+ \rho_2\frac{d_2}{dt}\left(u_2 + \frac{v_2^2}{2}\right) + n\frac{d_2 u_f{}^*}{dt} + \rho_{11}\mathbf{w}_{11}\nabla(u_{11} - u_{13}) + J\left(v_{13}u_{13} - v_{11}u_{11} - v_2 u_2 + v_2\frac{v_1^2 - v_2^2}{2}\right) \tag{2.4}$$

From the momentum equations of both phases (1.6), taking account of (1.8)-(1.10) there follows the theorem of the acting forces, or the equation of the kinetic energy of the mixture

$$\rho_1 \frac{d_1}{dt}\frac{v_1^2}{2} + \rho_2 \frac{d_2}{dt}\frac{v_2^2}{2} = -(\alpha_1 \mathbf{v}_1 + \alpha_2 \mathbf{v}_2)\nabla p - \mathbf{f}(\mathbf{v}_1 - \mathbf{v}_2) + J_2(\mathbf{v}_2 - \mathbf{v}_1)\mathbf{v}_1 \tag{2.5}$$

Further, we must introduce the heat-flux equations for each phase [7, 8]; these may be written in the form

$$\rho_1 \frac{d_1 u_1}{dt} = \rho_1 A_1 - J_2 x_1 + q_{f1} - \nabla \mathbf{q}_1 - \nabla \rho_{11} \mathbf{w}_{11}(u_{11} - u_{13})$$

$$\rho_2 \frac{d_2 u_2}{dt} = \rho_2 A_2 - J_2 x_2 + q_{f2}, \quad n\frac{d_2 u_f^*}{dt} = nA_f - J_2 x_f - q_{f1} - q_{f2} \tag{2.6}$$

where $A_i$ $(i = 1, 2, f)$ is the working capacity of the internal forces. The remaining terms are the heat fluxes; $x_i$ $(i = 1, 2, f)$ is the heat flux from the i-th phase to the substance undergoing chemical conversion, referred to its mass; $q_{fi}$ $(i = 1, 2)$ is the heat flux from the surface of the flame to the i-th phase, referred to unit volume of the mixture; $\mathbf{q}_1$ is the heat flux outside of the carrier phase, due to thermal conductivity. The last term of the first equation of (2.6) characterizes the corresponding change in the specific internal energy of the first phase due to the relative motion of its components, since the first phase itself is a two-velocity mixture.

Following [6-8], and taking account of the incompressibility of the drops and the particles and the absence of "surface tension" in the flame around a particle, and assuming that all the kinetic energy of the mixture dissipated in unit time as a result of friction (see (2.5)) between the phases, $\mathbf{f}(\mathbf{v}_1 - \mathbf{v}_2)$, goes over directly to the internal energy of the carrier phase, we have the following expressions for the work of the internal forces of the phases:

$$\rho_1 A_1 = -\rho_1 p\frac{d_1}{dt}\frac{1}{\rho_1^\circ} + \mathbf{f}(\mathbf{v}_1 - \mathbf{v}_2) + J_2\frac{(\mathbf{v}_2 - \mathbf{v}_1)^2}{2}, \quad A_2 = A_f = 0 \tag{2.7}$$

Taking (2.7) into account, the heat-flux equations (2.6) assume the form

$$\rho_1 \frac{d_1 u_1}{dt} = \frac{\alpha_1 p}{\rho_1^\circ}\frac{d_1 \rho_1^\circ}{dt} + \mathbf{f}(\mathbf{v}_1 - \mathbf{v}_2) + J_2\frac{(\mathbf{v}_2 - \mathbf{v}_1)^2}{2} - J_2 x_1 + q_{f1} - \nabla \mathbf{q}_1 - \nabla \rho_{11} \mathbf{w}_{11}(u_{11} - u_{13})$$

$$\rho_2 \frac{d_2 u_2}{dt} = -J_2 x_2 + q_{f2}, \quad n\frac{d_2 u_f^*}{dt} = -J_2 x_f - q_{f1} - q_{f2} \tag{2.8}$$

Starting from (2.4) and from Eqs. (2.5) and (2.8), we obtain an explicit expression for the substantive derivative of the total energy of the mixture

$$\rho \frac{dE}{dt} = J_2\left[u_1 - u_2 - (x_1 + x_2 + x_f) + p\left(\frac{1}{\rho_1^\circ} - \frac{1}{\rho_2^\circ}\right)\right] - \nabla p(\alpha_1 \mathbf{v}_1 + \alpha_2 \mathbf{v}_2) - \nabla \mathbf{q}_1 \tag{2.9}$$

The change in the total energy of the medium, described by the substantive derivative, in accordance with the definition of the latter is connected with the external action (described by the last two terms in (2.9)), but in no way with internal processes involving interaction of the phases. Therefore, the expression in square brackets in the right-hand part of (2.9), of the type of a source, connected with the chemical conversion, must revert to zero, i.e.,

$$x_1 + x_2 + x_f = i_1 - i_2 \tag{2.10}$$

where $i_i = u_i + p/\rho_i^0$ is the enthalpy of the corresponding phase. The values of $x_k$ depend on the combustion conditions and must be stipulated. These supplementary relationships will be called "accommodating."

In the case of purely heterogeneous conditions (combustion in the condensed phase, when there is no $f$-phase)

$$u_f^* \equiv 0, \quad x_f \equiv 0, \quad q_{f2} \equiv -q_{f1} = q_{12} \tag{2.11}$$

we assume that the first component (the oxidizer) arrives at the particles with an enthalpy determined by the temperature of the second phase, i.e., $\nu_{11} i_{11}$ $(p, T_2)$; the reacting mass of fuel enters into the reaction with an enthalpy $\nu_2 i_2$ $(p, T_2)$; the reaction products (the third component) leave the second phase with an enthalpy determined also by the temperature of the particles, $\nu_{13} i_{13}$ $(p, T_2)$. Thus, taking account of (2.10)

$$\nu_2 x_2 = \nu_{13} i_{13}(p, T_2) - \nu_{11} i_{11}(p, T_2) - \nu_2 i_2(p, T_2)$$

$$\nu_2 x_1 = \nu_2 i_1(p, T_1) - \nu_{13} i_{13}(p, T_2) + \nu_{11} i_{11}(p, T_2) \tag{2.12}$$

In the case of quasi-homogeneous conditions (combustion in the gas phase, when there is no $f$-phase and (2.11) holds), we assume that the fuel leaves a particle with an enthalpy $\nu_2 i \tau_{12}$ ($p_s$ ($T_2$), $T_2$), corresponding to vapors of the fuel in a state of saturation ($p_s(T_2)$ is the pressure of the saturated fuel vapors). As a result

$$\nu_2 x_2 = \nu_2 i_{12} (p_s (T_2), \ T_2) - \nu_2 i_2 (p, T_2)$$
$$\nu_2 x_1 = \nu_2 i_1 (p, T_1) - \nu_2 i_{12} (p_s (T_2), T_2) \tag{2.13}$$

