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NUMERICAL SIMULATION OF THE EXPLOSIVE COMPACTION OF MULTICOMPONENT MIXTURES

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ABSTRACT

The work considers the explosive compaction of a three-component mixture from aluminium, sulphur and carbon placed into a cylindrical steel ampoule. Behaviour of the mixture is described by a mathematical model of a multicomponent medium. The numerical computations have demonstrated that the thickness of the explosive layer essentially influences on the final result of explosive compaction. The insufficient or excessive thickness of explosives may be a reason for incompletely compacted final products or lead to the formation of cracks or damage.

Keywords: explosive compaction, multicomponent mixture, numerical simulation.

INTRODUCTION

Producing and using new advanced materials is often connected with extreme conditions such as fast processes, high pressures and temperatures (Eakins, 2009; Prümmer, 1989; Zelepugin, 2017). These processes are accompanied by structural changes and chemical reactions. At present, explosive technologies are commonly used in metal processing, including the technologies of shaping, welding, cutting, hardening, and compaction. Many of these technologies are already used in production, while the application of explosive compaction is restricted due to lack of ways to control and manage this process, and has not yet reached the level of technology so far. Many theoretical questions of explosive compaction of solid inert multi-component mixtures must be answered (Zelepugin, 2016).

This is caused by the complexity of studying the process of explosive compaction and inability to obtain reliable data on the dynamics of this phenomenon using final results of the experiments. The analysis of this process requires developing mathematical models, including the introduction of additional parameters and equations. There is a need also to take into account the initial parameters and characteristics of components in the mixture, and develop appropriate computational algorithms as well. This approach, together with the available experimental data, is to extend the range of application for numerical models and provide an opportunity to obtain reliable information on the mechanisms and dynamics of structural changes and ways to produce new advanced materials.

The aim of this paper is a study and numerical simulation of aluminum-sulfur-carbon mixtures under explosive compaction, considering the thickness of the explosive, using a multicomponent medium model (Ivanova, 2010). The numerical computations were carried out using the research computer code based on the modified finite element method without construction of the global stiffness matrix (Gorelski, 1997).

FORMULATION OF THE PROBLEM

The system of equations describing the nonstationary adiabatic motion of each component in a solid inert compressible mixture comprises the equations of continuity (Eq. 1), momentum (Eq. 2), and energy (Eq. 3) (Nigmatulin, 1991):

$$\frac{\partial}{\partial t}(\alpha_i\rho_i) + \nabla\alpha_i\rho_i\upsilon_i = 0, \ (i = 1, 2, \ldots, N), \tag{1}$$

$$\alpha_i\rho_i\frac{d_i\upsilon_i}{dt} = \nabla\sigma_i + \alpha_i\sum_{j=1}^{N}\alpha_j\mathbf{R}_{ji}, \ (i = 1, 2, \ldots, N), \tag{2}$$

$$\alpha_i\rho_i\frac{d_iE_i}{dt} = \sigma_i\varepsilon_i + \alpha_i\sum_{j=1}^{N}\alpha_j\Phi_{ji}, \ (i = 1, 2, \ldots, N), \tag{3}$$

where $\frac{d_i}{dt} \equiv \frac{\partial}{\partial t} + \upsilon_i^k\frac{\partial}{\partial x^k}$.

Here t is the time, ρ_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, υ_i is the velocity vector, E_i is the internal specific energy, ε_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_{ji} is the intensity of the momentum exchange between the j-th and i-th components, Φ_{ji} is the intensity of the energy exchange between the j-th and i-th components, N is the number of components.

Volume fractions of the mixture occupied by each component (Nigmatulin, 1991) are given by:

$$\alpha_1 + \alpha_2 + \ldots + \alpha_N = 1, \ (\alpha_i \geq 0), \ \alpha_i = \rho_i^*/\rho_i,$$

where ρ_i^* is the reduced density (mass of the i-th component per unit volume).

