A multicomponent one-velocity model for inert and reactive porous mixtures exposed to explosive detonation

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Abstract. The paper provides a multicomponent one-velocity model for numerical simulation of the behavior of inert and reactive porous mixtures exposed to explosive detonation. A system of equations describing the nonstationary adiabatic motion of both inert and reactive mixture components is presented. The relations for achieving mechanical equilibrium in a multicomponent mixture exposed to explosive detonation are considered within the framework of an elastic-plastic medium. To simulate explosive detonation, the upper part of the ampoule is exposed to pressure in an axial direction and the lateral side of the ampoule is exposed to pressure in a radial direction.

1. Introduction
Explosive loading is a promising direction for obtaining new materials with improved structure and properties [1−3]. Explosive detonation causes various physical and chemical transformations in substances, the behavior of which can not be predicted without special experimental and theoretical studies [4, 5]. Since the synthesis of materials and the formation of materials structure develop through stages, the explosive loading can selectively affect the various stages of these processes. This provides an opportunity to obtain final materials with different structures and properties using the same initial composition. The advantage of explosive loading is, first of all, a high and evenly distributed density of final materials [6]. At the same time various processes and their stages demand different time, therefore, not all processes will be able to develop for short time, which is typical for explosive loading and the substance will react to loading in another way in comparison with slow explosive loading. Consequences of explosive loading of substances are too diverse and complicated to be predictable. However, systematic fundamental investigations in physics and chemistry of shock waves give considerable opportunities to control structural chemical and phase transformations, improve the properties of materials, and produce new materials with unique properties.

In this work the finite element method is used to solve the spatial problems of explosive loading of reactive and inert porous multicomponent mixtures. Based on this method, a discrete model of a multicomponent mixture consisting of a set of finite elements connected with each other at node points is constructed. Within each element, all components are distributed over the volume occupied by the whole mixture and their center-of-mass velocities depend on different elastoplastic properties of the components. After the interaction of the components and their joint contribution to the nodal forces of the elements, the components of the mixture acquire the velocity of the corresponding element [7]. Equal pressure of the components is used as a condition for the joint deformation of the components in the mixture and for determining the volume actually occupied by the component. The time step is
chosen to ensure the stability of calculations. The calculation cycle can be repeated until either of the specified calculation criteria is reached.

The velocities and displacements of the nodes and, consequently, the new position of interacting components are determined by integrating the equations of motion taking into account the total contribution of the components to the nodal forces and the corresponding boundary conditions. The purpose of this paper is to use a multicomponent one-velocity model in the combination with the relations of the modified finite element method for the numerical study of the behavior of inert and reactive porous mixtures under explosive loading.

2. Formulation of the problem
The system of equations governing the nonstationary adiabatic motion of components in a space-fixed volume of a compressible solid mixture $V$ bounded by a surface $S$ with allowance for the exchange of momentum, energy and mass between components as well as the evolution of microdamages and chemical transformations comprises the continuity equation, the equation of motion, the energy equation [8]:

$$
\frac{\partial}{\partial t}(\alpha_i \rho_i) + \nabla \alpha_i \rho_i \mathbf{v}_i = 0, \quad (i=1, 2, \ldots, N),
$$

$$
\alpha_i \rho_i \frac{d \mathbf{v}_i}{dt} = \nabla \sigma_i + \alpha_i \sum_{j=1}^{N} \alpha_j \mathbf{R}_{ij}, \quad (i=1, 2, \ldots, N),
$$

$$
\alpha_i \rho_i \frac{d E_i}{dt} = \sigma_i \varepsilon_i + \alpha_i \sum_{j=1}^{N} \alpha_j F_{ij}, \quad (i=1, 2, \ldots, N),
$$