In the case of vapor-phase conditions (combustion in the $f$-phase), as in the preceding case, we assume that the fuel vapors move away from the particles into the flame which surrounds them (the $f$-phase) with an enthalpy $i_{12}(p_s(T_2), T_2)$, that the oxidizer leaves the carrier medium into the $f$-phase with an enthalpy $i_{11}(p, T_f)$, corresponding to the first component and determined by the temperature of the flame $T_f$, and that the reaction products leave the $f$-phase into the carrier medium at the temperature of the flame $T_f$, i.e.,

$$\nu_2 x_2 = \nu_2 i_{12} (p_s (T_2), \ T_2) - \nu_2 i_2 (p, T_2)$$
$$\nu_2 x_f = \nu_{13} (p, T_f) - \nu_2 i_{12} (p_s (T_2), T_2) - \nu_{11} (p, T_f)$$
$$\nu_2 x_1 = \nu_2 i_1 (p, T_1) + \nu_{11} (p, T_f) - \nu_{13} i_{13} (p, T_f) \tag{2.14}$$

Taking account of (1.7)-(1.10), (2.11)-(2.13), the system of equations (1.6), (2.8) describes the mutually interpenetrating motion of a two-phase disperse mixture, with combustion of the disperse phase under one of the three above-described sets of conditions. From this system, the equation for the conservation of energy of the mixture follows in the form

$$\rho_{11} \frac{d_1}{dt}\left(i_{11} + \frac{v_1^2}{2}\right) + \rho_{13} \frac{d_1}{dt}\left(i_{13} + \frac{v_1^2}{2}\right) + \rho_2 \frac{d_2}{dt}\left(i_2 + \frac{v_2^2}{2}\right) + n \frac{d_2 u_f^*}{dt} = \frac{\partial p}{\partial t} + \tag{2.15}$$
$$+ (i_{11} - i_{13}) \nabla \rho_{11} w_{11} + \nabla \rho_{11} w_{11} (u_{13} - u_{11}) + \nu_2 J \frac{v_2^2 - v_1^2}{2} - \nabla q_1 + J Q$$
$$(Q = \nu_{11} i_{11} (\rho_{11}°, \ T_1) + \nu_2 i_2 (p, \ T_2) - \nu_{13} (\rho_{13}° T_1) \ )$$

where Q is the heat of the chemical reaction under consideration. In the case of vapor-phase combustion conditions, it is often possible to neglect the heat capacity of the $f$-phase (the quantity $nd_2 u_f^*/dt$). Then, the heat-flux equation for this phase goes over into the algebraic relationship

$$- \nu_2 J x_f = q_{f1} + q_{f2} \tag{2.16}$$

which, taking account of (2.14), comes down to the equation for the temperature of the flame around the particles, $T_f$.

3. Interaction between Phases. For what follows, it is necessary to determine the mass (J), the force ($f$), and the thermal ($q_{fi}$) interaction between the phases, taking account of the structure of the phases, as well as of the combustion conditions. The corresponding expressions will be given by considerations with respect to the flow of a gas around an isolated sphere; the values of J and $q_{fi}$ will be determined in the approximation of a "reduced film" [9]. The force of the interphase friction can be written in the form

$$f = n \frac{\pi d^2}{4} C_d \rho_1° \frac{|v_1 - v_2| (v_1 - v_2)}{2} \left(C_d = C_d (N_{Re}, \ n), \ N_{Re} = \frac{\rho_1° |v_1 - v_2| d}{\mu_1}\right) \tag{3.1}$$

where $C_d$ is the friction coefficient; $N_{Re}$ is the Reynolds number; $\mu_1$ is the dynamic viscosity coefficient of the first phase, which can be taken as

$$\rho_1 \mu_1 = \rho_{11} \mu_{11} + \rho_{13} \mu_{13} \tag{3.2}$$

With Re < 1 and small volumetric contents of the second phase ($\alpha_2 \approx 0$), we can use Stokes law for laminar flow around a sphere

$$C_d = 24 / \text{Re} \tag{3.3}$$

The heat-transfer rate between the $f$-phase and the first and second phases, referred to unit volume of the mixture, can be represented in the form

$$q_{f1} = n \pi d_f^2 h_1 (T_f - T_1), \qquad q_{f2} = n \pi d^2 h_2 (T_f - T_2)$$
$$\left(h_1 = \frac{\lambda_{f1}}{d_f} \frac{2d_1}{d_1 - d_f}, \quad h_2 = \frac{\lambda_{f2}}{d} \frac{2d_f}{d_f - d}\right) \tag{3.4}$$

Here $h_1$ and $h_2$ are the heat-transfer coefficients between the flame and the gas or the particles, respectively; $d_1$ is the diameter of the reduced film; $d_f$ is the diameter of the surface of the flame. It is natural to assume

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$$\lambda_{f1} = \lambda_1(T_f), \qquad \lambda_{f2} = \lambda_{12}(T_f) \tag{3.5}$$

where $\lambda_1$ and $\lambda_{12}$ are the thermal conductivity coefficients of the first phase and of the fuel vapors; analogously to (3.2), we have

$$\rho_1\lambda_1 = \rho_{11}\lambda_{11} + \rho_{13}\lambda_{13} \tag{3.6}$$

In accordance with the definition of the reduced film, we have

$$\frac{2d_1}{d_1 - d} = N_{Nu} \tag{3.7}$$

Here $N_{Nu}$ is the diffusion Nusselt number, and we can use the Rants-Marshall relationship

$$N_{Nu} = 2 + 0.6 N_{Sl}^{1/3} N_{Re}^{1/2} \qquad N_{Sl} = \mu_1(\rho_1^\circ)^{-1} D_{11}^{-1} \tag{3.8}$$

where $N_{Sl}$ is the Schmidt number for a gas.

When there is no flame around the particles, we have

$$q_{12} = - q_{21} = n\pi d^2 h\,(T_1 - T_2) \qquad \left(h = \frac{\lambda_1}{d}\,\frac{2d_1}{d_1 - d}\right) \tag{3.9}$$

Here h is the heat-transfer coefficient between the particles.

We represent the mass-transfer rate between the second and $f$-phase in the form [10]

$$J_2 = n\pi d^2 \beta_2 \frac{p g_2}{R T_2} \ln \frac{p}{p - p_s} \qquad \left(\beta_2 = \frac{D_{12}}{d}\,\frac{2d_f}{d_f - d}\right) \tag{3.10}$$

where $\beta_2$ is the mass-transfer coefficient between the flame and the particles; $D_{12}$, $g_2$, and R are, respectively, the autodiffusion coefficient, the molecular weight of the fuel vapors, and the universal gas constant. Formula (3.10), known in the literature as the Stefan formula, determines the rate of vaporization by the rate of diffusion of the fuel vapors.

