Numerical modeling of thermodynamic parameters for mixtures with a few-parameter equation of state of their components

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Abstract. The results of numerical experiments on shock-wave loading of heterogeneous mixtures including tungsten and copper as a component are presented. Thermodynamically equilibrium model with a modified equation of state is used for modeling of thermodynamic parameters of pure materials and mixtures. The thermodynamic parameters for copper of different porosity are calculated for few-parameter equation of state, values of compression ratio and temperature along the shock adiabat are determined; the value of heat capacity at normal pressure is calculated. The results of calculations are compared with the known experimental results of different authors. The calculation of thermodynamic parameters under shock-wave loading for mixtures including tungsten and copper as a component is performed.

1. Introduction

Research of thermodynamic parameters of porous mixtures under shock-wave loading are of interest for many problems of modern science, which causes the emergence of new models for describing the behavior of mixtures, for example [1, 2]. Equations of state (EoSs) only for the components of the mixture are preferably used for describing of the behavior of powder mixtures given the wide variety of compounds, such as on the composition of the components and the porosities. Construction of EoS has been carried out for many years, but given the complexity and diversity of investigated materials, researching is continued in this direction [3–8]. Of particular interest in the simulation of thermodynamic parameters of mixtures is the construction of simple EoSs [9–16]. It is necessary to have a fairly simple model, which gives a good agreement to the experiment in a wide range of pressure values, both for solid and porous materials for modeling of thermodynamic parameters of mixtures. In the present paper, thermodynamically equilibrium model [17–20] is used for modeling of thermodynamic parameters of pure materials and mixtures. The results of calculations are compared with available experimental data of shock-wave loading of mixtures including tungsten and copper as a component.

2. Calculation model

Numerical modeling of thermodynamic parameters of shock-wave loading of both pure materials and mixtures is based on the assumption that all components of the mixture, including gas in
pores, under shock-wave loading are in thermodynamic equilibrium, which assumes equality of velocities, pressures and temperatures. This approach is used in [17–20]. Pure material is considered as a porous mixture with one condensed component in this case. We assume that the gas volume ratio is equal to zero for calculation of the behavior of a solid material. EoS of the Mie-Grüneisen type are used for condensed phases. The equations that determine the state of the condensed component are written as follows:

\[ P(\rho, T) = P_C(\rho) + P_T(\rho, T), \]
\[ E(\rho, T) = E_C(\rho) + E_T(T), \]
\[ P_T(\rho, T) = \Gamma \rho E_T(T). \]

Here \( P_C, E_C, P_T, \) and \( E_T \) are the potential and thermal components of pressure and specific energy, respectively. By taking into account the pressure region of applicability of this model 5–1000 GPa that is of interest to us, initial energy \( E_0 \) of a substance under normal conditions is considered to be equal to zero. Cold pressure component \( P_C \) is described by a Tait-type equation. Therefore, the thermal form of the EoS for a condensed component with current density \( \rho \) and initial density \( \rho_0 \) are as follows:

\[ P(\rho, T) = \rho_0 c_0^2/\rho \{[\rho/\rho_0]^n - 1\} + \Gamma \rho c v_0 (T - T_0). \]

Here, \( c_0 \) is the value of sound speed of under normal conditions, \( T_0 \) is initial temperature, \( c v_0 \) is specific heat capacity under normal conditions. The value \( n = (\partial K/\partial P)_T \) is determined by the derivative of the volume elasticity modulus under initial conditions. Thus, it remains only to determine the function \( \Gamma = P_T V/E_T \) reflecting the contribution of thermal components.

As a result of the analysis of experimental data of both monolithic and porous materials, an empirical dependence on the temperature \( \Gamma(T) \) was proposed, which was used in the development of the model TEC [17–20]. The parameters are chosen from the condition of compliance of the calculated shock adiabats with the known experimental results for each material. The conditions of dynamic compatibility at the wave front are prescribed: the conditions of mass flow preservation for each component of the mixture and the conservation of momentum and energy flows for the mixture as a whole. The equations with the EoS of each component are sufficient to find dependencies \( P(U) \) or \( D(U) \) \((P, U, \) and \( D \)-pressure, mass and wave velocities), which can be interpreted as shock adiabate of a multicomponent mixture. This approach allows to calculate not only the compression ratio of the mixture as a whole, but also to simulate the compression ratio of each component separately [18].

