

Ignition of a Cloud of Metal Particles in the Continuum Regime.

I. Adiabatic Flow

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A mathematical model is proposed to describe the motion of a mixture of a gas and reactive metal particles in the two-velocity, two-temperature approximation of mechanics of heterogeneous media. As an application of this model, a theory of wave ignition in a mixture of a gas and magnesium particles is developed, which extends N. N. Semenov's theory of thermal explosion to the case of a moving cloud of particles. A classification of the types of mixture flows behind the shock-wave front is given. The calculated induction period of the cloud correlates with experimental data. Stable propagation of a steady ignition wave and the possibility of its initiation are demonstrated.

1. GOVERNING EQUATIONS

We consider a unit volume of the mixture, which is filled by a gas and solid particles of a metal covered by an oxide film. We confine ourselves to the plane one-dimensional case, where all the parameters of the gas mixture depend on the spatial coordinate and time. We assume that the following components are present in the mixture: the gas phase including an oxidizer (subscript 11), an inert gas (12), and gaseous products of metal oxidation (13) and the disperse phase including a metal (22), which enters a heterogeneous chemical reaction with the oxidizer, and a condensed product of this reaction in the form of an oxide film (23). We write the following conservation equations for the mean parameters of the phases [1, 2]:

$$\begin{aligned} \frac{\partial \rho_1}{\partial t} + \frac{\partial \rho_1 u_1}{\partial x} &= \bar{\nu}_2 J, \\ \frac{\partial \rho_2}{\partial t} + \frac{\partial \rho_2 u_2}{\partial x} &= -\bar{\nu}_2 J \end{aligned} \quad (1.1)$$

for mass conservation,

$$\begin{aligned} \frac{\partial \rho_1 u_1}{\partial t} + \frac{\partial (\rho_1 u_1^2 + m_1 p)}{\partial x} &= p \frac{\partial m_1}{\partial x} + \bar{\nu}_2 J u_2 + R_1, \\ \frac{\partial \rho_2 u_2}{\partial t} + \frac{\partial (\rho_2 u_2^2 + m_2 p)}{\partial x} &= p \frac{\partial m_2}{\partial x} - \bar{\nu}_2 J u_2 + R_2 \end{aligned} \quad (1.2)$$

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for momentum conservation, and

$$\begin{aligned} \frac{\partial \rho_1 E_1}{\partial t} + \frac{\partial (\rho_1 u_1 E_1 + m_1 u_1 p)}{\partial x} &= -p \frac{\partial m_1}{\partial t} \\ &+ \bar{\nu}_2 J \left[-\chi_1 + h_1 + \frac{u_2^2}{2} \right] + Q_1 + R_1 (\beta u_1 + \bar{\beta} u_2), \\ \frac{\partial \rho_2 E_2}{\partial t} + \frac{\partial (\rho_2 u_2 E_2 + m_2 u_2 p)}{\partial x} &= -p \frac{\partial m_2}{\partial t} \\ &+ \bar{\nu}_2 J \left[-\chi_2 - h_2 - \frac{u_2^2}{2} \right] + Q_2 + R_2 (\beta u_1 + \bar{\beta} u_2) \end{aligned} \quad (1.3)$$

for energy conservation. Here ρ_i , u_i , E_i , h_i , and m_i are the mean density, velocity, total energy, enthalpy, and volume concentration of the i th phase, p is the pressure in the mixture, and R_i and Q_i are the terms defining the force and thermal interaction of the phases. The remaining notation is explained below.

The kinetic equations for the gas phase are

$$\rho_1 \frac{d_1 \xi_{11}}{dt} = -(\nu_{11} + \bar{\nu}_2 \xi_{11}) J,$$

$$\frac{\nu_{11} + \bar{\nu}_2 \xi_{11}}{\nu_{11} + \bar{\nu}_2 \xi_{11,0}} = \frac{\xi_{12}}{\xi_{12,0}}, \quad \xi_{11} + \xi_{12} + \xi_{13} = 1,$$

where $\xi_{1j} = \rho_{1j}/\rho_1$ is the mass fraction of the j th component of the gas phase.

We write the kinetic equations for the disperse phase in the form of the integrals

$$\frac{\xi_{22}(\alpha_\nu - \xi_{22,0})}{\xi_{22,0}(\alpha_\nu - \xi_{22})} = \left(\frac{r}{r_0}\right)^3, \quad \xi_{22} + \xi_{23} = 1,$$

where $\xi_{2j} = \rho_{2j}/\rho_2$, $\alpha_\nu = \nu_{22}/\bar{\nu}_2$, and $\bar{\nu}_2 = \nu_{22} - \nu_{23}$. Here ν_{ij} are stoichiometric coefficients of the oxidation reaction, which satisfy the relation

$$\nu_{11} + \nu_{22} = \nu_{13} + \nu_{23},$$

and r is the radius of the metal core of the particle, which is related to the total radius of the particle $R = r + h$ (h is the oxide film thickness) through the integral

$$R^3 - R_0^3 = a(r^3 - r_0^3)$$

($a = 1 - \nu_{23}\rho_{22}^0/\bar{\nu}_2\rho_{23}^0$). The following expression is valid for the source term J :

$$J = -\frac{3\rho_{22}}{r\nu_{22}}\frac{d_2r}{dt}.$$

We use the following closing relations:

