

Ignition of Gaseous Suspensions in an Interacting Continuum Regime

A. V. Fedorov¹

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A mathematical model is proposed for describing the flow of a mixture of gases and reactive solids including a heterogeneous chemical ignition reaction. The model is closed with an equation for the kinetics of oxide film growth. It is assumed that the heat of the chemical reaction can be released in both phases depending on the accommodation coefficients. The ignition of a motionless cloud of magnesium particles is studied in terms of this model. The model is tested with the use of experimental data on the maximum temperature of the medium as a function of the particle radius. Data on the dependence of the parameters of a heated particle cloud on the physical and chemical constants of the mixture and particles are presented.

Studies of the ignition of gaseous suspensions are of current interest in connection with the fire and explosion hazards of industrial dusts. From the standpoint of the general theory of heterogeneous media, of which gaseous suspensions composed of fine solid particles and a gas are a special case, the motions of aerosol suspensions can be described mathematically and physically in two approximations. The first is a single particle regime, in which the motion and heating of the discrete phase occur against a known flow field of the gas. This description is valid for gaseous suspensions with a sufficiently low dust content. The second approach is based on the assumption that the particles are quite numerous and can have a reciprocal effects, both dynamical and thermal, on the gas. Mathematical models have been proposed [1–4] for the ignition and combustion of gaseous suspensions under dynamic conditions behind advancing and reflected shock waves which include the different velocities and temperatures of the phases along with a heterogeneous low-temperature oxidation reaction. In order to close this model in the ignition state, it was assumed that the particle dimensions are roughly the same as the initial size and that the heat of the chemical reaction is released only in the condensed phase. In the following, we de-

velop a model for the ignition of an aerosuspension that is free of these assumptions.

BASIC EQUATIONS

As in [1], we shall consider a three-component two-phase medium on the basis of the general approach developed by Nigmatulin [5], in which a chemical reaction described by the stoichiometric relation

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

occurs, where ν_i and g_i are the stoichiometric coefficients and molecular masses of the phases and components. It is assumed that the gas is a mixture consisting of an oxidant ($i = 11$), an inert component ($i = 12$), gaseous oxidation products ($i = 13$), metal ($i = 22$), and condensed oxidation products ($i = 23$). Everywhere in the following $\nu_i \equiv \nu_i g_i$ and $\nu_2 \equiv \nu_{22}$.

The conservation equations for masses of the phases and components have the form

$$\begin{aligned} \partial_t \rho_i + \partial_x \rho_i u_i &= (-1)^{i+1} \bar{\nu}_2 J, \quad i = 1, 2, \\ \partial_t n + \partial_x n u_2 &= 0, \quad \rho_1 \partial_1 \xi_{11} = -(\nu_{11} + \bar{\nu}_2 \xi_{11}) J, \\ \frac{\nu_{11} + \bar{\nu}_2 \xi_{11}}{\nu_{11} + \bar{\nu}_2 \xi_{11,0}} &= \frac{\xi_{12}}{\xi_{12,0}}, \quad \sum \xi_{1i} = 1, \end{aligned} \quad (1)$$

¹Institute of Theoretical and Applied Mechanics, Siberian Division, Russian Academy of Sciences, Novosibirsk 630090.

$$\sum \xi_{2i} = 1, \quad \frac{\xi_{22}(\alpha - \xi_{22,0})}{\xi_{22,0}(\alpha - \xi_{22})} = \bar{r}^3,$$

$$\alpha = \frac{\nu_2}{\bar{\nu}_2}, \quad \bar{r} = \frac{r}{r_0}, \quad R^3 - R_0^3 = a(r^3 - r_0^3),$$

$$a = 1 - \frac{\nu_3 \rho_{22}^0}{\nu_2 \rho_{23}^0}, \quad \bar{\nu}_2 = \nu_2 - \nu_3.$$

Here $\rho_1 = m_1 \sum \rho_{1j}^0$ and $\rho_2 = m_{22} \rho_{22}^0 + m_{23} \rho_{23}^0 = m_2 \rho_2^0$ are the average densities of the gaseous and condensed phases, ρ_{1j}^0 is the true density of the j th gaseous component, ρ_2^0 is the apparent actual density of the condensed phase (c-phase); m_j ($j = 1, 2$) and m_{2j} ($j = 2, 3$) are the volume densities of the gases, c-phase, metal, and oxide; n is the number of particles per unit volume; $R = h + r$, where r is the particle radius and h is the thickness of the oxide film; $\xi_{ji} = \rho_{ji}/\rho_j$ ($j = 1, 2$ and $i = 1, 2, 3$); u_j are the velocities of the phases; $\partial_t = \partial/\partial t$, $\partial_x = \partial/\partial x$, and $\partial_j = \partial_t + u_j \partial_x$; a subscript 0 denotes the initial state; and, the first digit in a subscript with two digits denotes the number of the phase.