For the modified EoS of condensed component, \( P_C \) is described also by equation of Tait type, and \( P_T \) is considered in the following form:

\[ P_T(\rho, \tau) = c v_0 \rho_0 T_0 (\tau - 1) \sigma k \frac{1 + a_1 \tau}{1 + a_2 \tau}. \]

Here \( \tau = T/T_0 \) is the relative temperature, \( E_T \) is obtained by integrating the differential relation: \( (\partial E/\partial V)_T = T(\partial P/\partial T)_V - P \). As a result, we get:

\[ E_T(\rho, \tau) = F(\tau) - c v_0 T_0 k \frac{1 + 2a_2 \tau + (a_1 - a_2 + a_1 a_2) \tau^2}{(1 + a_2 \tau)^2} \ln(\sigma). \]

Function \( F(\tau) \) and heat capacity \( c V \) are defined from the relationship between heat capacities \( c P \) and experimental data on heat capacity \( c P, \sigma = \rho/\rho_0 \) is relative density:

\[ c_P(\rho, \tau) = c_V(\rho, \tau) - T_0 \sigma (\partial P/\partial T)_V^2 / (\partial P/\partial V)_T, \]
\[ F(\tau) = c v_0 T_0 \left[ (\tau - 1) \left( \lambda - \frac{1}{b_1} \frac{b_1}{b_2} \right) - \left( 1 - \frac{b_1}{b_2} \right) \ln \left( \frac{1 + b_2 \tau}{1 + b_2} \right) \right], \]
\[ c_V(\rho, \tau) = c v_0 (\lambda - \frac{1}{1 + b_1 \tau}) - c v_0 k \frac{2\tau(a_1 - a_2 + a_1 a_2 - a_2^2)}{(1 + a_2 \tau)^3} \ln(\sigma). \]
3. Simulation of shock-wave loading

The temperature values along the shock adiabat for solid copper are shown in figure 1 for model TEC2 and model TEC, as well as calculations from [22]. In the range of pressure values up to 300 GPa the calculations on the modified model are close to the values of [22] with an increase in the pressure value, the deviation of the calculations by model TEC2 is less than that obtained when estimating the temperature values on model TEC.

Data obtained on the basis of experiments for copper with different porosity values from 1 to
Figure 3. Change of heat capacity from temperature for copper. Calculation: solid line is dependence $c_P(T)$. Experimental data: open circles are from [21], dark triangles are from [24].

Figure 4. Shock adiabate (curves) and experimental data (points) of pressure on the compression ratio of porous mixture of W and Cu. Experimental data 1 – 9.691 g/cm$^3$; 2 – 12.315 g/cm$^3$; 3 – 13.812 g/cm$^3$; 4 – 14.852 g/cm$^3$ from the [23].

The change in the heat capacity $c_P(T)$ for copper along the isobar at normal pressure is shown in figure 3 for model TEC2. Here, for comparison, data from [21, 24] are shown. The model heat capacity values are in good agreement with the experimental data to temperature 2000 K. The deviation of the data [21] for values at 1500 K is associated with the transition to liquid phase of copper. The model does not take this transition into account at the moment.