If, in (3.10), we replace $d_f$ by $d_1$, we obtain an expression which determines the rate of mass transfer in the case of quasi-homogeneous combustion conditions.

The rate of mass transfer between the first and the $f$-phases, determined by the diffusion of the oxidizer and by the chemical kinetics, is represented in the form [10]

$$J_{11} = n\pi d_f^2 \frac{p_{11} g_{11}}{R T_1} \frac{1}{1/\beta_1 + 1/k} \qquad \left(\beta_1 = \frac{D_{11}}{d_f}\,\frac{2d_1}{d_1 - d_f}\right) \tag{3.11}$$

Here $\beta_1$ is the mass-transfer coefficient between the flame and the gas; $D_{11}$ and $g_{11}$ are the coefficient of autodiffusion and the molecular weight of the oxidizer; $p_{11}$ is the partial pressure of the oxidizer; k is the rate constant of the chemical reaction

$$k = z \exp\,(-E / R T_f) \tag{3.12}$$

where E is the activation energy; z is a pre-exponential factor.

Since, at the flame front, there is complete consumption of the arriving fuel vapors and oxidizer $(J_{11}\nu_2 = J_2\nu_{11})$, from this fact, and taking account of (3.10) and (3.11), an equation is also obtained which determines the diameter of the flame around the particles, $d_f$.

If, in (3.11), we replace $d_f$ by d, we obtain the rate of mass transfer between the phases, in the case of purely heterogeneous combustion.

For what follows, we need to determine the equations of state and the thermodynamic properties of the phases and the components. We postulate that the first phase and the fuel vapors consist of ideal gases, and that the second phase is an incompressible medium; then

$$\begin{aligned}
&i_{11} = c_{p1}(T_1 - T^\circ) + h_{11}^\circ, \quad p_{11} = \rho_{11}^\circ R_{11} T_1 \\
&i_2 = c_2(T_2 - T^\circ) + h_2^\circ + (p - p^\circ)/\rho_2^\circ, \quad \rho_2^\bullet = \text{const} \\
&i_{13} = c_{p3}(T_1 - T^\circ) + h_{13}^\circ, \quad p_{13} = \rho_{13}^\circ R_{13} T_1, \quad p = p_{11} + p_{13} \\
&i_{12}(p_s(T_2),\ T_2) = c_2(T_2 - T^\circ) + (p_s(T_2) - p^\circ)/\rho_2 + h_2^\circ + L_2(T_2), \quad p_s = \rho_{12}^\circ R_{12} T_2
\end{aligned} \tag{3.13}$$

where $h_i$ (i = 11, 13, 2) are the enthalpies of the components at $T = T^\circ$; $p = p^\circ$; $c_{p1} = c_{p3}$ are the mean (in the range from $T^\circ$ and $T_1$) specific heat capacities at constant pressure; $c_2$ is the specific heat capacity of the second

phase; $l_2(T_2)$ is the heat of vaporization; $\rho_{12}^\circ$ is the true density of the saturated vapor. For a majority of substances, the pressure of the saturated vapor is a function of the temperature of the particles, which is well described by the formula

$$p_s = p^* \exp(-T^*/T_2) \tag{3.14}$$

where $p^*$ and $T^*$ are empirical constants.

In accordance with (2.13), (3.13), the heat of the chemical reaction at $T_1 = T_2 = T^\circ$, and $p = p^\circ$, is determined by the formula

$$Q^\circ = \nu_{11}(h_{11}^* - h_{13}^\circ) + \nu_2(h_2^\circ - h_{13}^\circ) \tag{3.15}$$

### 4. Equations of One-Dimensional Fully Established Motion in the Case of Purely Heterogeneous Combustion Conditions. We go over to dimensionless variables

$$P = \frac{p}{p_0}, \quad U_i = \frac{v_i}{a_0}, \quad \theta_i = \frac{T_i}{T_0}, \quad M_k = \frac{m_k}{m_{110}}$$

$$(a_0 = \gamma_{10}p_0/\rho_{10}^\circ, \quad m_1 = \rho_1 v_1, \quad m_2 = \rho_2 v_2, \quad m_{11} = \rho_{11}v_1, \quad m_{13} = \rho_{13}v_1, \quad i = 1, 2; \quad k = 1, 11, 13, 2) \tag{4.1}$$

where the subscript 0 denotes that the corresponding parameter is taken in some fixed state, i.e., ahead of the front of the reaction, in an unperturbed state, which is assumed to be equilibrium $(v_1 = v_2 = v_0, T_1 = T_2 = T_0)$; $\alpha_0$ is the velocity of sound in the first phase; $\gamma_{10}$ is the adiabatic index of the first phase.

We introduce the reduced thermodynamic parameters

$$\lambda_k^* = \frac{\lambda_k T_0}{\rho_{10}^\circ a_0^3}, \quad C_1 = \frac{c_{p1}}{\gamma_{10}R_{10}}, \quad C_2 = \frac{c_2}{\gamma_{10}R_{10}}, \quad C_3 = \frac{c_{p3}}{\gamma_{10}R_{10}}, \quad Q^* = \frac{Q^\circ}{a_0^2} \tag{4.2}$$

as well as reduced terms, reflecting the phase interaction

$$J^* = \frac{J}{m_{10}}, \quad f^* = \frac{f}{m_{10}a_0}, \quad q^* = \frac{q_{12}}{\rho_{10}^\circ a_0^3} \tag{4.3}$$

In the case of the combustion of sufficiently large particles $(d_0 \geq 5~\mu)$, it is usually possible to neglect the velocities $w_{11}$ and $w_{13}$, characterizing the mutual diffusion of the gaseous components of the first phase in comparison with the velocities $v_1$ and $v_2$. Therefore, from Secs. 1 and 2, we obtain

$$\frac{dM_{11}}{dx} = -\nu_{11}J^*, \quad \frac{dM_2}{dx} = -\nu_2 J^*, \quad \frac{dM_{13}}{dx} = (\nu_{11} + \nu_2)J^*$$

$$M_1\frac{dU_1}{dx} + \frac{\alpha_1}{\alpha_{10}\gamma_{10}U_0}\frac{dp}{dx} = f_1^*, \quad M_2\frac{dU_2}{dx} + \frac{\alpha_2}{\alpha_{10}\gamma_{10}U_0}\frac{dP}{dx} = f^*$$

$$\frac{\lambda_1^*}{U_0}\frac{d\vartheta}{dx} - \frac{rM_2}{\gamma}\frac{dP}{dx} - M_1U_1\frac{dU_1}{dx} - M_2U_2\frac{dU_2}{dx} = b_3 \tag{4.4}$$

$$M_2\left[C_2 + \frac{dC_2}{d\theta_2}(\theta_2 - \theta^\circ)\right]\frac{d\theta_2}{dx} = b_5, \quad \frac{d\theta_1}{dx} = \vartheta$$

$$P\alpha_1\frac{dU_1}{dx} + \frac{\alpha_2PU_1}{U_2}\frac{dU_2}{dx} + \alpha_1U_1\frac{dP}{dx} = b_4$$