J is given in terms of the local flow characteristics by

$$J = -4\pi \rho_{22}^0 \frac{n r_2}{\nu_2} \partial_2 r = -\frac{3}{r} \frac{\rho_{22}}{\nu_2} \partial_2 r. \quad (2)$$

The source function J must be defined as a function of the average flow quantities. In an experiment there is generally some information on the rate of transformation of an individual fine particle. This is either a datum about the linear combustion velocity of the particle, which can be obtained from the empirical Sreznevskii law, or about the rate of growth of the oxide film thickness. Thus, it is necessary to obtain an expression for J of type (2). For this we shall assume that during the chemical transformation the particle consists of a metallic core of radius r coated with an oxide film of thickness h , i.e., the radius of the sphere is $R = r + h$. Here it was assumed that the finest oxide particles precipitate out on a larger metal particle. In addition, a conservation equation for the number of particles and one of the continuity equations for the c-phase were used. Based on these equations it is also possible to find the last of the integrals in Eq. (1).

The momentum conservation equations for the phases are written in the form

$$\partial_t \rho_i u_i + \partial_x (\rho_i u_i^2 + m_i p)$$

$$= p \partial_x m_i + (-1)^{i+1} \bar{\nu}_2 J + R_i, \quad i = 1, 2, \quad (3)$$

where R_i are the forces acting on the corresponding phase.

The energy conservation equation of the phases is written in the form

$$\partial_t \rho_i E_i + \partial_x (\rho_i u_i E_i + m_i p u_i)$$

$$= -p \partial_t m_i + (-1)^{i+1} \bar{\nu}_2 J \left(-k_i + i_i + \frac{u_i^2}{2} \right)$$

$$+ R_i (\beta u_1 + \bar{\beta} u_2) + Q_i, \quad i = 1, 2. \quad (4)$$

Here $E_i = e_i + u_i^2/2$ (e_i are the internal energies of the phases), β is the accommodation coefficient for the force interaction of the phases ($\bar{\beta} = 1 - \beta$), p is the pressure of the mix, and Q_i is a function describing the thermal interaction of the phases. Since the conservation equation for the total energy of the mixture does not contain sources, we have the basic energy equation [5] of the mechanics of reacting heterogeneous media,

$$k_1 + k_2 = i_1 + i_2,$$

where the k_i are the accommodation coefficients, which are to be determined, and the i_i are the enthalpies of the phases. The heat released in the chemical reaction is

$$q_* = \nu_{11} i_{11} + \nu_{21} i_{22} - \nu_{31} i_{23} - \nu_{13} i_{13}.$$

It is possible to go from the conservation equations for the total energies of the phases (4) to heat influx equations with inhomogeneous terms describing the heat sources, the frictional force between the phases, the kinetic energy of the masses which undergo phase changes (released only into the gas), heat transfer between the phases (Q_i), and the work of the pressure forces which develop from the change in the specific volumes of the phases. Note that for particles this is the variation in the apparent actual density of the particles.

In order to determine the k_i , we shall assume that heat $\alpha_1 q_*$ is released in the gas and $\bar{\alpha}_1 q_* = (1 - \alpha_1) q_*$ in the particles. Transforming to the enthalpies in the heat influx equations and using the representation of the right sides for determining k_i in them, we obtain the equations

$$(\nu_{11} + \bar{\nu}_2 \xi_{11}) i_{11} + \bar{\nu}_2 \xi_{12} i_{12}$$

$$- (\nu_{13} + \bar{\nu}_2 \xi_{13}) i_{13} - \bar{\nu}_2 k_1 = \alpha_1 q_*,$$

$$(\nu_2 - \bar{\nu}_2 \xi_{22}) i_{22} - (\nu_2 - \bar{\nu}_2 \xi_{22}) i_{23} - \bar{\nu}_2 k_2 = \bar{\alpha}_1 q_*.$$

The solution of this system has the form

$$k_1 = [-\alpha_1 q_* + (\nu_{11} + \nu_2 \xi_{11}) i_{11} + \nu_2 \xi_{12} i_{12}$$

$$- (\nu_{13} - \nu_2 \xi_{13}) i_{13}] / \nu_2,$$

$$k_2 = i_1 - i_2 - k_1.$$

In this way the accommodation equations have been determined.