— the caloric equation of state in the form

$$(p = \mathcal{R}T_1\rho_1^0),$$

where

$$\mathcal{R} = \mathcal{R}_\mu \sum_{i=1}^3 \frac{\xi_{1i}}{\mu_i} = \sum_{i=1}^3 \xi_{1i}\mathcal{R}_{1i}$$

(\mathcal{R}_μ is the universal gas constant) and

$$\rho_1^0 = \rho_1/m_1, \quad m_1 + m_2 = 1, \quad m_2 = 4/3\pi R^3 n;$$

— the thermal equations of state for internal energies of the phases

$$e_1 = \sum_{i=1}^3 \xi_{1i}e_{1i}, \quad e_{1i} = c_{v,1i}(T_1 - T_0) + e_{1i}^0,$$

$$e_2 = \sum_{j=2}^3 \xi_{2j}e_{2j}, \quad e_{2j} = c_{v,2j}(T_2 - T_0) + e_{2j}^0;$$

— the relationships between the enthalpies and internal energies in the form

$$h_{1i} = e_{1i} + \frac{p_{1i}}{\rho_{1i}} = c_{p,1i}(T_1 - T_0) + h_{1i}^0,$$

$$h_{1i}^0 = e_{1i}^0 + \mathcal{R}_{1i}T_0 \quad (i = 1, 2, 3);$$

— the condition of incompressibility of the particles

$$\rho_{2j}^0 = \text{const} \quad (j = 2, 3).$$

Here $c_{p,1i}$ is the heat capacity of the i th component of the gas phase at constant pressure, $c_{v,1i}$ is the same at constant volume, and $c_{v,2j} = c_{p,2j}$ is the heat capacity of the j th component of the disperse phase.

In Eqs. (1.2) and (1.3), the conditions $R_1 = -R_2$ and $Q_1 = -Q_2$ are imposed on the functions R_i and

Q_i (see also below); the expression $E_i = e_i + u_i^2/2$, where e_i is the internal energy, is valid for the total energy of a phase. The quantity β defines the fraction of heat released in the disperse phase due to the work of the friction force, and $\bar{\beta} = 1 - \beta$ is a similar quantity for the gas phase. The parameters χ_1 and χ_2 are the accommodation coefficients and allow for distribution of the heat of the chemical reaction between the phases. The values of χ_i are found from the following condition of conservation of the total energy of the mixture:

$$\chi_1 + \chi_2 = h_1 - h_2.$$

By definition, the heat of the chemical reaction is

$$q_* = \nu_{11}h_{11} + \nu_{22}h_{22} - \nu_{13}h_{13} - \nu_{23}h_{23}$$

with $\alpha_q q_*$ going to the gas and $(1 - \alpha_q)q_*$ going to the particles. Here α_q is the fraction of the heat of chemical reaction that goes to the gas. We can easily obtain the following expressions

$$\chi_1 = [-\alpha_q q_* + (\nu_{11} + \bar{\nu}_2 \xi_{11})h_{11} + \bar{\nu}_2 \xi_{12}h_{12} - (\nu_{13} - \bar{\nu}_2 \xi_{13})h_{13}]/\bar{\nu}_2,$$

$$\chi_2 = h_1 - h_2 - \chi_1.$$

In contrast to [1], the heat of the chemical reaction is distributed between the phases in the present model in accordance with the quantity α_q . In addition, it is not assumed here that the total radius of the particle remains constant, which is important for slow oxidation processes proceeding in the medium.

In accordance with [3], we perform a thermodynamic analysis of the mathematical model proposed. For this purpose, we introduce the specific entropy of the mixture

$$\rho S = \rho_1 S_1 + \rho_2 S_2,$$

where S_1 and S_2 are the specific entropies of the phases. This allows us to find the particle derivative of S , which characterizes the variation of entropy in a constant-mass volume of a two-phase medium:

$$\rho \frac{DS}{Dt} = \rho_1 \frac{d_1 S_1}{dt} + \rho_2 \frac{d_2 S_2}{dt} - \bar{\nu}_2 J(S_2 - S_1).$$

Here, we take into account the equations of mass conservation (1.1) for each phase. Assuming local thermodynamic equilibrium within each phase, we can use the Gibbs relations

$$\rho_i T_i \frac{d_i S_i}{dt} = \rho_i \frac{d_i e_i}{dt} - \frac{m_i p}{\rho_i^0} \frac{d_i \rho_i^0}{dt} \quad (i = 1, 2),$$

whose right sides can be determined using the following equations of heat addition to the phases:

$$\begin{aligned} \rho_1 \frac{d_1 e_1}{dt} - \frac{m_1 p}{\rho_1^0} \frac{d_1 \rho_1^0}{dt} &= R_1 \beta (u_2 - u_1) \\ &+ \bar{v}_2 J \left[-\chi_1 + \frac{(u_2 - u_1)^2}{2} \right] + Q_1, \\ \rho_2 \frac{d_2 e_2}{dt} - \frac{m_2 p}{\rho_2^0} \frac{d_2 \rho_2^0}{dt} &= R_1 \beta (u_2 - u_1) \\ &- \bar{v}_2 J \chi_2 + Q_1. \end{aligned}$$

