

# ENGINEERING MATHEMATICS

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## SIMULATION OF SHOCK COMPRESSION AND THERMAL EXPANSION OF SIMPLE SUBSTANCE AND COMPLEX COMPOUNDS

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Mathematical modeling of physical processes using modern computer technology is applied for studying the behavior of continuous media with dynamic loads. The system of equations for the mechanics of a continuous medium is the laws of conservation of mass, momentum, and energy. This system of equations is closed by the equation of state constructed for a elementary substance or a complex chemical compound. A new method of the formulation of state equations in the area of not very big pressures is offered at this paper. Basic parameters of the equation of state are selected for complex chemical compounds using the original version of the Simplex-method. The method uses linear dependences of the shock wave velocity against the substance velocity and thermal expansion data under constant pressure. For the target function a sum of quadratic differences between calculated and experimental values has been selected. coincidence of theoretical and experimental values is obtained. Satisfactory coincidence of theoretical and experimental values is obtained. The paper was supported by RFBR, Grant 13-01-00072.

*Keywords:* equation of state; Simplex-method; shock compression; thermal expansion.

### Introduction

Now in literature [1–3] a large number of the equations of a state of substances (EOS) from very simple to very difficult is described. When studying the behavior of continuous media that are exposed to dynamic loads, mathematical modeling is used, which is performed on computers. The number of components in difficult models of multicomponent media with chemical reactions and phase transitions can reach several tens, and even hundreds. When calculating a mixture in such models, computer time can be stretched for a considerable time even with the use of modern computers. The proposed low-parametric EOS will significantly reduce the calculation time on the computer of complex physical processes. The paper was supported by RFBR. Grant 13-01-00072.

### 1. Equations at the Surface of a Strong Discontinuity

The laws of conservation for mass, pulse, and energy at the surface of a strong discontinuity (shock wave) in the case of an ideal medium (the deviator of the stress tensor is zero and there is no thermal conductivity) have the following form

$$\rho \cdot (D - U) = \rho_0 \cdot (D - U_0), \quad (1)$$

$$\rho \cdot (D - U)U - P = \rho_0 \cdot (D - U_0)U_0 - P_0, \quad (2)$$

$$P_0 = 0. \quad (3)$$

Values without an index in equations (1)–(3) characterize the state behind the discontinuity,  $D$  – the velocity of the shock wave. Values with index 0, such as  $\rho_0$  – density,  $U_0$  – mass velocity,  $P_0$  – pressure,  $E_0$  – specific internal energy describe the state of the substance before discontinuity. Let us consider a shock wave in a substance at rest. According to [1], the equation of state was considered under the assumption that the quantities  $P_0$  and  $E_0$  are negligible in comparison with  $P$  and  $E$ . Equations (1)–(3) take the form of  $P_0 = 0$ ,  $E_0 = 0$  and  $U_0 = 0$ .

$$\rho \cdot (D - U) - \rho_0 D = 0, \quad \rho_0 D U = P, \quad (4)$$

$$E = \frac{1}{2} D U \cdot \left( 1 - \frac{\rho_0}{\rho} \right). \quad (5)$$

The system consists of three equations (4), (5) and contains five quantities  $P$ ,  $\rho$ ,  $E$ ,  $U$ ,  $D$ . If any two of them are obtained from experiments, the remaining quantities can be found from expressions (4) and (5). The point on the Hugoniot adiabat is completely determined. The dependence between experimentally measured and known for more than fifty years and is satisfactorily described by a linear ratio

$$D = C_0 + b \cdot U. \quad (6)$$

On the basis of a large number of processed experimental data, the reference book [2] contains information on the  $D(U)$  ratio for elements and compounds.

Pressure is defined by the caloric equation of a state  $P = P(\rho, E)$  form in case  $\rho$  and  $E$  are independent thermodynamic variables. Complex and labor-consuming modern EOS are considered in [3, 4]. However, for the express calculations it is possible to use rather simple EOS.

In [1] the EOS of a form is considered

$$P = P_X(\rho) + P_T(\rho, S), \quad E = E_X(\rho) + E_T(\rho, S), \quad (7)$$

where

$$P_X = \frac{\rho_0 C_0^2}{n} (x^{-n} - 1), \quad P_T = \rho_0 C_0^2 \cdot f(S) \cdot x^{-\gamma}, \quad (8)$$

$$E_X = \frac{C_0^2}{n-1} \left( \frac{x^{1-n}}{n} + \frac{x(n-1)}{n} - 1 \right), \quad E_T = \frac{C_0^2 \cdot f(S)}{\gamma-1} x^{1-\gamma}. \quad (9)$$

$C_0$  – sound speed before shock wave for  $P = P_0$ ,  $\rho = \rho_0$ ,  $S$  – entropy,  $n = \text{const}$ ,  $\gamma = \text{const}$ ,  $x = \rho_0/\rho$ .