The equations of state of the phases are easily expressed in terms of the average characteristics of the flow of the suspension:

$$\begin{aligned}
 p &= \frac{\rho_1 T_1 \bar{R}}{m_1} \left(\sum \frac{\xi_{1i}}{\mu_i} \right), \quad m_1 + m_2 = 1, \\
 m_2 &= \frac{\rho_2}{\rho_2^0}, \quad \rho_{2j}^0 = \text{const}, \quad j = 2, 3, \\
 \rho_2^0 &= \frac{\rho_{22}^0 r^3 + (R^3 - r^3) \rho_{23}^0}{R^3} \equiv \rho_2^0(r), \\
 e_1 &= c_{v1} \Delta T_1 + h_1^0, \quad c_{v1} = \sum \xi_{1i} c_{vi}, \quad (5) \\
 h_1^0 &= \sum \xi_{1i} h_{1i}^0, \quad \Delta T_i = T_i - T^0, \\
 e_2 &= c_2 \Delta T_2 + h_2^0, \quad c_2 = \sum \xi_{2j} c_{2j}, \\
 h_2^0 &= \sum \xi_{2i} h_{2i}^0, \quad \Delta T_j = T_j - T^0, \quad j = 2, 3,
 \end{aligned}$$

T^0 is the equilibrium temperature in the standard state, h_{ij}^0 are the heats of formation of the phases and components, c_{p1} is the specific heat of the gas mixture, c_{pj} is that of the gas component, c_2 is that of the condensed phase, and c_{2j} is that of the solid phase.

We shall consider the unknowns to be 11 components of the vector function $\Phi(\rho_i, u_i, T_i, p, r, \xi_{11}, h, n)$, which is defined by the seven partial differential equations which express the conservation of mass, momentum and energy of the phases and components in Eqs. (1), a single equation of state from Eqs. (5), and the algebraic relation between r and h expressed by the last of Eqs. (1), and, finally, the mathematical model is closed by the kinetic equation for the growth of the oxide film,

$$\partial_2 h = G(h, T_2, \dots). \quad (6)$$

Thus, system (1)–(6) for determining the 11 unknowns in the solution vector Φ is closed.

Remark. The number of differential equations in (1)–(6) can be reduced through the integral

$$\frac{n}{n_0} = \frac{\rho_2 \xi_{22}}{\rho_{20} \xi_{22,0} \bar{r}^3}.$$

We now consider the following problem as an application.

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Point Model and Its Transformations

We consider a cloud of magnesium particles that fills unit volume uniformly and exchanges through

the walls of a vessel with surroundings heated to a temperature \tilde{T} . When the initial parameters of the cloud and characteristics of the external interaction are changed, the gaseous suspension may exhibit different types of heating dynamics. We shall establish these using a point model for the above equations supplemented by heat transfer with the external medium:

$$\begin{aligned}
 d_t \rho_i &= (-1)^{i+1} \bar{\nu}_2 J, \quad i = 1, 2, \\
 d_t \xi_{11} &= -(\nu_{11} + \bar{\nu}_2 \xi_{11}) J, \quad \frac{\xi_{22}(\alpha - \xi_{22,0})}{\xi_{22,0}(\alpha - \xi_{22})} = \bar{r}^3, \\
 \frac{\nu_{11} + \bar{\nu}_2 \xi_{11}}{\nu_{11} + \bar{\nu}_2 \xi_{11,0}} &= \frac{\xi_{12}}{\xi_{12,0}}, \quad \sum \xi_{1i} = 1, \\
 \sum \xi_{2i} &= 1, \quad R^3 - R_0^3 = a(r^3 - r_0^3), \quad (7) \\
 d_t(\rho_1 e_1 + \rho_2 e_2) &= -Sk(T_1 - \tilde{T}), \\
 \rho_2 d_t e_2 - \frac{m_2 p}{\rho_0^2} d_t \rho_0^2 &= -\bar{\nu}_2 k_2 J + Q_2, \\
 Q_2 &= -m_2 \frac{3}{R} \alpha_{12}(T_2 - T_1),
 \end{aligned}$$

where k is the coefficient of heat transfer from the gas to the tube, α_{12} is that from the gas to a particle, and S is the inner surface area of the tube. Combining the equations of continuity for the phases, we find the first integral, i.e., the conservation of mass for the mixture as a whole,

$$\rho_1 + \rho_2 = \rho_{10} + \rho_{20} = C_1. \quad (8)$$

Substituting the expression for J in the continuity equation for the c-phase, we obtain an equation with separable variables which yields the integral

$$\frac{\rho_2}{\rho_{2,0}} = \frac{\alpha + \xi_{22,0}(\bar{r}^3 - 1)}{\alpha}. \quad (9)$$

Using Eqs. (8) and (9), it is easy to obtain the dependence of the average gas density on the particle radius,

$$\frac{\rho_1}{\rho_{1,0}} = \frac{\alpha - \rho_{21}^0 \xi_{22,0}(\bar{r}^3 - 1)}{\alpha}, \quad \rho_{21}^0 = \frac{\rho_{2,0}}{\rho_{1,0}}. \quad (10)$$

Equation (10) substituted in the third of Eqs. (1) makes it possible to find the integral of this equation, as well:

$$\frac{\nu_{11} + \bar{\nu}_2 \xi_{11}}{\nu_{11} + \bar{\nu}_2 \xi_{11,0}} = \frac{\alpha}{\alpha - \rho_{21}^0 \xi_{22,0}(\bar{r}^3 - 1)}. \quad (11)$$

Therefore, the average densities and relative concentrations of the phases and components are expressed explicitly in terms of the relative particle radius.