As a result, we find the change in the entropy of the mixture

$$\begin{aligned} \rho \frac{DS}{Dt} &= \left(\frac{\bar{\beta}}{T_1} + \frac{\beta}{T_2} \right) R_1 (u_2 - u_1) + Q_1 \left(\frac{1}{T_1} - \frac{1}{T_2} \right) \\ &- \bar{v}_2 J \left[-S_2 + S_1 + \frac{\chi_1}{T_1} + \frac{\chi_2}{T_2} - \frac{(u_2 - u_1)^2}{2T_1} \right] \\ &= \rho \frac{D^{(i)}S}{Dt} + \rho \frac{D^{(e)}S}{Dt}, \end{aligned}$$

where $\rho D^{(e)}S/Dt = 0$ because of the neglect of momentum and heat fluxes related to dissipation processes in the gas phase (viscosity and heat conductivity) and $\rho D^{(i)}S/Dt = \sigma$, where $\sigma = j_R X_R + j_Q X_Q + j_{12} X_{12}$ is the dissipation function. We have the following expressions for thermodynamic forces and fluxes entering into σ :

$$\begin{aligned} X_R &= (u_2 - u_1) \left(\frac{\bar{\beta}}{T_1} + \frac{\beta}{T_2} \right), \quad j_R = R_1; \\ X_Q &= \frac{1}{T_1} - \frac{1}{T_2}, \quad j_Q = Q_1; \\ X_{12} &= -S_1 + S_2 + \frac{\chi_1}{T_1} + \frac{\chi_2}{T_2} - \frac{(u_2 - u_1)^2}{2T_1}, \\ j_{12} &= -\bar{v}_2 J. \end{aligned}$$

To establish the relationships between the fluxes and forces, we can use, for example, the linear Onsager relations, where the force and thermal interactions between the phases are described in the form

$$R_1 \sim (u_2 - u_1), \quad Q_1 \sim (T_2 - T_1).$$

2. UNSTEADY MODEL OF AN IGNITION WAVE

We consider the application of this mathematical model to the problem of propagation of an ignition wave over a gas mixture of metal particles. Let a one-dimensional space be filled by a mixture of a gas and magnesium particles. When a shock wave

(SW) acts on the cloud, conditions for particle ignition can occur in the mixture. This phenomenon was previously studied within the framework of numerical experiment [1, 4, 5]; laboratory experiments were conducted for a gas mixture of magnesium particles in oxygen [6]. Boiko et al. [4] and Medvedev et al. [5] calculated the dependence of the ignition delay in the mixture on the SW Mach number, but the analytical criteria of cloud ignition were not determined there. The problems of initiation of an ignition wave in the mixture were not analyzed either.

The theoretical study of the ignition wave in a mixture of a gas and reacting magnesium particles moving behind the SW front, which is presented below, complements papers [1, 4, 5] in the aspect mentioned above.

We begin to construct the theory of ignition of a cloud of particles from an asymptotic one-velocity variant of the flow of the gas mixture. We assume that the particles are rather small and the difference in phase velocities can be ignored. Therefore, to describe the motion of the mixture, we use the above generic mathematical model in the one-velocity approximation of mechanics of heterogeneous media in the form of the mass, momentum, and energy conservation laws for the mixture as a whole:

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} &= 0, \quad \frac{\partial \rho u}{\partial t} + \frac{\partial (\rho u^2 + P)}{\partial x} = 0, \\ \frac{\partial \rho E}{\partial t} + \frac{\partial (\rho E + P)u}{\partial x} &= 0. \end{aligned} \quad (2.1)$$

We write the equation of heat addition for the disperse phase in the nondivergent form

$$\rho \left(\frac{\partial T_2}{\partial t} + u \frac{\partial T_2}{\partial x} \right) = G(T_1, T_2) \quad (2.2)$$

and add the closing relations in the form of the thermal and caloric equations of state

$$\begin{aligned} E &= e + \frac{u^2}{2}, \quad e = \bar{c}_{v,1} T_1 + \bar{c}_{v,2} T_2 + \bar{Q}, \\ P &= \rho T_1. \end{aligned} \quad (2.3)$$

All the quantities here correspond to the partial parameters of the phases in the known manner and are normalized to the initial state ahead of the SW front. The scales of density, pressure, and temperature are $\rho_M = \rho_0$, $p_M = p_0$, and $T_M = T_0$. The characteristic velocity $u_M = \sqrt{p_M/\rho_M}$, energy $e_M = u_M^2$, time t_M , and length $x_M = u_M t_M$ are introduced. The function $G(T_1, T_2)$ determines the addition of the heat of the chemical oxidation reaction of magnesium particles at the stage of ignition and the interphase heat transfer:

$$G(T_1, T_2) = B_2 (T_m - T_2) \exp \left(-\frac{E_a}{T_2} \right) - A_2 (T_2 - T_1).$$

