EXPLOSIVE GENERATION OF HETEROGENEOUS DETONATION WAVES IN AEROCOLLOIDS OF A UNITARY FUEL

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The process of explosive initiation of spherical, heterogeneous detonation waves in monodisperse, homogeneous aerocolloids of a unitary fuel is modeled mathematically. It is shown that regimes of decaying and detonating combustion of the reacting disperse mixtures are possible, depending on the initial mass concentration and initial particle size in the mixture. It is established that the laws governing the mass transfer of burning particles have a significant influence on the patterns of explosive generation and propagation of detonation waves in unitary fuel aerocolloids. The critical (maximum) diameter of the unitary fuel particles, below which the shock initiation of heterogeneous combustion is possible, is determined as a function of the particular value of their relative mass concentration in the mixture.

The nonimpact initiation and evolution of plane heterogeneous detonation waves in aerocolloids of a unitary (oxidizer-containing) fuel have been analyzed theoretically in several papers [1-3]. In this article we analyze numerically the explosive initiation and subsequent evolution of spherical and cylindrical detonation waves in aerocolloids of a unitary fuel.

BASIC EQUATIONS

We consider a mixture of an inert gas and, suspended in it, solid particles of a unitary fuel, whose combustion results in the formation of gaseous products of chemical reaction. The customary assumptions of the mechanics of multiphase disperse continua are used to describe the motion of the mixture [3]: The ranges of appreciable variation of the parameters of the motion are much greater than the characteristic particle diameters and the distances between them; viscosity and heat-conduction effects are significant only in processes of interaction between the carrier and disperse phases; the unitary fuel particles are incompressible, monodisperse, and spherical; the volume content of particles of the disperse in the mixture is very small; the particles do not collide or form clusters (agglomerate); the contributions of unsteady Basset forces, buoyancy, and additional masses to the total force of interaction between phases are negligible.

Furthermore, in accordance with [1, 2], we adopt the following assumptions as to the mechanism of ignition and combustion of individual unitary fuel particles: A particle ignites when it heats up to the ignition temperature, during which time the temperature distribution in the particle interior is uniform (an elementary chemical reaction of the type C \rightarrow G takes place, where C and G are the chemical symbols of the condensed unitary fuel and its gaseous combustion products); the temperature of a burning particle remains constant, i.e., the entire heat input to its surface is spent in gasification of the fuel.

Within these assumptions the system of differential equations of one-dimensional motion of the gas and unitary fuel particles can be written in the divergent form [3]

\[
\frac{\partial \rho_{1k}}{\partial t} + \frac{1}{z' \nu} \frac{\partial \rho_{1k} v_1 z'}{\partial z} = (k - 1) J, \quad \rho_1 = \sum_{k=1}^{2} \rho_{1k},
\]
\[
\begin{align*}
    \frac{\partial \rho_2}{\partial t} + \frac{x}{x^\nu} \frac{\partial \rho_2 v_2 x^\nu}{\partial x} &= -J, \\
    \frac{\partial n}{\partial t} + \frac{1}{x^\nu} \frac{\partial n v_2 x^\nu}{\partial x} &= 0, \\
    \frac{\partial \rho_i v_i}{\partial t} + \frac{1}{x^\nu} \frac{\partial \rho_i v_i x^\nu}{\partial x} + (2 - i) \frac{\partial \rho}{\partial x} &= (-1)^i (F_{12} - J v_2), \\
    \frac{\partial p_{2e_2}}{\partial t} + \frac{1}{x^\nu} \frac{\partial p_{2e_2} x^\nu}{\partial x} &= Q_{12} \eta(-J) - J e_2, \\
    \frac{\partial}{\partial t} \sum_{i=1}^2 \rho_i E_i + \frac{1}{x^\nu} \frac{\partial}{\partial x} \sum_{i=1}^2 (\rho_i E_i v_i + p a_i v_i) x^\nu &= 0, \\
    \rho_{1k} = \rho_{0k} \alpha_k, \quad \rho_i = \rho_{0i} \alpha_i, \quad E_i = e_i + 0.5 v_i^2, \quad (i, k = 1, 2), \quad \alpha_2 = \frac{1}{6} \pi d^3 n, \quad \alpha_1 + \alpha_2 = 1.
\end{align*}
\]}