Transformation of the Equations for the Energies of the Phases. The particle energy conservation

equation, i.e., the next to the last of Eqs. (1), has the following enthalpy form:

$$\rho_2 \sum \xi_{2j} d_i i_{2j} - m_2 d_i p = J \bar{\alpha}_1 q_*. \quad (12)$$

Given the representations

$$i_{2j} = c_{2j}(T_2 - T^0) + \frac{p}{\rho_{2j}} + h_{2j}^0, \quad j = 2, 3,$$

and substituting them in Eq. (12), we obtain the energy equation for the solid particles in the following form:

$$\rho_2 c_2 d_i T_2 = Q_2 + J \bar{\alpha}_1 q_*. \quad (13)$$

Similarly, the conservation equation for the gas can be written as

$$\rho_1 c_p d_i T_1 = Q_1 + J \alpha_1 q_* - Sk(T_1 - \tilde{T}). \quad (14)$$

We supplement Eqs. (13) and (14) with the kinetic equation for the growth of the oxide layer and the geometric relationship between R and r :

$$d_i h = K \exp\left(-\frac{E}{RT}\right), \quad R^3 - R_0^3 = a(r^3 - r_0^3). \quad (15)$$

System (13)–(15) for the three unknowns T_1 , T_2 , and r is closed.

Asymptotic Approximation for the Mathematical Model (13)–(15). We shall use the fact that during the chemical transformations in the preignition period the thickness of the oxide film changes very little, i.e., $h/r \ll 1$. Expanding the last of Eqs. (15) in a series and limiting ourselves to the linear approximation, we find the representation

$$(a - 1)(r - r_0) = h - h_0, \quad (16)$$

which yields

$$d_i r = (a - 1)^{-1} d_i h = \frac{K}{a - 1} \exp\left(-\frac{E}{RT}\right). \quad (17)$$

Note that since the thickness of the oxide layer varies little, the coefficients in Eqs. (13) and (14) can be “frozen” in the first stage of this study and we shall use the representation (17) for determining the source term J for magnesium particles. This makes it possible to represent two of the unknowns (the temperatures of the gas and solid particles) by the asymptotic model

$$\begin{aligned} \rho_2 c_2 d_i T_2 &= -a_1(T_2 - T_1) \\ &+ b \exp\left(-\frac{E}{RT_2}\right) \equiv A(T_2, T_1), \end{aligned} \quad (18)$$

$$\rho_1 c_{p1} d_i T_1 = a_1(T_2 - T_1) - c(T_1 - \tilde{T}) \equiv B(T_2, T_1),$$

where $a_1 = m_2 \frac{3}{R} \alpha_{12}$, $b = \frac{3\rho_{22}K}{R\nu_2(1-a)} q_*$, and $c = Sk$. Equations (18) must satisfy the initial conditions

$$T_2(0) = T_{2,0}, \quad T_1(0) = T_{1,0}. \quad (19)$$

These conditions describe the different possible thermal effects on the cloud. For example, if the particles are ejected into some volume containing a high temperature gas, then $T_{2,0} < T_{1,0}$.

As the cloud evolves thermally, the temperature can vary regularly or irregularly. This depends on the form of the catastrophe (ignition) manifold, which we now investigate.

Zero Isoclines of Eqs. (18). On equating the right-hand sides of Eqs. (18) to zero, we obtain a system of equations for determining the stationary points of our mathematical model:

$$\begin{aligned} \Delta T_1 &= \frac{a_1}{a_1 + c} \Delta T_2, \quad \Delta T_i = T_i - \tilde{T}, \\ b \exp\left(-\frac{E}{RT_2}\right) &= a_1 \frac{c}{c + a_1} \Delta T_2. \end{aligned} \quad (20)$$

The last equation, when differentiated with respect to T_2 , can be used to obtain the convolution curve on the catastrophe/ignition manifold. In the case of the ignition of a cloud under study here, the doubly degenerate critical points on this manifold coincide with the analytic form of the Semenov condition,

$$\alpha = a_1 \frac{c}{(c + a_1)b} = \alpha_- = \Delta T_{2-} \exp\left(-\frac{E}{RT_{2-}}\right)$$

and have been discussed previously [6]. Here ΔT_{2-} is the smallest root of the equation

$$G(T_2) = \frac{E}{RT_2^2} \Delta T_2 + 1 = 0.$$

It is known from the general theory of thermal explosions that the last of Eqs. (20) is a nonunique curve in the (T_2^0, α) plane for the interval $\alpha \in (\alpha_-, \alpha_+)$. Its properties have been discussed in detail elsewhere [7, 8].