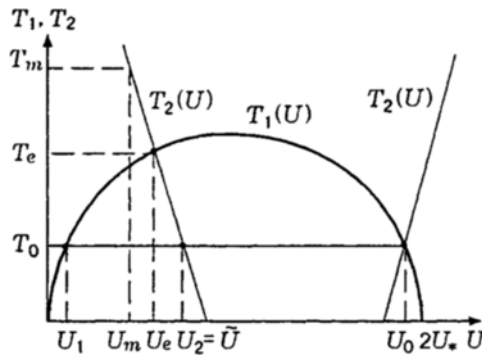


Fig. 1. Qualitative form of phase temperatures versus the velocity of the mixture [relation (3.4)].

Here

$$A_2 = \frac{3m_2 Nu_{12} \lambda_1 t_M}{2\xi_2 \rho_M c_{v,2} T^2}, \quad B_2 = \frac{3\xi_{11} \rho_{22} q t_M K_{00}}{\xi_2 \rho_M c_{v,2} T},$$

$$K_{00} = \frac{K_0}{1-a}, \quad q = \frac{q_*}{\nu_{22}}, \quad E_a = \frac{E_A}{R_\mu T_0},$$

K_0 , q_* , and E_A are the preexponent, the thermal effect, and the activation energy of the oxidation reaction, respectively, the factor $T_m - T_2$ is introduced in [7], $\xi_2 = \rho_2/\rho$ is the mass concentration of the disperse phase, ρ_{22} is the mean density of the metal component, Nu_{12} is the Nusselt number of the inter-phase heat transfer, and λ_1 is the thermal conductivity of the gas phase (see also [2]). We introduce the constants

$$\bar{c}_{v,1} = \frac{1}{\gamma_1 - 1}, \quad \bar{c}_{v,2} = \frac{\xi_2 c_{v,2}}{\xi_1 c_{v,1}} \bar{c}_{v,1}, \quad \bar{Q} = \frac{Q_0}{e_M},$$

where $Q_0 = \xi_2 Q - (\xi_1 c_{v,1} + \xi_2 c_{v,2})T_0 + e_{11}^0$. For simplicity, we assume that the entire heat of the oxidation reaction is released in the disperse phase ($\alpha_q = 0$). For the magnitude of heat release, we propose the following statement.

Statement 1. Let the following conditions be satisfied for the physicochemical and thermophysical parameters of the mixture:

$$e_{11}^0 = e_{12}^0 = e_{13}^0, \quad e_{22}^0 = e_{23}^0,$$

$$\nu_{11} c_{p,11} = \nu_{13} c_{p,13}, \quad \nu_{22} c_{p,22} = \nu_{23} c_{p,23}.$$

The heat release due to the chemical reaction is determined in the form

$$q_* = \bar{\nu}_2 Q - (\nu_{13} c_{v,13} - \nu_{11} c_{v,11})T_0 = \text{const},$$

$$Q = e_{22}^0 - e_{11}^0 = \text{const},$$

i.e., in this specific case, q_* is a constant quantity independent of the phase temperatures.

We show that system (2.1)–(2.3) with the corresponding initial and boundary conditions allows the solution of the travelling ignition-wave type.

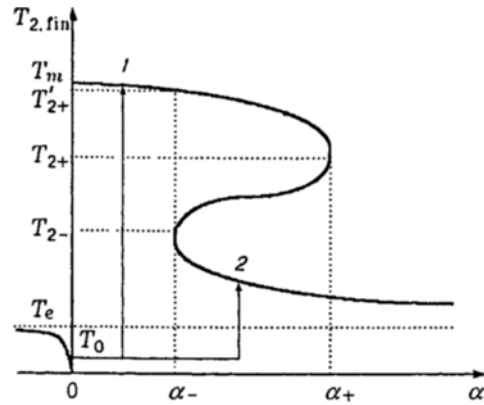


Fig. 2. Dependence of the final equilibrium temperature of the disperse phase on the parameter α : curves marked by arrows indicate the direction of particle heating for $\alpha < \alpha_-$ (1) and $\alpha > \alpha_+$ (2).