The allowance for porosity in model TEC for mixture of W and Cu (elkonite) [17, 23] made it possible to obtain an adequate description of available experimental data for all values of elkonite density. Figure 4 shows the shock adiabat of the porous mixture. For a better and clearer presentation, the calculated and experimental curves for different values of porosity are 10 are presented in [23]. Porosity $m$ is defined as the ratio of the normal density of a monolithic substance to the initial density of the sample. The calculated curves and data obtained from the experiment for porous copper $m = 4, 7.2, 10$ in the pressure–density coordinates are shown in figure 2. The simulation results show that the model TEC2 describe reliably the data obtained from the experiment to pressure values of 3000 GPa. On the other hand, it can be seen that at pressures up to 300 GPa both models describe well the available data within the accuracy of the experiments. Thus, a simpler model TEC can be used in this pressure range in the absence of the necessary data $c_P(T)$ to determine the dynamic parameters of shock wave loading.
Figure 5. Calculated (lines) and experimental data [25] (points) of pressure dependence on the specific volume of the mixture of tungsten and paraffin: 1–4 are the results of calculations using different methods (1 – SC-criterion; 2 – KEA-method; 3 – TE-method [26]; 4 – model TEC [17]).

plotted in figure 4 with a shift along the compression ratio axis. Parameters and calculations of shock-wave loading of pure W and Cu are given in [20] for model TEC. The difference between the calculations on model TEC and model TEC2 in this case is insignificant taking into account the pressure value up to 300 GPa for which the comparison is made.

The calculated and experimental dependences of pressure on the density of the mixture of paraffin and tungsten are given in figure 5. The figure from [26] is used, on which the calculated curve obtained from the model TEC is added. The results of calculations on the principle of additivity at a pressure of less than 100 GPa are in good agreement with the experimental data, at a higher pressure they are in better agreement with the results of the calculation by the method TE which, however, is not reliable at a pressure below 100 GPa. Only the model TEC [17] allows to describe experimental data in the whole range. The EoS coefficients for paraffin obtained within the framework of the model are as follows: \( \rho_0 = 0.917 \text{ g/cm}^3 \), \( A = 3.8 \text{ GPa} \), \( n = 3.0 \), \( c_V = 2.9 \text{ J/(g K)} \), \( \Gamma(T_0) = 1.70 \), \( \Gamma(T_s) = 1.10 \), \( \Gamma(T_{\infty}) = 0.50 \), \( T_s = 5000 \text{ K} \).

The model TEC allows to describe shock adiabats in region of phase transition [27–29]. The calculations of mixture of quartz with tungsten \( \rho_0 = 10.19 \text{ g/cm}^3 \) and the experimental data from [23] are shown in figure 6. The calculations for pure quartz and for mixtures with quartz as a component are shown in [30].

The data for the shock wave loading of periclase MgO are given by [31] up to a pressure of 1000 GPa. In addition to the new field of dynamic parameters, a region of high-pressure phase transition is discovered. The presence of a high-pressure phase transition for oxides holds great promise for the analysis of the internal structure of the Earth with consideration for a large content of oxides in its composition [32, 33]. It is preferable to use model TEC2 for describing thermodynamic characteristics of materials in this pressure range.

The possibility of a fairly simple model to reliably describe the behavior of materials in a wide range of porosities allows us to simulate shock-wave loading of multicomponent porous mixtures in a wide range of parameters, both in pressure and porosity. In [34] it was shown that the model allows to estimate the temperature values for high-porous mixtures, taking into account the consistency of model calculations of temperature values as the data obtained from experiments and direct measurements, as well as estimates from other models. For example, a
mixture of copper and tungsten in terms of volume (90/10) and a mixture of copper, tungsten and aluminum – (50/25/25) are similar in density, but temperature for these mixtures are markedly different. This means that it is possible to determine the compositions of mixtures that allow for same pressure value to significantly raise temperature of resulting mixture, practically without changing total mass of metal in it.

4. Conclusion
The modified model of shock-wave loading of porous materials with few-parameter EoS of condensed components allows to carry out reliable calculations for materials and mixtures with large porosity values. Comparison of calculations with experimental data and calculations of other authors shows that the model of dynamic loading of porous materials considered in this paper adequately describes the known experimental results for materials with high porosity in the range of pressure values from 5 to 3000 GPa. This model describes thermodynamic properties of the mixtures over whole region investigated in shock-wave experiments. The data of such calculations allow to determine the compositions of mixtures for obtaining the necessary values of pressures and temperatures.

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