Jacobi Matrix and Eigenvalues. The Jacobi matrix at the stationary points of system (19) has the form

$$J = \begin{vmatrix} A_{1,T_2} = -a_2 u(G + v) & A_{1,T_1} = a_2 \\ B_{1,T_2} = \xi a_2 & B_{1,T_1} = \frac{\xi a_2}{uv} \end{vmatrix}$$

where $u = c/(a_1 + c)$, $v = a_1/c$, $\xi = \rho_2 c_2 / \rho_1 c_{p1}$, and $a_2 = a_1 / \rho_2 c_2$. The eigenvalues λ of this matrix are found from the equation ($\lambda = \tilde{\lambda}/a_2$)

$$\lambda^2 + \text{tr} J \lambda + \det J = 0, \quad (21)$$

where $\text{tr} J = u(G + d)$, $\det J = \xi G/v$, and $d = v(1 + \xi/u^2 v^2)$. The existence of a root of Eq. (21)

depends on the sign of the discriminant $D(G) = \text{tr}J^2 - 4\det J = G^2 + 2Gl + d^2$, where $l = v(1 - \xi/u^2 v^2)$. We shall treat it as a function of G . Its sign, in turn, is determined by that of $D_1 = -2\xi/u^2$, which is non-positive. This implies that the discriminant is a positive function. Therefore, the roots of Eq. (21) are always real.

We examine the behavior of $\det J(T_2)$ as a function of whether the point T_2 belongs to the stationary states curve. It is easy to show that

$$\det J \begin{cases} > 0, & T_2 \in (0, T_-) = A, & T_2 \in (T_-, \infty) = C, \\ \leq 0, & T_2 \in (T_-, T_+) = B. \end{cases}$$

Based on the above remarks, we can formulate

Proposition 1. The eigenvalues of Eq. (21) for $T_2 \in A$ and $T_2 \in B$ are both negative; for $T_2 = T_{+,-}$ one of the eigenvalues is zero and the second is negative; for $T_2 \in (T_-, T_+)$ the eigenvalues have different signs.

Therefore, on A and B the stationary points of the equations are stable nodes, while on the negative branch the stationary points are saddle points, and for $T = T_-, T_+$ they are degenerate nodes.

Initial and Boundary-Value Problems for Eqs. (18) and (19)

Based on Proposition 1, we can describe the possible types of solutions of Eqs. (18) and (19). First we consider the solution of the boundary-value problem for the temperature of the gaseous phase as a function of the temperature of the c-phase. It is obtained by dividing the first of Eqs. (18) by the second. Here it is possible to state an auxiliary boundary-value problem which can be used to give a classification of the types of heating dynamics for the particles:

$$T_2(T_1) = T^A, \quad T_1 = \frac{a_1}{a_1 + c} \Delta T^A + \tilde{T},$$

$$T_2(T_1) = T^B, \quad T_1 = \frac{a_1}{a_1 + c} \Delta T^B + \tilde{T}.$$

We now show how to solve it. First, we choose the slope of the trajectory from a point belonging to the unstable branch B corresponding to a positive eigenvalue. Upon specifying a negative temperature increment for the particles on this trajectory, we find the corresponding increment in the gas temperature. Taking the resulting values of the unknowns as initial data, we can integrate the equation and, as T_1 approaches T^B , the trajectory enters a stationary point belonging to the stable branch of the catastrophe manifold, $T = T^A$. In the case of a positive increment of the particle temperature, the solution,

which is a semitrajectory, will approach T^C , which is also a stable node.

In a similar fashion, it is possible to construct a second trajectory that passes through the saddle point T^B before intersecting the straight lines $T_2 = 0$ and $T_1 = 0$. We denote the region lying between the axes and this trajectory by D_1 and above, by D_2 . Then the solution of the Cauchy problem with initial data T^0 from D_1 approaches T^A , while for $T^0 \in D_2$, the solution approaches T^C . Based on these remarks, we formulate

Proposition 2. The solution of the Cauchy problem for $\alpha \in (\alpha_-, \alpha_+)$ and $T^0 \in D_1$ stabilizes on branch A; if $T^0 \in D_2$, it stabilizes on C. There is a trajectory which joins the unstable state T^B with T^A and T^C . The solution of the Cauchy problem for $\alpha \notin (\alpha_-, \alpha_+)$ stabilizes on T^C and T^A , respectively.