3. ADIABATIC STEADY IGNITION WAVE IN THE MIXTURE

3.1. Governing Equations and Formulation of the Problem. We attach the coordinate system to the SW front and write the steady variant of Eqs. (2.1) and (2.2):

$$\rho U = C_1, \quad C_1 U + P = C_2, \tag{3.1}$$

$$e + \frac{U^2}{2} + \frac{P}{\rho} = C_3,$$

$$\frac{dT_2}{d\zeta} = B \left\{ (T_m - T_2) \exp\left(-\frac{E_a}{T_2}\right) - \alpha(T_2 - T_1) \right\}. \tag{3.2}$$

Here $\zeta = x - Dt$ is a self-similar coordinate, D is the shock-wave velocity, C_1 , C_2 , and C_3 are the fluxes of mass, momentum, and total energy of the mixture in the initial state, $\alpha = A_2/B_2$, and $B = B_2/C_1$. The following initial conditions are used for the mixture:

$$\Phi = \Phi_0 \quad \text{as } \zeta \rightarrow -\infty \tag{3.3a}$$

ahead of the front of a frozen SW,

$$\Phi = \bar{\Phi} \quad \text{for } \zeta = 0 \tag{3.3b}$$

behind the SW front, and the condition of steadiness at $+\infty$

$$\frac{d\Phi}{d\zeta} \rightarrow 0 \quad \text{as } \zeta \rightarrow +\infty. \tag{3.3c}$$

Here Φ is the vector of the solution [$\Phi = (\rho, U, P, T_1, T_2)$].

Thus, the problem of determination of the travelling ignition wave in the mixture reduces to the solution of boundary-value problem (3.1)–(3.3) in the

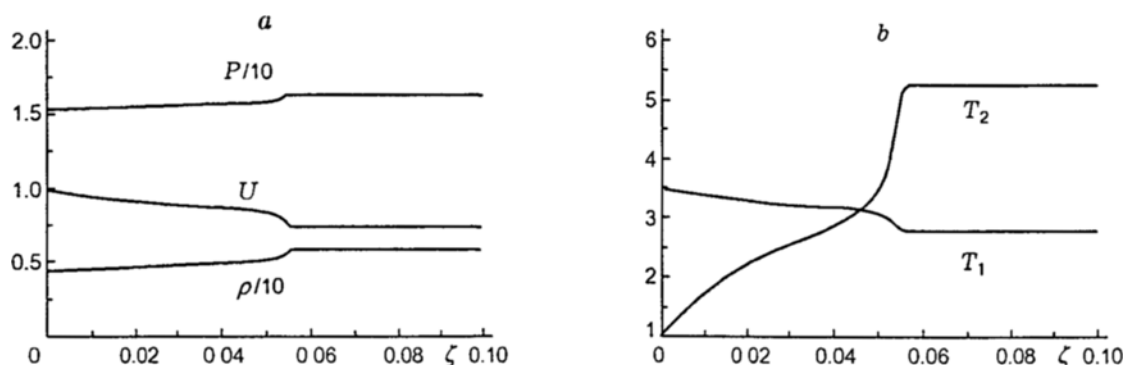


Fig. 3. Steady structure of the ignition wave for $\alpha = 0.276 \cdot 10^{-4} < \alpha_- = 1.58 \cdot 10^{-4}$ and $M_{f0} = 3.63$.

region $(-\infty, +\infty)$. We note that system (3.1), (3.2) can be reduced to one differential equation for the temperature T_2 or velocity U .

3.2. Classification of Flow Regimes of the Mixture. Using (3.1), we can obtain the following algebraic expressions for the phase temperatures through the velocity of the mixture:

$$T_1(U) = U(2U_* - U), \quad T_2(U) = a_2 U^2 - a_1 U + a_0,$$

$$U_* = \frac{C_2}{2C_1}, \quad a_0 = \frac{C_3 - \bar{Q}}{\bar{c}_{v,2}}, \quad (3.4)$$

$$a_1 = 2U_* \frac{\bar{c}_{v,1} + 1}{\bar{c}_{v,2}}, \quad a_2 = \frac{\bar{c}_{v,1} - 0.5}{\bar{c}_{v,2}}.$$

It is useful to introduce the velocity of the mixture U_e in the case of temperature equilibrium $T_1(U_e) = T_2(U_e) = T_e$, and also the velocities U_1 , U_2 , and U_m determined from the conditions $T_1(U_1) = T_0$, $T_2(U_2) = T_0$, and $T_2(U_m) = T_m$. It can be easily seen that U_2 coincides with \bar{U} , i.e., with the velocity of the mixture behind the SW front. In what follows, we assume that $U_m < U_e$ (or $T_m > T_e$). Relations (3.4) allow us to inspect the flow parameters of the mixture represented as functions of its velocity. It is necessary for the analysis of the final equilibrium states of the system (Fig. 1). We impose a natural requirement: the final temperatures of the phases $T_{1,\text{fin}}$ and $T_{2,\text{fin}}$ cannot be lower than the temperature of the initial state T_0 . This allows us to conclude that the velocity of the mixture in the final state U_{fin} is within the interval from U_1 to U_2 . To determine whether U_{fin} is greater or smaller than U_e , we construct a bifurcation diagram for the equilibrium states of Eq. (3.2) (Fig. 2). The form of the dependence $T_{2,\text{fin}} = T_{2,\text{fin}}(\alpha)$ is known [7]. The difference is that the role of the temperature of external action belongs now to the quantity T_e . For $T_{2,\text{fin}} < T_e$ [which corresponds to the velocity of the mixture within the interval (U_e, U_2) in Fig. 1], thermal equilibrium is

impossible: the heat-transfer parameter α becomes unphysical (negative). Therefore, from the fact that $T_{2,\text{fin}}$ cannot exceed T_m , we conclude that the final velocity of the mixture U_{fin} belongs to the interval (U_m, U_e) . The final temperature of the disperse phase is always greater than the final temperature of the gas phase: $T_{2,\text{fin}} > T_{1,\text{fin}}$. For the value of $T_{2,\text{fin}}$, using the analysis of the catastrophe/ignition manifold shown as cross sections $T_e = \text{const}$ in Fig. 2, we establish the following statement.