Here

$$f_1^* = -f^* + \nu_2 J^*(U_2 - U_1), \quad b_3 = \nu_1 J^*(C_3 - C_1)(\theta_1 - \theta^\circ)$$

$$+ \nu_2 J^*\left[C_3(\theta_1 - \theta^\circ) - C_2(\theta_2 - \theta^\circ) + \frac{U_1^2 - U_2^2}{2}\right] - J^*Q^* + (M_{11}C_1 + M_{13}C_3)\vartheta$$

$$- \frac{\vartheta^2}{U_0}\frac{d\lambda_1^*}{d\theta_1} + \frac{\vartheta J^*(\nu_{13}M_{11} + \nu_{11}M_{13})}{U_0M_1^2}(\lambda_{11}^* - \lambda_{13}^*) + \left(M_{11}\frac{dC_1}{d\theta_1} + M_{13}\frac{dC_3}{d\theta_1}\right)$$

$$\times (\theta_1 - \theta^\circ)\vartheta + b_5, \quad b_5 = \frac{1}{U_0}q^* + J^*Q^* + J^*(\theta_2 - \theta^\circ)[\nu_{11}(C_1' - C_3') + \nu_2(C_2 - C_3')]$$

$$b_4 = \alpha_{10}U_0\theta_1 J^*\left[\frac{g_{11}}{g_{13}}(\nu_{11} + \nu_2) - \nu_{11}\right] - \frac{\alpha_2PU_1}{M_2}\nu_2 J^* \tag{4.5}$$

$$+ \alpha_0U_0\left(M_{11} + \frac{g_{11}}{g_{13}}M_{13}\right)\vartheta \qquad (r = \rho_{110}^\circ/\rho_2^\circ, \quad C_1' = C_1(\theta_2), \quad C_3' = C_3(\theta_2))$$

The last equation of (4.4) is the equation of state of the first phase in differential form.

The system (4.4) has four primary integrals

$$M_{11} + M_2 + M_{13} = S_1, \quad M_{11} - \frac{\nu_{11}}{\nu_2}M_2 = S_4, \quad M_1U_1 + M_2U_2 + \frac{P}{\alpha_{10}\gamma_{10}U_0} = S_2$$

$$\frac{\lambda_1^*}{U_0}\vartheta - \frac{M_1U_1^2}{2} - \frac{M_2U_2^2}{2} - (M_{11}C_1 + M_{13}C_3)(\theta_1 - \theta^\circ) - M_2C_2(\theta_2 - \theta^\circ) - M_2\frac{r}{\gamma_{10}}(P - 1) + M_{13}\frac{\nu_2 r}{\gamma_{10}\nu_{13}} + M_{13}\frac{Q^*}{\nu_{13}} = S_3$$

$$\left(M_{11} + M_{13} = M_1, \quad \alpha_2 = 1 - \alpha_1 = r\alpha_{10}U_0\frac{M_2}{U_2} = \frac{\alpha_{20}U_{20}}{M_{20}}\frac{M_2}{U_2}\right) \tag{4.6}$$

Solving system (4.4) with respect to derivatives, we obtain

$$\frac{dM_{11}}{dx} = -\nu_1 J^*, \qquad \frac{dM_2}{dx} = -\nu_2 J^*, \qquad \frac{dM_{13}}{dx} = \nu_{13} J^*$$

$$\frac{dU_1}{dx} = \frac{1}{M_1}\left(f_1^* - \frac{\alpha_1}{\alpha_{10}\gamma_{10}U_0}\frac{\Delta_p}{\Delta}\right), \qquad \frac{dU_2}{dx} = \frac{1}{M_2}\left(f^* - \frac{\alpha_2}{\alpha_{10}\gamma_{10}U_0}\frac{\Delta_p}{\Delta}\right)$$

$$\frac{d\theta_1}{dx} = \vartheta, \qquad \frac{d\theta_2}{dx} = \frac{b_5}{M_2 C_2}, \qquad \frac{dP}{dx} = \frac{\Delta_p}{\Delta}$$

$$\frac{d\vartheta}{dx} = \frac{U_0}{\lambda_1^*}\left[(b_3 + U_1 f_1^* + U_2 f^*) - \left(\frac{\alpha_1}{\alpha_{10}\gamma_{10}U_0}U_1 + \frac{\alpha_2}{\alpha_{10}\gamma_{10}U_0}U_2 - \frac{r}{\gamma_{10}}M_2\right)\frac{\Delta_p}{\Delta}\right]$$

$$\left(\Delta = \alpha_1 U_1 M_1 - \frac{P\alpha_1^2}{\alpha_{10}\gamma_{10}U_0} - \frac{rPU_1\alpha_2 M_1}{\gamma_{10}U_2^2}, \quad \Delta_p = b_4 M_1 + \alpha_1 P f_1^* - \frac{r\alpha_{10}U_0 PU_1 M_1 f_1^*}{U_2^2}\right) \qquad (4.7)$$

Introducing the dimensionless variables

$$d^* = \frac{d}{d_0}, \qquad \mu^* = \frac{\mu_1}{\mu_0}, \qquad z^* = \frac{z}{a_0}, \qquad D_{11}^* = \frac{D_{11}}{a_0 d_0}, \qquad \theta_A = \frac{E}{RT_0} \qquad (4.8)$$

we obtain expressions for $f^*$, $q^*$, $J^*$

$$f^* = \frac{3}{4}\frac{r\alpha_{10}}{\alpha_1 d_0}\frac{U_0 M_2 M_1}{U_1 U_2}\frac{C_d}{d^*}\frac{(U_1 - U_2)^3}{|U_1 - U_2|}, \qquad q^* = \frac{6m_{10}}{\rho_2^0 d_0^2 \alpha_0}\frac{\lambda_1^* M_2}{d^{*2} u_2}N_{Nu}(\theta_1 - \theta_2)$$

$$J^* = \frac{6m_{10}}{\rho_{26}d_0\alpha_0}\frac{M_1 M_2}{L_1 U_1}\left[\frac{d^*}{N_{Nu}D_{11}^*} + \frac{\exp(\theta_A/\theta_2)}{z^*}\right]^{-1}$$

$$\left(\text{Re} = \frac{\rho^0{}_{10}a^0{}_0 d_0}{\mu_0}\frac{d^*}{\mu^*}\frac{\alpha_{10}M_1}{\alpha_1}\frac{U_0}{U_1}|U_1 - U_2|, \quad d^* = \left(\frac{M_2}{M_{20}}\right)^{1/3}\right) \qquad (4.9)$$