This system includes equations for: conservation of mass of the inert gas \((k = 1)\), the gaseous products of chemical reaction \((k = 2)\), and the unitary fuel particles; conservation of the number of unitary fuel particles; the heat input to the fuel particles; conservation of the total energy of the entire mixture; the law of conservation of momenta of the carrier phase (the mixture of the inert gas and the chemical reaction products). The subscripts \(1\) and \(2\) refer to the parameters of the gaseous and disperse phases, \(\rho_{1k}\) and \(\rho_{0k}\) are the average and true densities of the gaseous components, \(\rho_1, \rho_{01}, v_1, e_1,\) and \(E_1\) are the average and true densities, particle velocity, volume content, and specific internal and total energies of the \(i\)-th phase \((i = 1, 2)\), \(n\) is the number of particles per unit volume of the mixture, \(d\) is the particle diameter, \(p\) is the pressure of the gaseous carrier phase, \(F_{12}\) is the intensity of the force interaction between the carrier phase and the disperse particles, \(Q_{12}\) is the heat input rate to the unitary fuel particles, \(J\) is the rate of mass transfer between the carrier and disperse phases per unit volume of the mixture, \(\nu\) is a symmetry parameter, which takes the values 0, 1, and 2 for planar, cylindrical, and spherical symmetry, respectively, and \(\eta\) is the Heaviside unit step function.

To close the system of differential equations (1), we introduce the equations of state of an ideal, calorifically perfect gas [4] as the equations of state of the inert gas and the products of combustion of the unitary fuel particles:

\[
\begin{align*}
    p_{1k} &= \rho_{0k} R_{1k} T_1, \\
    e_{1k} &= c_{v1k} (T_1 - T_0) + e_{1k}^0, \\
    (R_{1k}, c_{v1k}, e_{1k}^0, T_0 = \text{const}, k = 1, 2), \quad (2)
\end{align*}
\]

where \(R_{1k}, c_{v1k},\) and \(p_{1k}\) are the gas constant, the specific heat at constant volume, and the partial pressure of the \(k\)-th component of the gas mixture, \(T_1\) is the temperature of the gaseous phase, and \(e_{1k}^0\) is the specific internal energy of the \(k\)-th component of the gas mixture at a certain fixed temperature \(T_0\).

The equations of state of the carrier gas, on the whole, are specified in accordance with Dalton's law and the condition of additivity of the internal energy of the carrier phase with respect to the masses of its constituent gas components [5]:

\[
\begin{align*}
    p &= \sum_{k=1}^2 p_{1k} = \rho_1 R_1 T_1, \quad R_1 = \sum_{k=1}^2 x_{1k} R_{1k}, \\
    e_1 &= \sum_{k=1}^2 x_{1k} e_{1k} = c_{v1}(T_1 - T_0) + e_{11}, \\
    c_{v1} &= \sum_{k=1}^2 c_{v1k} x_{1k}, \\
    e_{11} &= \sum_{k=1}^2 x_{1k} e_{1k}^0, \quad x_{1k} = \frac{\rho_{1k}}{\rho_1} \quad (k = 1, 2). \quad (3)
\end{align*}
\]

The following equations of state are used for incompressible disperse phase particles [4]:

\[
\begin{align*}
    \rho_2^0 = \text{const}, \quad e_2 = c_2 (T_2 - T_0) + e_2^0, \quad (c_2, e_2^0 = \text{const}), \quad (4)
\end{align*}
\]

where \(c_2\) and \(T_2\) are the specific heat and temperature of the unitary fuel particles. The constants \(e_{12}^0\) and \(e_2^0\) in the equations of state (2) and (3) obey the normalization condition [4]

\[
e_2^0 - e_{12}^0 = Q^0 - \left( \frac{p_0}{\rho_{10}} - \frac{p_{120}}{\rho_{120}} \right). \quad (5)
\]