Statement 2. If the bifurcation parameter α in the ignition wave in the flow of the mixture is smaller than α_- , then the final temperature of the particles $T_{2,\text{fin}}$ lies between T'_{2+} and T_m . If $\alpha > \alpha_-$, then the final temperature $T_{2,\text{fin}}$ lies between T_e and T_{2-} . The first case ($\alpha < \alpha_-$) corresponds to the flow of the mixture behind the SW with ignition of the disperse phase (the course of particle heating is shown by curve 1 in Fig. 2); the second case ($\alpha > \alpha_-$) corresponds to the flow with "regular" heating of the particles (curve 2). Here α_{\pm} are uniquely determined through the parameters of the initial state of the mixture.

3.3. Numerical Examples. The following values of the parameters are used in the calculations: $\rho_0 = 1.2 \text{ kg/m}^3$, $p_0 = 10^5 \text{ Pa}$, $\rho_{20} = 0.17 \text{ kg/m}^3$, $r = 5 \cdot 10^{-7} \text{ m}$, $t_M = 10^{-3} \text{ sec}$, $\bar{Q} = 4 \cdot 10^7 \text{ J/kg}$, $E_A/\mathcal{R}_\mu = 10^4 \text{ K}$, and $K_0 = 10^{-5} - 10^{-4} \text{ m}/(\text{sec} \cdot \text{K})$.

We give some numerical illustrations of steady flow structures of a gas mixture behind the SW. Figure 3 shows the distribution of the parameters of the mixture behind the SW front for a flow with ignition of the disperse phase for Mach number $M_{f0} = 3.63$ and $\alpha \cdot 10^4 = 0.276 < \alpha_- \cdot 10^4 = 1.58$. During the motion of the mixture, the particles are heated and ignited owing to energy extraction from the gas phase. Therefore, the profiles of temperature T_1 and velocity U are monotonically decreasing. The particle temperature T_2 monotonically increases and has two

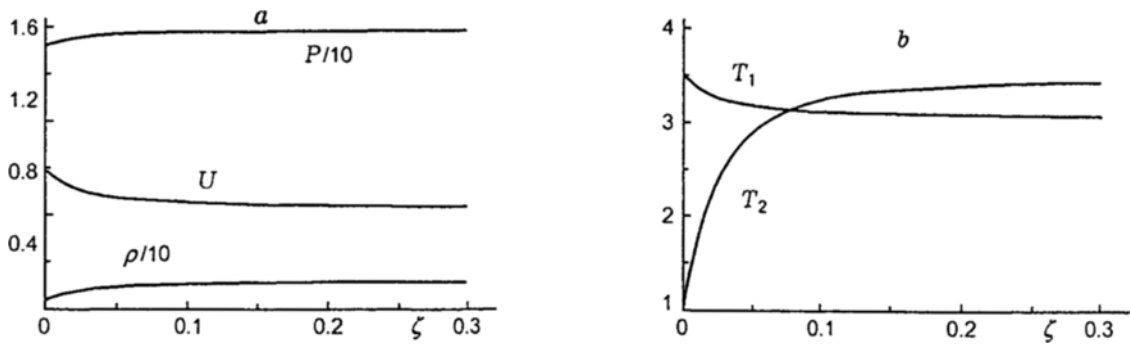


Fig. 4. Steady flow structure behind the shock wave upon regular heating of particles for $\alpha_- = 1.58 \cdot 10^{-4} < \alpha = 2.76 \cdot 10^{-4}$ and $M_{f0} = 3.63$.

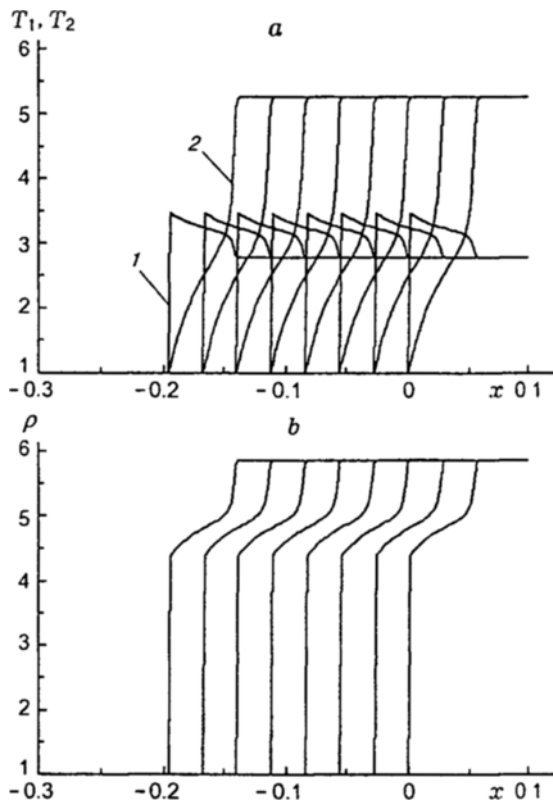


Fig. 5. Propagation of a steady ignition wave: (a) temperature of gas (1) and disperse (2) phases; (b) density of the mixture.