where

$$
\frac{d}{dt} = \frac{\partial}{\partial t} + \mathbf{v}_i \cdot \nabla.
$$

Here, $t$ is the time, $\rho_i$ is the density of the $i$-th component equal to the mass of the $i$-th component per unit volume of the $i$-th component, $\mathbf{v}_i$ is the velocity vector, $E_i$ is the internal specific energy, $\varepsilon_i$ is the strain rate tensor, $\sigma_i=P_i \delta_i+S_i$ is the stress tensor, $P_i$ is pressure, $S_i$ is the stress deviator, $R_{ij}$ is the intensity of the momentum exchange between the $j$-th and $i$-th components, $F_{ij}$ is the intensity of the energy exchange between the $j$-th and $i$-th components, $N$ is the number of components.

To simulate fracture in multicomponent media, a damaged medium model characterized by the presence of microcavities (pores, cracks) is used. The total volume of each component $W_i$ contains an undamaged part occupying the volume $W_s$, and characterized by the density $\rho_s$, and the microcavities (voids) occupying the volume $W_f$, in which the material density is assumed to be zero. The average density of the damaged component is related to the parameters introduced by the relation $\rho_i = \rho_s \left( \frac{W_s}{W_i} \right)$. The damage of the component is characterized by the specific volume of microdamages $V_f = W_f / W_i$. All microcavities are assumed to be inside the components and are not connected with their external surface, and the damaged medium model is applied independently for each component in the mixture.

Chemical reactions are simulated using a zeroth-order kinetic relation characterized by a constant rate of chemical transformations [9, 10]:

$$
J_{ij} = \frac{dn}{dt} = \begin{cases} 0, & \text{if } \eta = 1 \text{ or } (T_i < T_\eta \text{ and } P < P_\eta) \\ f(P_\eta), & \text{if } \eta < 1 \text{ and } (T_i \geq T_\eta \text{ or } P \geq P_\eta) \end{cases},
$$

$$
f(P_\eta) = \begin{cases} K_0, & \text{if } P < P_\eta \\ K_p P_\eta, & \text{if } P \geq P_\eta, \end{cases}
$$

2
where \( T_i \) is the temperature, \( P \) is the matched pressure of components, and \( T_\eta, P_\eta, K_\eta, K_0 \) are the constants, \( \eta \) is the conversion degree.

The equation describing the change in the specific volume of pores is as follows [11]:

\[
\frac{dW_{i_1}}{dt} = \begin{cases} 
0, & \text{if } |P_{s_i}| \leq P_* \text{ or } (P_{s_i} > P_* \text{ and } W_{i_1} = 0) \\
-\text{sign}(P_{s_i}) \frac{K_{f_i}}{|P_{s_i} - P_*|} (V_{s_i} + W_{i_1}), & \text{if } P_{s_i} < -P_* \text{ or } (P_{s_i} > P_* \text{ and } W_{i_1} > 0),
\end{cases}
\]

here \( P_{s_i} \) is the pressure in a solid component of the mixture, \( V_{s_i}, V_2, P_{k_i}, K_{f_i} \) are the experimental material constants.

Pressure in the undamaged component of the mixture is a function of specific volume and internal energy and is determined by the Mie-Grüneisen equation of state according to the formula [12]:

\[
P = \rho_0 u_{e_i}^2 \mu_j + \rho_0 u_{e_i}^2 \left[ 1 - \gamma_0 / 2 + 2 (b_i - 1) \right] \mu_j^2 + \rho_0 u_{e_i}^2 \left[ 2 (1 - \gamma_0 / 2) (b_i - 1) + 3 (b_i - 1)^2 \right] \mu_j^3 + \gamma_0 \rho_0 E_i,
\]

Here \( \mu_j = V_j / (V_j - V_{f_i}) - 1, \ \gamma_0 \) is the Grüneisen coefficient, \( V_0 \) and \( V_i \) are the initial and current specific volumes, respectively, and \( u_{e_i} \) and \( b_i \) are the constants of the Hugoniot shock adiabat described by the relation [1]:

\[
u_{s_i} = u_{e_i} + b_i u_{p_i},
\]

here \( u_{s_i} \) is the shock wave velocity and \( u_{p_i} \) is the particle velocity of a component behind the shock wave front.