5. The Problem of the Normal Propagation of a Flame in a Gas Suspension. The flame front in a gas suspension is a region in which particles undergo preliminary heating, are ignited, and burn. It is always possible to indicate a region in which the rate of a chemical reaction is negligibly small, i.e., to introduce some temperature $T_b$ (or $\theta_b$) below which the chemical reaction does not proceed. The presence of $T_b$ (which may be arbitrarily called the ignition temperature, and which must be substantially lower than the temperature at which combustion takes place at an appreciable rate) is a necessary condition for singularity of the solution of the steady-state problem of the normal propagation of a flame [10]. This is bound up with the fact that the boundary conditions of the corresponding boundary value problem are given at singular points of the differential equations. In the case of the combustion of a gas suspension, the disclosure of these special characteristics is complicated by two-phase effects.

The above-mentioned boundary conditions characterize the state of the system before ($x = -\infty$, state 0) and after ($x = +\infty$, state e) of the reaction front. In the one-dimensional steady-state statement, the system of coordinates will be connected with the flame front, and the rate of propagation of the flame is determined by the velocity of the flow of fresh mixture ($x = -\infty$). From a mathematical point of view, the solution comes down to seeking the above velocity, $v_0$, (or $U_0$), which corresponds to solution of the steady-state equations satisfying the given boundary conditions at 0 and e.

We postulate that the conditions $U_1 = U_2$, $\theta_1 = \theta_2$ are satisfied in the states 0 and e; in addition, we assume that there is no third component (reaction products) ahead of the front. Thus, 0 and e are characterized by the parameters

$$P_0 = 1, \; U_0, \; \theta_0 = 1, \; M_{110}, \; M_{20}, \; M_{130} = 0, \; \vartheta = 0$$
$$P_e, \; U_e, \; \theta_e, \; M_{11e}, \; M_{2e}, \; M_{13e}, \; \vartheta_e = 0 \qquad (5.1)$$

The values of the parameters at the point e are determined from the given parameters at point 0 on the basis of the primary integrals (4.6), whence, if it is taken into account that $U_0 \ll 1$ (the velocity of the flame is considerably less than the velocity of sound), we have

$$P_e = 1, \quad \theta_e = 1 + \frac{M_{3e}Q^*}{\nu_{13}(M_{11e}C_1 + M_{13e}C_3 + M_{2e}C_2)}, \quad U_e = \alpha_0 U_0 \theta_e\left(M_{11e} + \frac{g_{11}}{g_{13}}M_{13e}\right) \qquad (5.2)$$

Since points 0 and e are singular points of the system of differential equations (4.4), or (4.7), we must investigate the asymptotic behavior of the integral curves in the neighborhood of 0 and e.

The vicinity of point 0 ($\theta < \theta_b$) is characterized by a zero combustion rate ($J^* = 0$). In addition, for sufficiently large particles, the change in their velocity and temperature may be neglected in comparison with the change in the corresponding parameters of the gas. Then

$$P = 1, \quad \theta_1 = 1 + (\theta_b - 1)\exp(C_1 U_0 x / \lambda_1^*), \; U_1 = U_0\theta_1$$
$$U_2 = U_0, \; \theta_2 = 1 \qquad (5.3)$$
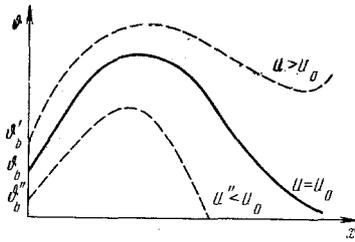
Fig. 1
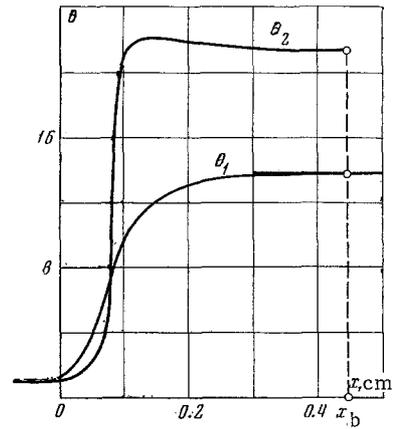


Fig. 2
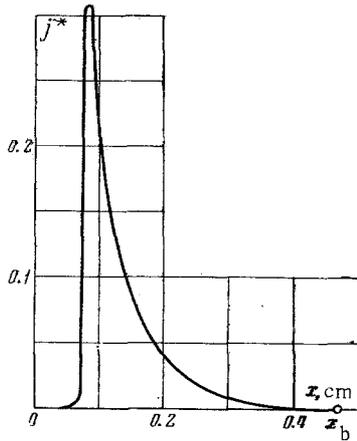


Fig. 3
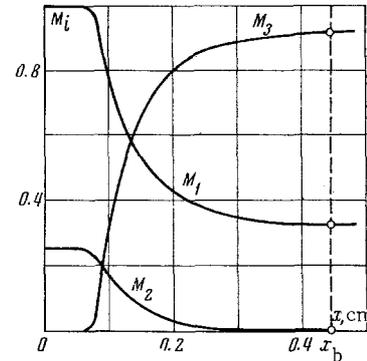


Fig. 4

The vicinity of point e is characterized by the asymptotic approach of the reaction rate to zero. As a first approximation, we shall assume that the reaction goes to completion, i.e., up to complete combustion of the fuel or the oxidizer, and that the combustion takes place under diffusion conditions $(k \gg \beta_1,\ N_{Nu} = 2)$, as a result of the rather high temperature. Under these conditions, we can isolate three cases, depending on the composition of the starting mixture.