Remark. Let $\alpha \in (\alpha_-, \alpha_+)$. The solutions passing through the stationary points (T^B, T^A) and (T^B, T^C) describe the regimes of dispersive quenching and dispersive ignition, respectively. The solution of the Cauchy problem with initial data from region D_1 can describe both quenching and regular heating of a particle in the cloud; if the initial data are taken from D_2 , then this solution describes the ignition of the cloud. If $\alpha \leq \alpha_-$, then for initial data lying below T^C the cloud ignites and if $\alpha \geq \alpha_+$, regular heating or quenching occurs, depending on whether the initial point lies below or above T^A .

Discussion of Numerical Results

Before proceeding to solving the direct problem, we stop to determine the kinetic constants E and K

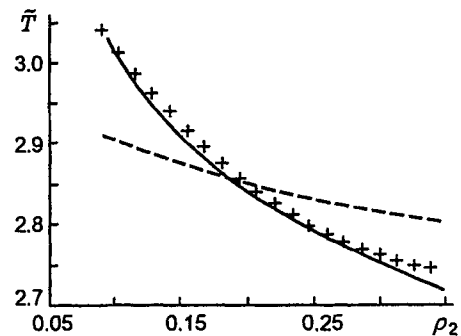


Fig. 1. The limiting temperature \tilde{T} of the medium as a function of the average density of manganese particles: particle radius $5 \mu\text{m}$ and radius of containment vessel 1.5 cm ; points + denote experimental data [9], the dashed curve refer to the calculation with the constants developed for describing the oxidation of solid magnesium in air and the solid curve refer to the author's calculations.

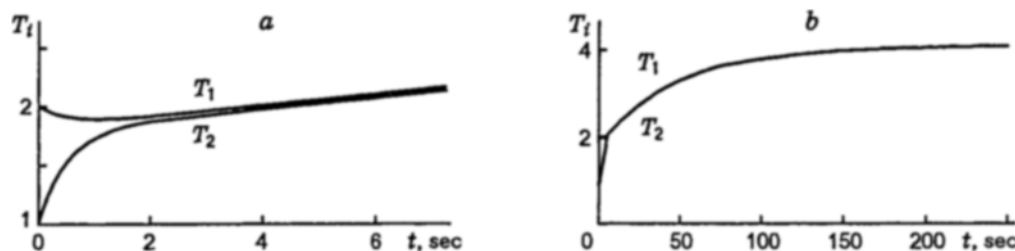


Fig. 2. Particle temperature as a function of time: (a) nonequilibrium thermal regime at the initial times, (b) quasiequilibrium heating of the phases and the approach to a stationary state B.

TABLE 1

t_{ign} and α as Functions of the Particle Radius for $T_{1,0} = T_{2,0} = 1$, $\bar{T} = 3.03$, and $\alpha_- \cdot 10^5 = 1.598$

| $r, \mu\text{m}$ | 0.01 | 0.1 | 1 | 5 | 6 | 7 | 8 | 9 | 10 | 15 | 16 | 17 |
|-----------------------|-------------------|-------------------|-------------------|-------|-------|-------|------|-------|-------|-------|-------|------|
| t_{ign}, sec | 3.99 | 5.81 | 9.58 | 17.06 | 18.85 | 20.76 | 22.8 | 25.21 | 27.93 | 66.19 | 91.32 | none |
| $\alpha \cdot 10^5$ | $9.55 \cdot 10^4$ | $9.55 \cdot 10^3$ | $9.55 \cdot 10^2$ | 0.48 | 0.57 | 0.67 | 0.76 | 0.86 | 0.95 | 1.42 | 1.52 | — |

in the cloud ignition formula. To do this, by analogy with [7, 8], we write down the Semenov conditions on the catastrophe/ignition manifold for the two radii of the particles and for the limiting temperatures of the region surrounding the exploding cloud. These two equations have an analytic solution for the unknowns, $E = 48.54$ and $K = 3.054$. Figure 1 shows the dependence of the limiting temperature of the medium on the average density of magnesium particles obtained using these parameter values. In this and the remaining figures, the temperatures are relative to 300 K.