To achieve mechanical equilibrium in the components of the mixture, the approach proposed below is used. In this case, it is necessary to find a new pressure that is the same to all components, and mechanical equilibrium is achieved when the condition \( \alpha_1 + \alpha_2 + \ldots + \alpha_N = 1 \) is satisfied. Such mechanical equilibrium can be achieved by solving the system of equations as follows:

\[
P = P_i + \Delta P_i = P_i - \frac{K_i}{\alpha_i} \Delta \alpha_i,
\]

\[
\sum_{i=1}^{N} \Delta \alpha_i = 0,
\]

where \( K_i = a_i \rho_i c_i^2 \) is the volume compression modulus, and \( c_i \) is the volume velocity of sound. The new value of the volume fraction of the components \( \Delta \alpha_i \) is determined from the equations as follows:

\[
P = \sum_{i=1}^{N} \frac{a_i P_i}{K_i} / \sum_{i=1}^{N} \frac{a_i}{K_i},
\]

\[
\Delta \alpha_i = \frac{a_i}{K_i} (P_i - P).
\]

\[
\alpha_i \rho_i E_i = \alpha_i \rho_i E_i - P \Delta \alpha_i.
\]

After equalizing the pressures of the components, a new value of the internal energy \( E_i \) is determined:
To provide the mass conservation of the mixture, it is necessary to obtain a new value of density:

$$\rho_i = \frac{\alpha_i \rho_i}{\alpha_i + \Delta \alpha_i}.$$ 

All equations are applied iteratively with an appropriate evaluation of the equation of state for determining the pressure and volume compression modulus of each component. The change in porosity is assumed to be caused only by the spherical stress component or pressure, whereas the components of the stress deviator are bounded by the independent deviatoric yield function [13]:

$$2G_i \left( \varepsilon_{ij} - \frac{1}{3} \varepsilon_{kk} \delta_{ij} \right) = \frac{dS^0_{ij}}{dt} = \lambda S_{ij},$$

where $dS^0_{ij}/dt$ is the Jaumann derivative given by:

$$\frac{dS^0_{ij}}{dt} = \frac{dS_{ij}}{dt} - S_{ij} W_{ij} - S_{ij} W_{kk},$$

and $2W_{ij} = \partial u_i/\partial x_j - \partial u_j/\partial x_i$. The parameter $\lambda$ is zero for elastic deformation, and for plastic deformation is determined from the Mises yield criterion [13]:

$$S_{ij} S_{ij} = \frac{2}{3} \sigma_i^2.$$ 

Here $G_i$ is the shear modulus and $\sigma_i$ is the dynamic yield point [11, 12, 14]:

$$G_i = G_{0i} K_{Ti} \left( 1 + \frac{c_i P_i}{(1 + \mu_i)^{1/3}} \right) \frac{V_{ij}}{(V_{ij} + V_{i3})},$$

$$\sigma_i = \begin{cases} \sigma_{0i} K_{Ti} \left( 1 + \frac{c_i P_i}{(1 + \mu_i)^{1/3}} \right) \left( 1 - \frac{V_{ij}}{V_{i4}} \right), & \text{if } V_{ij} \leq V_{i4}, \\ 0, & \text{if } V_{ij} > V_{i4} \end{cases},$$

$$K_{Ti} = \begin{cases} 1, & \text{if } T_0 \leq T_i \leq T_l, \\ \frac{T_{i0} - T_i}{T_{i0} - T_{i1}}, & \text{if } T_{i1} < T_i < T_{i0}, \\ 0, & \text{if } T_i \geq T_{i0}. \end{cases}$$

Here $T_{i0}$ is the melting point of components and $c_i, V_{ij}, V_{i4}, T_i$ are the constants of components. In the computations, the function $K_{Ti}(T_i)$ was chosen to model the nonthermal character of plastic deformation and dynamic strength of solids at high strain rates ($10^5$ sec$^{-1}$ or higher).