1. A mixture of stoichiometric composition

$$M_{2\bullet} = \nu_2 / \nu_{11}, \quad M_{11e} = 0, \quad M_{2e} = 0, \quad M_{12e} = 1 + \nu_2 / \nu_{11} \tag{5.4}$$

in which the asymptotic behavior of the system in the vicinity of the point is described as follows:

$$M_2 = \frac{27 M_2{}^\circ}{[3 + (x - x^\circ)/\delta]^3} \qquad \left( \delta = \frac{d_0 U_e{}^2}{18 \alpha_0 U_0 \nu_2 r D_{11}* M_{12}{}^{2/3} M_2{}^{\circ 1/3}} \right)$$

$$\frac{U_2 - U_e}{U_2{}^\circ - U_e} = \exp\left[ c\left( \frac{1}{M_2{}^\circ} - \frac{1}{M_2} \right) \right] \qquad \left( c = \frac{3 \alpha_e U_e a_0 \mu_1}{2 \nu_2 D_{11}} \right)$$

$$\theta_2 - \theta_e = \left[ (\theta_2{}^\circ - \theta_e) \exp \frac{a}{M_2{}^\circ} - b \int_{M_2{}^\circ}^{M_2} \frac{1}{\xi} \exp \frac{a}{\xi} \, d\xi \right] \exp\left( -\frac{a}{M_2} \right) \tag{5.5}$$

$$\left( a = \frac{\lambda_1* \alpha_e \nu_{11} U_e}{d_0 \alpha_0 C_2 D_{11}* U_0}, \quad b = \frac{Q_2*}{\nu_2 C_2}, \quad Q_2* = Q* + (\theta_{2e} - \theta_0) [\nu_{11} (C_1' - C_3') + \nu_2 (C_2' - C_3')] \right)$$

where the degree signs denote the parameters of particles corresponding to some fixed state, serving as a starting point for the asymptotic solution. It follows from (5.5) that at $x \to \infty$, $M_2 \to 0$, $U_2 \to U_e$, $\theta_2 \to \theta_e$.

2. A mixture with an excess of oxidizer

$$M_{20} < \frac{\nu_2}{\nu_1}, \quad M_{11e} = M_{110} - \frac{\nu_{11}}{\nu_2} M_{20}, \quad M_{2e} = 0, \quad M_{13e} = \left( 1 + \frac{\nu_{11}}{\nu_2} \right)$$

$$\frac{M_2}{M_2{}^\circ}=\left(\frac{x_\delta-x}{x_\delta-x^\circ}\right)^{3/2},\quad \frac{U_e-U_2}{U_e-U_2{}^\circ}=\left(\frac{M_2}{M_2{}^\circ}\right)^c,\quad \frac{\theta_2-\theta_{2e}}{\theta_2{}^\circ-\theta_{2e}}=\left(\frac{M_2}{M_2{}^\circ}\right)^a \qquad (x\leqslant x_\delta)$$

$$\left(c=\frac{3\mu_{10}\nu_{11}\alpha_e}{2m_{110}d_0\nu_2 D_{11}{}^*}\frac{\mu^* U_e}{M_{11e}},\quad a=\frac{\lambda_1{}^*\alpha_e\nu_{11}U_e}{d_0\alpha_0 C_2 D_{11}{}^* U_0 M_{11e}},\quad \theta_{2e}=\theta_e+\frac{Q_2{}^*}{\nu_2 C_2}\right.$$

$$\left. x_\delta=x^\circ+\left(\frac{M_2{}^\circ}{M_{20}}\right)^{1/2}\frac{\nu_{11}\alpha_e U_e{}^2 d_0}{8\alpha_0 r U_0\nu_2 D_{11}{}^* M_{11e}}\right) \tag{5.6}$$

It follows from Eqs. (5.6) that at $x\to x_\delta$, $M_2\to 0$, $U_2\to U_e$, $\theta_2\to\theta_{2e}\neq\theta_e$; this means that the temperature of the particles, in distinction to their velocity, cannot be equated with the temperature of the gas at the moment of their complete combustion.

### 3. A mixture with an excess of fuel

$$M_{20}>\frac{\nu_2}{\nu_{11}},\quad M_{11e}=0,\quad M_{2e}=M_{20}\frac{\nu_2}{\nu_{11}}M_{110},\quad M_{13e}=M_{110}\left(1+\frac{\nu_2}{\nu_{11}}\right)$$

$$\frac{M_2-M_{2e}}{M_2{}^\circ-M_{2e}}=\exp\left(-\frac{x-x^\circ}{\delta}\right),\quad \frac{U_e-U_2}{U_e-U_2{}^\circ}=\left(\frac{M_2-M_{2e}}{M_2{}^\circ-M_{2e}}\right)^c$$

$$\frac{\theta_2-\theta_e}{\theta_2{}^\circ-\theta_e}=\left(\frac{M_2-M_{2e}}{M_2{}^\circ-M_{2e}}\right)^a+\frac{b(M_{20}{}^\circ-M_{2e})}{(a-1)(\theta_2{}^\circ-\theta_e)}\left[\frac{M_2-M_{2e}}{M_2{}^\circ-M_{2e}}-\left(\frac{M_2-M_{2e}}{M_2{}^\circ-M_{2e}}\right)^a\right]$$

$$\left(c=\frac{3\mu_{10}}{2m_{110}d_0}\frac{\mu^*\alpha_e U_e}{D_{11}{}^* M_{2e}},\quad a=\frac{\lambda_1{}^*\alpha_e U_e}{d_0\alpha_0 C_2 D_{11}{}^* M_{2e}},\quad b=\frac{Q_2{}^*}{\nu_2 C_2 M_{2e}},\quad \delta=\frac{d_0\alpha_e U_e{}^2}{12x_0 r U_0 D_{11}{}^* M_{20}{}^{2/3}M_{2e}{}^{1/3}}\right) \tag{5.7}$$

From Eqs. (5.7) it follows that at $x\to\infty$, $M_2\to M_{2e}$, $U_2\to U_e$, $\theta_2\to\theta_e$.

**6. Calculation of the Structure of a Reaction Front in a Gas Suspension.** The parameters in a reaction front vary continuously; the state of the system ahead of the front ($x=-\infty$) and behind the front ($x=+\infty$ or $x=x_\delta$) is known. To find the corresponding integral curve numerically, it is necessary to carry out ranging with respect to the parameter $U_0$ (the eigenvalue of the problem). Since the integral curves permit displacement along the x axis, for $x=0$, we fix some value of $\theta_b$, which is such that $1<\theta_b<\theta_e$; $\theta_b$ must be taken close enough to unity so that the asymptotic solution (5.3) is satisfied in the region $x\leq 0$. At $x=0$, the solutions yield parameters of the system which are used as starting conditions for solution of the Cauchy problem at $x>0$.

Further, we select $U_0$ in such a manner that, with integration of the system to the right of $x=0$, the values of the parameters at the limit ($x\to\infty$ or $x\to x_\delta$) arrive at values corresponding to the state e, i.e., $\vartheta_e=0$ (see Fig. 1, which shows the typical course of the integral curves in the plane $x\vartheta$, where $\vartheta$ is the temperature gradient), here

$$\vartheta_b=C_1 U_0(\theta_b-1)/\lambda_1{}^* \tag{6.1}$$

The solutions of (5.5)-(5.7) are used to determine the asymptotic behavior of the particles. Numerical solution of the system of equations (4.7) was carried out in an electronic computer, using the Runge-Kutta method; in this case, the integrals (4.6) were used to verify the accuracy of the computations.