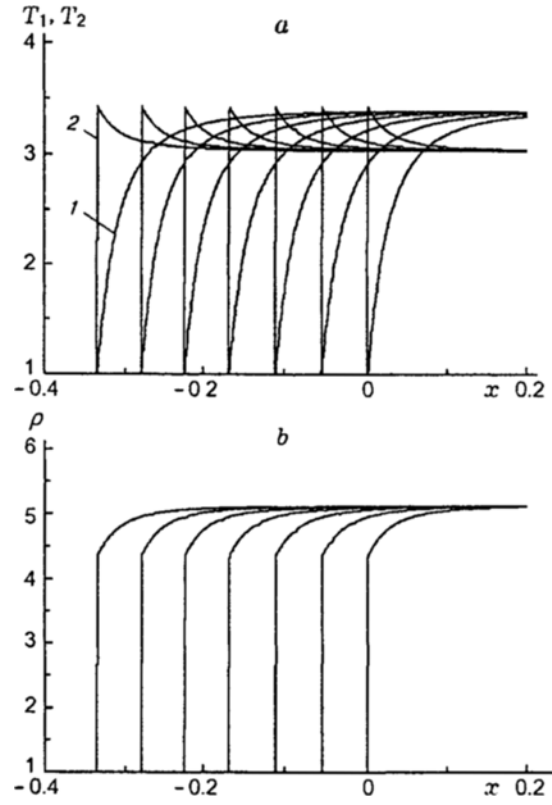


Fig. 6. Propagation of the steady flow structure of the mixture upon regular heating of the disperse phase: (a) temperature of the gas (1) and disperse (2) phases; (b) density of the mixture.

points of inflection. In accordance with the classical concepts, which are also valid for a moving medium, we associate the last point of inflection with ignition:

$$\left. \frac{dT_2}{d\zeta} \right|_{\zeta=\zeta_{ign}} \rightarrow \max, \quad \left. \frac{d^2T_2}{d\zeta^2} \right|_{\zeta=\zeta_{ign}} = 0.$$

In this variant, the ignition coordinate is $\zeta_{ign} \approx 0.055$, so the ignition delay is $t_{ign} \approx 100 \mu\text{sec}$, which coincides with experimental data [6] in order of magnitude. The phase temperatures are significantly dif-

ferent in the entire flow region, though there is an equilibrium temperature point $T_1 = T_2 = T_e$. However, this point is unstable because of the presence of a chemical source of heat. The heat release from reacting particles does not have enough time to increase the gas temperature to the point of ignition, since the characteristic time of convective interphase heat transfer is much greater than the characteristic "chemical" time ($\alpha^{-1} \gg 1$).

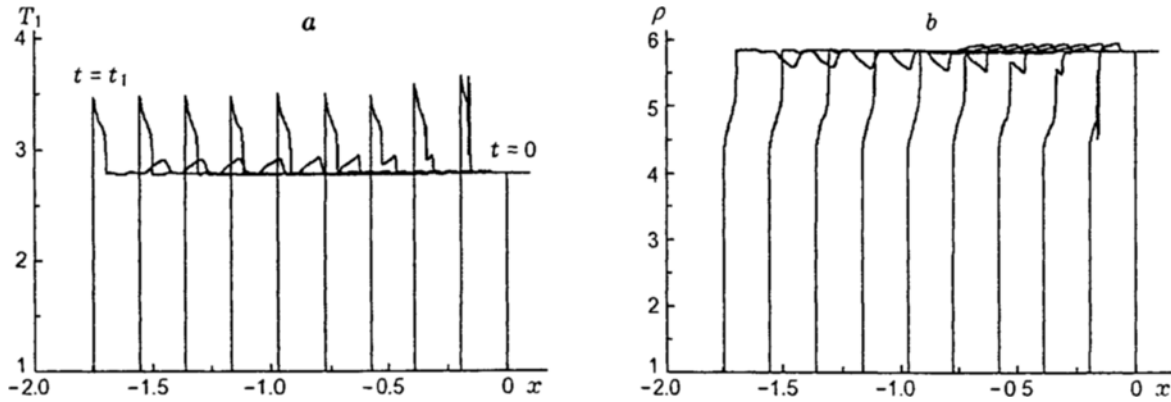


Fig. 7. Initiation of an ignition wave: (a) temperature of the gas phase; (b) density of the mixture.