Evolution of porosity in the material (compression and growth of pores) is simulated using a kinetic model of the active type, which determines changes in specific volume of pores influencing on the material properties and causing stress relaxation (Kanel, 2007):

$$\frac{dV_{fi}}{dt} = \begin{cases} 0, \ \text{if} \ |P_{si}| \leq P_i^* \ \text{or} \ (P_{si} > P_i^* \ \text{and} \ V_{fi} = 0) \\ -\operatorname{sign}(P_{si})K_{fi}(|P_{si}| - P_i^*)(V_{2i} + V_{fi}), \\ \text{if} \ P_{si} < -P_i^* \ \text{or} \ (P_{si} > P_i^* \text{and} \ V_{fi} > 0), \end{cases}$$

where $P_i^* = P_{ki}V_{1i}/(V_{fi} + V_{1i})$, P_{si} is the pressure in the solid (undamaged) part of the i-th component in the mixture, V_{1i}, V_{2i}, P_{ki}, K_{fi} are experimentally determined constants of the material.

Studying the deformation of multicomponent media, it is necessary to take into account the state and response of each component, as well as, in contrast to a homogeneous mixture, not only the displacement of the external boundaries of the selected volume, but also the displacement of components in the selected volume of the mixture. In this paper, we consider the equality of pressures during the interaction of components to be a condition for joint deformation of components in the mixture, which determines volume concentrations of the components:

$$P = P_i(V_i, E_i) = P_j(V_j, E_j) = \ldots = P_N(V_N, E_N).$$

The temperature was calculated using the following ratio:

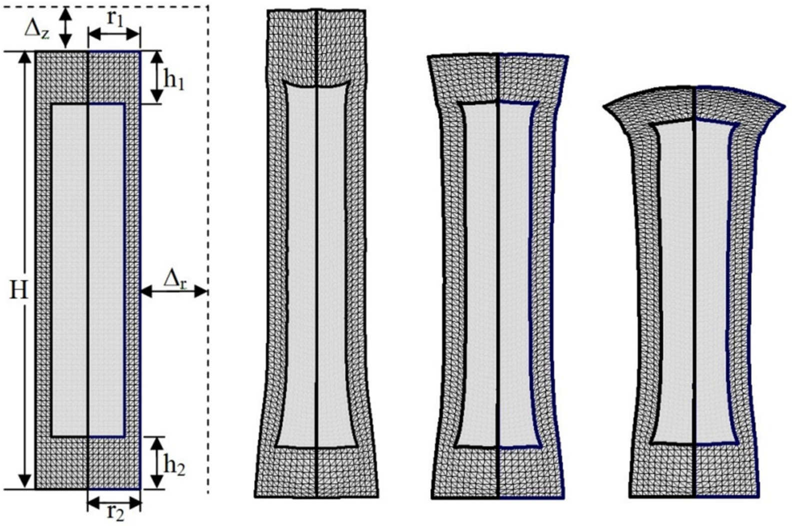
$$dT_i = \begin{cases} d(E_i - E_{0xi})/c_{pi}, & \text{if } T_i < T_{mi} \\ 0, & \text{if } T_i = T_{mi}, \\ d(E_i - E_{0xi} - \Delta H_{mi})/c_{pi}, & \text{if } T_i > T_{mi} \end{cases}$$

where the specific heat capacity c_{pi} increases linearly with increasing the temperature up to the melting point of a substance, E_{0xi} is the "cold" component of the specific internal energy, T_{mi} is the melting temperature, ΔH_{mi} is the specific melting heat of the i-th component.

RESULTS AND DISCUSSION

We consider the axisymmetric problem of explosive compaction of a three-component mixture from aluminium, sulphur and carbon placed into a cylindrical steel ampoule. The inert substance (graphite) was added to the mixture of aluminum and sulfur in a proportion of 2/1 to avoid the reaction between aluminum and sulfur. The mass fractions of the components in the sample (mixture) were taken in proportion: Al 11.5, S - 21.5, C - 67.0; the volume fractions: Al - 9.55, S - 23.35, C - 67.1. The porosity of the mixture was 0.4 (ratio between the volume of pores and total volume). The height of the cylindrical sample was 64 mm, the diameter was 14 mm. The thickness of the lateral wall of the ampoule was 3 mm, the thickness of top and bottom lids was 10 mm. The height of the ampoule (H) was 84 mm, the external diameter was 20 mm (Figure 1a).

In the computations the actions of the detonation products surrounding the ampoule was simulated by the action of pressure on the upper part of the ampoule in a vertical (axial) direction and on the lateral surface of the ampoule in a horizontal (radial) direction. In the axial direction the action started at the initial moment of the process, and in the radial direction the action stated during propagation of the detonation wave from top to bottom (Ivanova, 2014). The detonation velocity was D = 2.8 km/s on the basis of experimental data. The P_0 = 3.2 GPa value was chosen on the basis of numerical and experimental evaluations.



a b c d

Fig. 1 - Explosive compaction of the ampoule for different thickness of the axial layer of explosives at the initial moment of time (a) and 80 μs: Δ_z = 5 mm (b); Δ_z = 30 mm (c); Δ_z = 40 mm (d).