**7. Results of Calculations.** As an example, a study was made of the combustion of particles of carbon (electrode carbon) in an oxygen atmosphere. It was assumed that [11, 12] a chemical reaction of complete combustion takes place under purely heterogeneous conditions

$$O_2+C=CO_2 \tag{7.1}$$

Figures 2-5 give the results of a numerical integration, reflecting the structure of the reaction front ($v_0=17.8$ cm/sec) in a gas suspension with a starting composition $M_{20}=0.25$ (excess of oxidizer) and an initial particle size $d_0=50\ \mu$, with the following thermodynamic data:

$$p_0=1_{\text{atm}},\quad T_0=300^\circ\text{ K},\quad \gamma_{10}=1.41,\quad \rho_{10}{}^\bullet=0.131\cdot 10^{-2}\text{ g/cm}^3$$
$$\rho_2{}^\circ=1.5\text{ g/cm}^3,\quad c_{p1}=0.915\text{ J/g}\cdot\text{deg},\quad c_2=0.714\text{ J/g}\cdot\text{deg}$$
$$c_{p3}=0.84\text{ J/g}\cdot\text{deg},\quad \lambda_{11}{}^\circ=5.89\cdot 10^{-5}\text{ cal/cm}\cdot\text{sec}\cdot\text{deg}$$
$$\lambda_{13}{}^\circ=3.28\cdot 10^{-5}\text{ cal/cm}\cdot\text{sec}\cdot\text{deg},\quad D_{110}=0.186\text{ cm}^2/\text{sec}$$
$$\mu_{11}{}^\circ=202\cdot 10^6\text{g/cm}\cdot\text{sec},\quad \mu_{13}{}^\circ=146\cdot 10^{-6}\text{ g/cm}\cdot\text{sec},\quad Q^\circ=94052\text{ cal}.$$

The dependence of the thermodynamic coefficients ($c_p$, $\lambda$, D, $\mu$) on the temperature was taken in accordance with [13]. As a result of the small velocity effects in the combustion front ($N_{Re}<1$), the Stokes friction law may be used in the form $C_d=24/N_{Re}$. The corresponding kinetic constants (see (3.12)) were taken from [11], equal to $E=4\cdot 10^4$ cal/mole, $x=5\cdot 10^9$ cm/sec.

It follows from the curves that, at the start, in a certain region there is a gradual heating-up of the particles (Fig. 2) due to heat transfer with the gas which, in turn, is heated by heat transfer from a zone
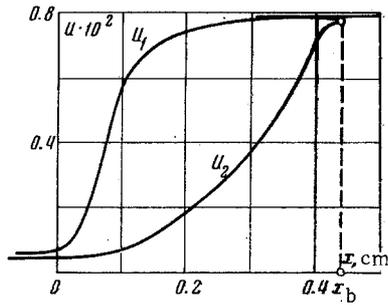
Fig. 5
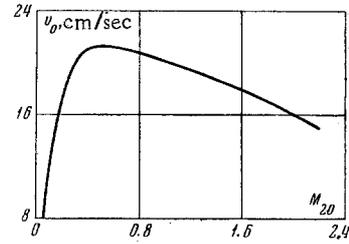


Fig. 6
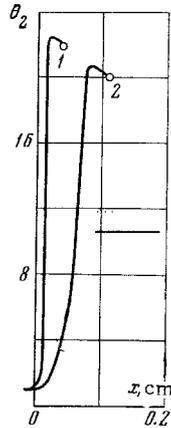


Fig. 7
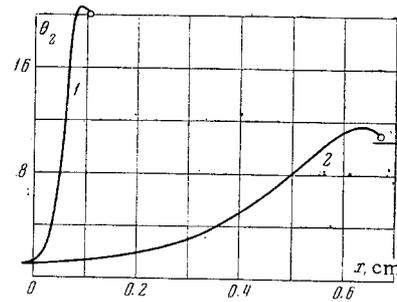


Fig. 8
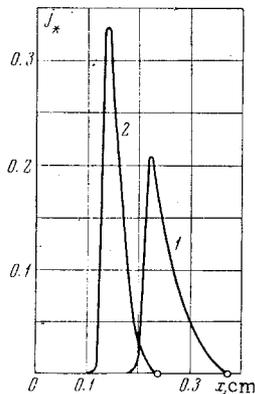


Fig. 9
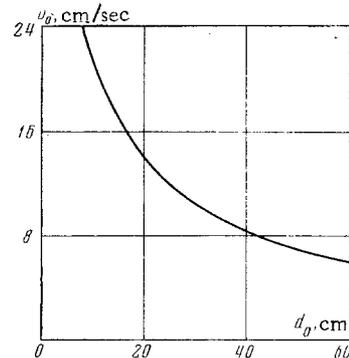


Fig. 10

with a higher temperature. In this region, the rate of the reaction J* (Fig. 3) is small. Further on, the reaction rate starts to rise appreciably and becomes so great that the heat evolved in the particles cannot be removed into the gas, and the particles start to heat up spontaneously. This heating up constitutes ignition of the particles. As the result of ignition, the particles attain their highest temperature. The slowing down of the rise in the temperature of the particles and the formation of a maximum of the curve of $\theta_2(x)$ is explained by a decrease in the reaction rate resulting from a decrease (Fig. 4) in the mass of carbon (curve $M_2(x)$) and oxygen (curve $M_1(x)$) present. After the particles have attained their maximal temperature, further combustion takes place in the diffusion region.

The change in the temperature of the gas in the reaction front is described by the curve of $\theta_1(x)$ on Fig. 2, which has a point of inflection corresponding to the maximal value of the temperature gradient $\vartheta$ (see the curve of $\vartheta(x)$). Up to the point of inflection, each element of the gas is a heat sink, i.e., it receives from hotter elements a greater amount of heat than it gives up to colder elements; after the point of inflection, the element of the gas is transformed into a heat source, i.e., it gives up to colder elements a greater amount of heat than it receives from hotter elements.

Acceleration of the gas (the curve of $U_1(x)$ on Fig. 5) takes place as the result of thermal expansion. The velocity of the particles themselves (the curve of $U_2(x)$) varies only under the action of the force of friction. After the relative velocity becomes sufficiently great, the particles are entrained into the motion of the gas; this process is reinforced with combustion of the particles. As a result of the small velocities, the pressure in the reaction front is practically invariable.

Figure 6 shows the effect of the composition ($M_{20}$) of the initial mixture (the other parameters are the same as those given at the beginning of this section) on the rate of propagation of a flame in the mixture. The maximum of the curve is located not at the stoichiometric composition ($M_{20} = 0.375$), but is shifted somewhat toward the side of mixtures richer in fuel, and occurs at a value of $M \approx 0.5$. This fact is explained, above all, by an increase in the total reaction surface in richer mixtures. An anlogous shift has been observed also with the combustion of homogeneous mixtures [11].