To calculate the temperature, the relations are used as follows:
\[ dT_i = \begin{cases} 
\frac{d(E_i - E_{i0})}{c_p}, & \text{if } T_i < T_{i0} \\
0, & \text{if } T_i = T_{i0}, \\
\frac{d(E_i - E_{i0} - \Delta H_{i0})}{c_p}, & \text{if } T_i > T_{i0} 
\end{cases} \]

where specific heat \( c_{p_i} \) increases linearly as the temperature increases to the melting point of the substance:

\[
c_{p_i} = \begin{cases} 
c_{p_i}^0 + \frac{c_{p_i}^L - c_{p_i}^0}{T_{i0} - T_{i0}}(T_i - T_{i0}), & \text{if } T_{i0} \leq T_i < T_{i0} \\
c_{p_i}^L, & \text{if } T_i \geq T_{i0} \end{cases}
\]

3. Numerical results

The axisymmetric problem of explosive loading is considered for multicomponent mixtures such as Al/Tf, Al/S and Al/S/C placed into a cylindrical steel ampoule. The porosity of all mixtures was 0.4. The height and diameter of the cylindrical samples were 64 mm and 14 mm, respectively. The thickness of the lateral wall of the ampoules was 3 mm and the thickness of top and bottom lids was 10 mm. The height and external diameter of the ampoules was 84 mm and 20 mm, respectively. The detonation velocity used in the numerical computations was measured experimentally and was equal to \( D = 2.8 \) km/s. The \( P_0 = 3.2 \) GPa value was chosen from numerical and experimental estimations.

In the numerical computations the thickness of the explosive \( \Delta z \) in the axial direction was varied to study the effect on a final shape and size of the ampoules. The value \( \Delta r \) for the explosive acting radially on the lateral wall of the ampoule was a constant and was equal to 18 mm.

Figure 1 shows the change in the shape of cylindrical ampoules depending on the thicknesses of the explosive acting in the vertical direction on the upper part of the ampoule at the time of 80 microseconds after explosive loading.

![Figure 1](image)

**Figure 1.** Shape of cylindrical ampoules depending on the thicknesses of the explosive acting on the upper part of the ampoule at the time of 80 microseconds after explosive loading: \( \Delta z = 5 \) mm (a); \( \Delta z = 30 \) mm (b); \( \Delta z = 40 \) mm (c).
The numerical computations show a significant effect of the explosive layer on explosive loading. For the small value of the thickness $\Delta z$, elongation of the ampoules is observed in the axial direction (figure 1a). When the thickness $\Delta z$ is large, the upper part of the ampoule is subjected to additional load and the top lid of the ampoules is deformed (figure 1c). Based on the numerical computations, we can conclude that the use of the explosive layer with a thickness of $0\div13$ mm in the axial direction increases the height of the ampoule. The use of the explosive layer with a thickness of $35\div40$ mm strongly deforms the ampoules for all cases. The parameters of the ampoule obtained for the axial explosive layer with a thickness of $30$ mm have demonstrated the positive explosive loading. The bottom lid of the ampoules is not deformed for all cases.

4. Conclusion
The numerical computations obtained using the developed one-velocity multicomponent model and experimental data have shown that the chosen parameters of explosive loading provides the obtaining of materials with desired properties. For an example, the effect of the thickness of the explosive layer on explosive loading is clearly observed. The insufficient or excessive thickness of explosives may be a reason for incompletely compacted final products or leads to cracks in products. Explosive synthesis in reactive mixtures has been also found to depend on the dispersity of components in mixtures and the duration of explosive loading. A decrease in the particle size of reagents simplifies and accelerates reactions.

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