Next, the calculations were done for the direct problem, i.e., the heating dynamics of the components of the mixture were determined. As the above remarks show, regular and catastrophic heating of the cloud occur. Thus, let $T_{1,0} = 2$, $T_{2,0} = 1$, $r = 5 \mu\text{m}$, $R_1 = 1.5 \cdot 10^{-3} \text{ m}$, and $\bar{T} = 4$. For this case, $\alpha_- \cdot 10^4 = 2.3 \leq \alpha \cdot 10^{-4} = 4.43$, ignition does not occur, and the particles undergo regular heating out of thermal equilibrium (the quantity $A = nS\alpha_{12}/\alpha_1 S_1 \approx 10$ is not too large), as shown in Fig. 2. In the first stage of heating of the system, the gas transfers heat to the particles so its temperature drops (see Fig. 2a), and then the temperatures of the phases approach one another, but the gas has a higher temperature. The rates of change of the temperatures of the phases do not differ greatly here, and the phases subsequently approach thermal equilibrium on the lower branch of the ignition manifold. This is shown in Fig. 2b for later times.

Decreasing the vessel radius to $R_3 = 1.5 \cdot 10^{-4} \text{ m}$ causes the zone where the gas temperature is re-

duced to vanish because of more rapid heating of the smaller volume of gas; there the temperature relaxation time is about 4 msec.

Let us see if this mathematical model for the ignition of a magnesium cloud describes the scale factor described in [9], i.e., the reduction in the limiting ignition temperature of the system as its size is increased. This situation can be illustrated by this sort of computational data. Let $T_{1,0} = 2$ and $T_{2,0} = 1$; then for $R_3 = 1.4 \text{ cm}$ ignition sets in within the interval $\bar{T} \in (832.835)$ and for $R_3 = 1.5 \text{ cm}$, the cloud ignites for $\bar{T} \in (823.825)$.

We study the effect of the particle radius on the ignition delay time t_{ign} . Calculations were done for different particle radii (see Table 1) and for a constant average density of the particles. The third row of the Table 1 lists a dimensionless characteristic of the process which controls the onset of ignition in the system for $r \leq 17 \mu\text{m}$. For $r \geq r_* \geq 17 \mu\text{m}$ ignition is not observed in this system. This happens because the convective heat transfer coefficient is proportional to r^{-2} , i.e., decreases with increasing particle radius. As a consequence, the heating of the particle extends to temperatures where there is significant heat release from the chemical reaction, so that the ignition delay increases.

The effect of the ambient temperature on the ignition delay was studied. The results of these calculations are shown in Table 2. Evidently, when the temperature is not high enough ignition does not occur in the system (the first column of Table 2) and as \bar{T} increases the preignition period is reduced.

The dependence of the heating dynamics on the

TABLE 2

| t_{ign} and α as Functions of Ambient Temperature for $T_{1,0} = 2$, $T_{2,0} = 1$, and $R_3 = 1.5$ cm | | | | | | | |
|--|-------------|-------|-------|------|-------|-------|------|
| \bar{T} | 2.67 | 3.03 | 3.17 | 3.3 | 3.5 | 3.67 | 4 |
| t_{ign} , sec | no ignition | 14.86 | 11.66 | 9.34 | 7.86 | 6.8 | 5.44 |
| $\alpha \cdot 10^5$ | 1.6 | 2.57 | 4.4 | 7.11 | 10.96 | 23.05 | 0.32 |

initial gas temperature was determined by varying the latter. The results are shown in Table 3. The temperatures of the phases behave as follows: for equal initial temperatures of the phases, the gas heated at the vessel walls transfers heat to the particles and the phases essentially arrive at thermal equilibrium. This is related to the fact that the zero isocline of the energy equation for the gas can be used to determine $\Delta T_1 = A\Delta T_2/(1+A)$, where $A = nS\alpha_{12}/\alpha_1 S_1$. Since $A \gg 1$ in these calculations, the gas temperature approaches that of the particles and then the cloud of particles, which is in thermal equilibrium, ignites.

The reaction of the cloud to preliminary heating of the particles, i.e., when the initial temperature $T_{2,0}$ is changed, is similar. Thus, for $r = 5 \mu\text{m}$ and $T_{1,0} = 1$, the ignition delays are 9.55, 9.21, 8.84, 8.71, and 8.43 for $T_{2,0} = 300, 600, 900, 1000,$ and 1200 K, respectively. The dependence of the induction time on the amount of particles in the cloud is shown in Fig. 3. It can be seen that as ρ_2 increases with the other conditions held constant, t_{ign} decreases. This happens because of increased heat transfer from the

gas to the particles in the first convective stage of the heat transfer process, as well as because of increased heat release from the chemical reaction.

Increasing the radius of the reaction vessel leads to the establishment of an adiabatic ignition process. In fact, increasing R_3 over an order of magnitude, beginning at 15 cm, yields induction times of 21.27, 23.26, 23.28, and 23.28 with a gas temperature of 900 K and, of the ambient, 1050 K. At the same time, the Nusselt number for the typical vessel sizes [9] has no effect on the development of ignition. This is because $A \gg 1$ and the effective heat transfer coefficient for the mixture ceases to depend on the heat transfer mechanism between the gas and particles.