It must be noted that, generally speaking, the combustion of carbon is accompanied by secondary reactions which, in the final analysis, lead to the formation of carbon monoxide, CO [11]. This situation is particularly important for mixtures with a composition close to the stoichiometric, whose combustion takes place at higher temperatures, and for mixtures with a large excess of fuel. The formation of carbon monoxide during the combustion process must inevitably be taken into account, and must lead to a decrease in the equilibrium temperature $T_e$, and, consequently, to a change in the rate of propagation of the reaction front.

Figures 7 and 8 give the dependences of the temperature of the particles, $\theta_2(x)$ for different values of the kinetic constants z and E. The results given correspond to an initial diameter $d_0 = 5\ \mu$, and to a density of the material of the particles $\rho_2{}^\circ = 2.2$ g/cm$^3$, typical of graphite, as well as to $M_{20} = 0.154$. It is evident from the curves that a decrease in the pre-exponential factor from $z = 5 \cdot 10^9$ cm/sec to $z = 5 \cdot 10^6$ cm/sec, at $E = 4 \cdot 10^4$ cal/mole (curves 1 and 2 in Fig. 7), leads to a longer lag in ignition of the particles and, by virtue of this, to a decrease in the rate of propagation of the flame from $v_0 = 29$ cm/sec to $v_0 = 11.2$ cm/sec. However, in both cases, there are regions in which the temperatures of the gas and of the particles differ considerably, i.e., there are two-temperature effects. An increase in the activation energy from $E = 4 \cdot 10^4$ cal/mole to $E = 5 \cdot 10^4$ cal/mole, at $z = 5 \cdot 10^6$ cm/sec (curves 1 and 2 in Fig. 8), leads to qualitative changes. In this case, the combustion takes place in the kinetic region, which leads to a significant increase in the thickness of the reaction front, and to a decrease in the rate of propagation from $v_0 = 29$ cm/sec to $v_0 = 4.3$ cm/sec. In this case, the difference in the temperatures of the gas and the particles over the whole length of the front is not great (i.e., the two-temperature effects are less considerable). In this case, generally speaking, it has no meaning to talk about ignition of the particles, since the temperature of the particles varies rather smoothly along the whole length of the front.

The same may be said about the value of the two-velocity effects. In the case when the particles burn in the kinetic region, their effect is not great. At the same time, with combustion in the diffusion region, the relative rate of movement (in spite of the small dynamic effects) of the particles and the gas ($N_{Re} \sim 1$) leads to higher rates of heat and mass transfer between the gas and the particles. This is illustrated in Fig. 9, which gives dependences of $J^*(x)$, obtained by calculation using the single-velocity approximation ($v_1 = v_2$, curve 1) and with the friction law $C_d = 24/Re$ (curve 2), with the following values of the parameters:

$$M_{20} = 0.154, \quad d_0 = 25\ \mu,$$
$$z = 5 \cdot 10^6\ \text{cm/sec}, \quad E = 4 \cdot 10^4\ \text{cal/mole}.$$

In this case, failure to take account of two-velocity effects leads to a lowering of the velocity of the flame to 6.6 cm/sec, in comparison with 11.8 cm/sec. The effect of two-velocity effects assumes more importance the larger the particle diameter. Thus, at $d_0 = 50\ \mu$, the single-velocity approximation gives $v_0 = 3.9$ cm/sec, instead of the value $v_0 = 6.9$ cm/sec given by the two-velocity model.

Figure 10 shows the dependence of the rate of propagation of the front on the initial particle diameter, with a fixed composition of the fresh mixture ($M_{20} = 0.154$). The fact of a decrease in the velocity ($v_0 \sim d_0{}^{-m}$, $m = 0.5$–$0.8$) is explained by the fact that, with an increase in the particle size, there is an increase in the combustion time of a fixed mass of fuel. The result obtained is in qualitative agreement with the results of [1]. This same article gives data on the propagation of a flame in a gas-carbon mixture at atmospheric pressure, with reference to a graphite-oxygen mixture. The mixture consisted of graphite dust ($d_0 \leq 5\ \mu$) and oxygen, in the amount of 1 liter per 0.2 g graphite (this corresponds to $M_{20} = 0.154$). From a comparison of experimental data and the data of the present article, a conclusion may be drawn with respect to

their qualitative agreement. However, for a quantitative comparison, we need a complete solution of the inverse problem of the theory of combustion and, consequently, a more broadly determined and accurate set of experimental data.

LITERATURE CITED

1. I. O. Leipunskii, "The pressure dependence of the combustion of black powder on pressure," Zh. Fiz. Khim., 34, No. 1 (1960).
2. É. N. Rumanova and B. I. Khaikin, "Critical conditions for the autoignition of an accumulation of particles," Fizika Goreniya i Vzryva, 5, No. 1 (1969).
3. L. A. Klachko, "Ignition of an accumulation of particles with a heterogeneous reaction," Teploénergetika, No. 8 (1966).
4. T. H. Burgoyne and L. Cohen, "The effect of drop size on flame propagation in liquid aerosols," Proc. Roy. Soc., A255, No. 1162, 357-392 (1954).
5. F. A. Williams, "Spray combustion theory," Combustion and Flame, No. 2, pp. 215-228 (1959).
6. R. I. Nigmatulin, "Equations of the hydromechanics and for a compression wave in a two-velocity and two-temperature medium with phase transitions," Izv. Akad. Nauk SSSR, Mekhan. Zhidk. i Gaza, No. 5 (1967).
7. R. I. Nigmatulin, Methods in the mechanics of a continuous medium for the description of multiphase media," Prikl. Mat. i Mekhan., 34, No. 6 (1970).
8. R. I. Nigmatulin, "Small-scale flows and surface effects in the hydromechanics of multiphase media," Prikl. Mat. i Mekhan., 35, No. 3 (1971).
9. G. A. Varshavskii, "The combustion of drops of liquid fuel," Tr. NII-1, No. 6 (1945).
10. D. A. Frank-Kamenetskii, Diffusion and Heat Transfer in Chemical Kinetics [in Russian], Izd. Nauka, Moscow (1967).
11. L. N. Khitrin, The Physics of Combustion and Explosion [in Russian], Izd. MGU, Moscow (1957).
12. B. V. Kantorovich, "Problems in the Theory of the combustion of a flow of fuel," in: The Combustion of Two-Phase Systems [in Russian], Izd. Akad. Nauk SSSR, Moscow (1958).
13. Chemist's Handbook [in Russian], Izd. Goskhimizdat, Moscow-Leningrad (1962-1964).