In the computations we varied the thickness of the explosive Δ_z in the axial direction, that act on the upper part of the ampoule in order to study the influence of the parameter on a final shape and size of the ampoule. The value Δ_r for the explosive acting radially on the lateral wall of the ampoule was constant and equal to 18 mm.

Figures 1b-d show the evolution process for explosive compaction of a cylindrical ampoule with an inert mixture for different thicknesses of an axial layer of the explosive. Figures are given at the time of 80 microseconds. This moment of time illustrates the final stage of explosive compaction of the inert mixture in the cylindrical ampoule. The results of computations show a significant influence of the axial explosive layer on the final results of explosive loading. When the thickness Δ_z is low, the influence of lateral load prevails, which leads to elongation of the ampoule in the axial direction (Figure 1b). When the thickness Δ_z is high, there is an additional load on the upper part of the ampoule, which causes deformation of the top lid of the ampoule (compaction in the axial direction and elongation in the radial direction) and a portion of the mixture.

Table 1 shows the numerical results for the loaded cylindrical ampoule with an inert mixture from aluminum, sulfur and carbon, when the thickness of the explosive layer is varied in the axial direction. Here Δ_z is the thickness of the axial layer, H is the height of the ampoule after loading, h_1, r_1 and h_2, r_2 are the height and radius of top and bottom lids of the ampoule. The initial values of the parameters are as follows: H=84 mm; $h_1 = h_2 = 10$ mm; $r_1 = r_2 = 10$ mm.

Table 1 - Results of computations.

№	Δ_z, mm	H, mm	h_1, mm	h_2, mm	r_1, mm	r_2, mm
1	0	92.8	17.2	9.0	7.6	11.1
2	5	89.0	13.9	9.0	8.8	11.1
3	10	85.4	11.9	9.0	9.8	11.1
4	15	83.2	10.8	8.9	10.3	11.1
5	20	80.9	10.0	8.9	10.5	11.1
6	25	78.6	9.3	8.7	11.0	11.2
7	30	76.1	8.2	8.7	11.9	11.2
8	35	73.2	6.9	8.8	13.4	11.1
9	40	69.6	5.5	8.9	15.4	11.0

Analyzing the data in Table 1, we can conclude that for positive results of compaction it is necessary to select a number of parameters for explosive loading. It is important to choose appropriate explosives and the thickness of explosives. Insufficient thickness of explosives, as well as excessive thickness will lead to unsatisfactory results of explosive compaction, in particular, the incompletely compacted final product, cracks and damages. In addition, the excessive thickness of explosives in the axial direction strongly distorts the shape of the ampoule during explosive compaction.

The computation results show that the change in thickness of the layer Δ_z within the range of $0 \div 13$ mm is not sufficient for compaction of the ampoule in the axial direction and leads to an increase in height of the ampoule. Using the thickness of the axial explosive layer within the range of 35÷40 leads to a strong distortion of the shape of the ampoule, in particular, the top lid of the ampoule and the mixture in this area. The parameters of ampoule, obtained for the thickness of the axial explosive layer $\Delta_z = 30$ mm, have shown that in this case the degree of compaction for the sample of the mixture was about 97%. The parameters for the bottom lid of the ampoule changed insignificantly for all cases.

CONCLUSIONS

We numerically investigated the explosive compaction of a cylindrical ampoule that contained a solid three-component mixture of aluminum, sulfur and graphite. The inert substance (graphite) was added to the mixture to avoid the reaction between aluminium and sulphur.

We studied the influence of the initial thickness of the explosive layer in the axial direction on the final shape of the ampoule. We found the essential influence of the thickness of the explosive layer on the final result of explosive compaction. When the thickness of the explosive layer is low, the influence of lateral load prevails, which leads to the elongation of the ampoule in the axial direction. When the thickness of the explosive layer is high, there is an additional load on the upper part of the ampoule, which causes the large deformation of the ampoule (compaction in the axial direction and elongation in the radial direction). We can conclude that the insufficient or excessive thickness of explosives may be a reason for an incompletely compacted final product or lead to the formation of cracks or damage.

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