The effect of the heat release in both phases was studied. In particular, for $\sigma = 0$, which corresponds to heat release at the particles alone, $t_{\text{ign}} = 9.55$. As σ increases, the ignition delay increases up to the point where the particles in the cloud do not ignite. Thus, for $\sigma = 0.5, 0.6, 0.7,$ and 0.8 , respectively, $t_{\text{ign}} = 11.9, 12.9, 14.6, 17.83$. If, on the other hand, $\sigma = 0.95$, the cloud does not ignite.

TABLE 3

t_{ign} as a Function of the Initial Gas Temperature for $T_{2,0} = 1$, $\bar{T} = 3.5$, $\alpha \cdot 10^5 = 0.48$, and $R_3 = 1.5$ cm

| $T_{1,0}$ | 1 | 2 | 3 | 3.5 | 4 |
|------------------------|------|------|------|------|------|
| t_{ign} , sec | 9.55 | 7.86 | 5.06 | 2.87 | 1.07 |

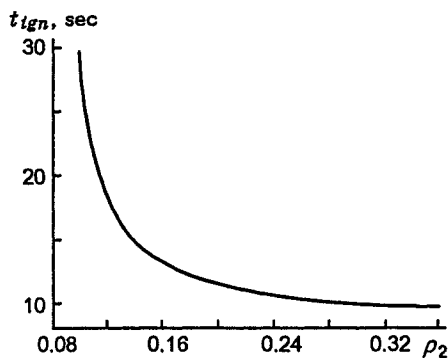


Fig. 3. Ignition delay as a function of the average particle density.

CONCLUSIONS

A distributed mathematical model for the ignition of gaseous suspensions of metal particles has been proposed which takes into account the heat release in both phases.

In the framework of a point approximation for this model, we have obtained the conditions for various types of heating dynamics of the gaseous suspension and determined the kinetic constants in an empirical formula for the growth of the oxide film which made it possible to describe the experimental dependence of the limiting temperature of the medium on the average density of particles in a magnesium cloud.

It has been shown numerically that when the volumes enclosing the cloud of particles are small, nonequilibrium regular heating of the mixture occurs leading asymptotically to an equilibrium state lying on the lower branch of the catastrophe/ignition curve and when the vessel size is increased, ignition occurs.

It has been found quantitatively and qualitatively that, with the other parameters fixed, there is

a critical radius r_* for the particles in the cloud, such that for smaller radii than this, the cloud ignites and for greater, regular heating takes place.

Increasing the fraction of heat released in the gas leads to regular heating of the particles in the cloud.

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REFERENCES

1. A. E. Medvedev, A. V. Fedorov, and V. M. Fomin, "Description of ignition and combustion of gaseous suspensions using the methods of continuum mechanics," *Fiz. Goreniya Vzryva*, **20**, No. 2, 3-9 (1984).
2. V. M. Boiko, A. V. Fedorov, V. M. Fomin, et al., "Ignition of small solid particles behind shock waves," in: J. R. Bowen, N. Manson, and R. Soloukhin (eds.), *Progress in Astronautics and Aeronautics*, Vol. 87: *Shock Waves, Explosions, and Detonations* (1983), pp. 71-87.
3. Yu. V. Kazakov, A. V. Fedorov, and V. M. Fomin, "Mathematical modeling of ignition in dusty gases," *Arch. Combust.*, **7**, Nos. 1 and 2, 7-17 (1987).
4. A. V. Fedorov and V. M. Fomin, "Mathematical modeling of ignition of aerosuspension," in: *Int. Colloquium on Advanced Computation and Analysis of Combustion*, Moscow, Russia, May 12-15 (1997).
5. R. I. Nigmatulin, *Dynamics of Multiphase Media*, Parts 1 and 2, Hemisphere Publ., New York (1991).
6. É. I. Rumanov and B. I. Khaikin, "Critical conditions for self-ignition of particle aggregates," *Fiz. Goreniya Vzryva*, **5**, No. 1, 129-136 (1969).
7. A. V. Fedorov, "Physical and mathematical modeling of the ignition of fine magnesium particles," Preprint No. 12-94, Inst. of Theor. and Appl. Mech., Russian Acad. of Sci., Sib. Div., Novosibirsk (1993).
8. A. V. Fedorov, "Numerical-analytic study of the ignition of magnesium particles," *Fiz. Goreniya Vzryva*, **32**, No. 1, 75-84 (1996).
9. A. M. Matsko, K. M. Kopeika, D. I. Polishchuk, et al., "Effect of external heat transfer on the critical conditions for ignition of a gaseous suspension of magnesium particles," in: *The Physics of Aerodispersed Systems* [in Russian], No. 20 (1980), pp. 53-56.