Figure 4 illustrates the distribution of the parameters of the mixture in a flow with “regular” heating of the disperse phase at $M_{f0} = 3.63$ and $\alpha_- \cdot 10^4 = 1.58 < \alpha \cdot 10^4 = 2.76$. Temperature nonequilibrium of the phases is also observed here in the region behind the SW. Nevertheless, the profiles of the parameters are smoother here than in the previous case. In particular, there is no dramatic change in the particle temperature, which corresponds to ignition of the disperse phase. The special feature of the flow structure is that the pressure and other parameters of the mixture reach equilibrium values earlier than the particle temperature.

4. STABILITY AND INITIATION OF A STEADY IGNITION WAVE

The problem of initiation and stable propagation of a steady ignition wave within the framework of the unsteady approximation of mechanics of heterogeneous media is of significant interest.

4.1. Stability of the Ignition Wave. The stability was investigated by numerical simulation of the initial-boundary problem for unsteady equations (2.1) and (2.2) with a steady solution of the travelling wave type as the initial conditions. The problem was formulated as follows.

Find the vector of the solution $\Phi = (\rho, u, P, T_1, T_2)$, which, within the region $\{(x, t) : x \in (-\infty, \infty), t \geq 0\}$, satisfies system (2.1)–(2.3), the initial conditions

$$\Phi = \begin{cases} \Phi_0, & x < 0, \\ \Phi_{st}(x), & x \geq 0 \end{cases}$$

for $t = 0$ and the boundary conditions

$$\Phi = \Phi_0 \text{ as } x \rightarrow -\infty,$$

$$\frac{\partial \Phi}{\partial x} \rightarrow 0 \text{ as } x \rightarrow +\infty.$$

Here $\Phi_{st}(x)$ is a steady distribution of the parameters in a travelling ignition wave.

The system of equations of nonequilibrium gas dynamics (2.1) was solved using a finite-difference TVD-scheme [8]. The kinetic equation of ignition (2.2) was integrated along the trajectory using the method proposed by Fedorov and Khmel’ [9]. The algorithm of the TVD-scheme was preliminary tested on the Riemann problem for a perfect gas and on the problem of propagation of a frozen SW in a gas mixture of inert particles (a two-temperature model).

It was found that the resultant steady structures propagate steadily during the calculation period. Figure 5 shows the ignition-wave parameters (the temperatures of the phases and the density of the mixture) at different times with a time step $\Delta t = 6.5 \cdot 10^{-3}$ (the data correspond to Fig. 3). The leading shock wave in the structure of a steady ignition wave is located at the point $x = 0$ at $t = 0$. Figure 6 illustrates the stability of the steady structure, which describes the “regular” heating of the disperse phase behind the SW ($\Delta t = 6.46 \cdot 10^{-3}$; the data correspond to Fig. 4). We note that conditions of the subsonic piston type were maintained at the right boundary of the flow region, which guaranteed the steadiness of the process. In experimental studies, this is ensured by quasi-steadiness of the plug in the shock tube.

4.2. Initiation of an Ignition Wave. In a region of space filled by a mixture of a gas and particles, a zone of elevated pressure and temperature of the gas phase is created at the initial time (for example, due to instantaneous localized heat release). We have to find under which conditions an ignition wave arises in the mixture. Mathematically, the problem consists in solving the problem of decay of an arbitrary discontinuity for system (2.1), (2.2).

We consider an example of initiation of an ig-

nitiation wave from the initial discontinuity whose parameters are correlated with a steady structure, i.e., when all the parameters of the mixture in the high-pressure region are set equal to their final equilibrium values in the wave:

$$\Phi = \begin{cases} \Phi_0, & x < 0, \\ \Phi_{\text{fin}}, & x \geq 0. \end{cases}$$

The calculation results for this variant of the flow corresponding to the data in Figs. 3 and 5, i.e., for the condition $\alpha < \alpha_-$ satisfied, are plotted in Fig. 7. The ignition wave is formed over a length of several dozen of its thickness and becomes practically steady at the time $t_1 = 0.403$. A perturbation of the density of the mixture is seen in the tail of the wave. This perturbation lags behind the frozen leading SW with time and decays in terms of the amplitude. The appearance of this perturbation is probably related to the manner of initiation of the ignition wave by the method of a pushing piston.

CONCLUSIONS

The one-dimensional motion of a mixture of a gas and reacting metal particles has been considered. A two-velocity, two-temperature mathematical model has been proposed. This model takes into account the chemical oxidation reaction of the disperse phase with heat release in both phases.

On the basis of the model proposed, a theory of an ignition wave in a gas mixture of magnesium particles has been developed, which extends N. N. Semenov's theory of explosion to the case of moving continua of reacting particles. The flow of the mixture behind the shock-wave front has been classified into two basic regimes:

- with ignition of the disperse phase by the method of thermal explosion;
- without ignition, with "regular" heating.

The calculated delay of ignition of the gas mixture corresponds to experimental data in order of magnitude. Within the framework of the unsteady approach, a stable propagation of the resultant steady ignition wave over the mixture has been demonstrated. A numerical example of ignition-wave initiation in a mixture with the help of a pushing piston is given.

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