The dependencies  $P_X(x)$ ,  $E_X(x)$  and  $P_T(E_T, x)$  follow from (8) and (9)

$$P_X = \frac{(n-1)\rho_0 E_X}{x} + \rho_0 C_0^2 \cdot \left( \frac{1-x}{x} \right), \quad P_T = \frac{(\gamma-1)\rho_0 E_T}{x}. \quad (10)$$

EOS is obtained by substituting (10) into (7), which takes the following form

$$P = (\gamma-1)\rho_0 E x^{-1} + \rho_0 C_0^2 \cdot \phi(x), \quad (11)$$

where

$$\phi(x) = \frac{n - \gamma}{(n - 1)n} x^{-n} + \frac{\gamma - 1}{(n - 1)x} - \frac{\gamma}{n}.$$

According to [1], equation (11) is called an "equation with matched  $\gamma$  and  $n$ " if  $\gamma = n$ . Thus, equation (11) takes the form

$$P = (n - 1) \rho_0 E \cdot x^{-1} + \rho_0 C_0^2 \frac{1 - x}{x}, \quad (12)$$

where  $\rho_0$  and  $n$  have constant values.

Let us consider under what conditions the equations (4), (5), (12) agree with the linear ratio  $D(U)$ . The dependence  $D(U)$  is obtained by elimination  $P$ ,  $E$  and  $x$  in expressions (4), (5) and (12)

$$D = \frac{n + 1}{4} U + \sqrt{C_0^2 + \left(\frac{n + 1}{4} U\right)^2}. \quad (13)$$

Comparing expression (13) to expression (6), it is possible to see that these dependencies differ. The smallest differences are in area

$$\frac{n + 1}{4} U \ll C_0.$$

As the assumption of constancy  $n$  in EOS (12) leads to a nonlinear dependence in expression (13) which, in turn, does not agree with the linear ratio  $D(U)$  (6), we do the opposite. Linear ratio  $D(U)$  (6) is taken as a basis. Values  $P$  and  $E$  are expressed through  $C_0$  and  $b$  from equations (4)–(6). After that, we will substitute the received expressions in (11) and we will find the equation in which  $n$  along a Hugoniot adiabat can't be a constant quantity

$$n = 2b \cdot (2 - b \cdot (1 - x)) - 1. \quad (14)$$

## 2. Equation of State

The behavior of the substance in place of EOS (12) will be described by an equation in which the assumption that  $n$  depends on  $x$

$$P = (n(x) - 1) \cdot \rho_{0K} x^{-1} E + \rho_{0K} C_{0K}^2 \cdot \phi(x). \quad (15)$$

In the expression (15)  $\rho_{0K}$ ,  $C_{0K}$  is density and sound speed at the point of  $P = 0$ ,  $T = 0$ ,  $x = 1$ .

In [5–7], EOS of the type (15) was used, where the value  $n$  depends on  $x$ . In equation (14), the quantity  $n$  is linearly dependent  $x$  on the range  $D$  and  $U$  in which relation  $D(U)$  (6) is valid. From the expressions (4), (5) and (15) follows the dependence  $n(x)$  (14), hereinafter named as experimental.

The function  $n(x)$  must have a maximum in the neighborhood  $x \approx 1$  according to [2] and [3]. Thus, if  $x = 0$  and  $n = n_0$ , then it is true that  $n_m > n_0$ . We will use a simple function of the form.

$$n(x) = n_0 + (n_m - n_0) \frac{ax^2}{ax^2 + (x^2 - x_m^2)^2}, \quad (16)$$

where

$$a = \frac{16x_m^2}{4 - (n_m - n_0)^2}.$$

Knowing that for  $x = 0$ , and  $x = \infty$   $n(x) = n_0$  also for  $x = x_m$   $n(x) = n_m$ , from (16), we find the derivative  $n(x)$  in the form

$$\frac{dn}{dx} = \frac{(n_m - n_0) \cdot 2ax^2 (x_m^2 - x^2)}{(ax^2 + (x^2 - x_m^2)^2)^2}. \quad (17)$$

The derivative  $n(x)$  is equal to zero for  $x = 0$ ,  $x = \infty$  and  $x = x_m$ . Value  $n_0$ , as well as values  $n_m$ ,  $x_m$  we select from the condition of the best description of the experimental data. It is made because the area of applicability of low-parametrical EOS is limited to final compression. We take the function  $\phi(x)$  from (15) in the form closest to expression (12)

$$\phi(x) = \frac{1 - x}{x^{n_0+1}}. \quad (18)$$

We divide the pressure and energy into cold and thermal components to determine the temperature and heat capacity

$$P = P_X(x) + P_T(x, T), \quad E = E_X(x) + E_T(x, T). \quad (19)$$

In accordance with [7], we take the dependence  $E_T(x, T)$  in the form

$$E_T = \frac{AT^2}{\theta(x) + T}, \quad (20)$$

where  $A$  – individual characteristics of the substance, for simple substances close to  $\frac{3R}{\mu}$ ;  $R$  – universal gas constant;  $\mu$  – molecular mass. Differentiating expression (20), we obtain the heat capacity at constant  $x$

$$C_V = \frac{AT \cdot (2\theta(x) + T)}{(\theta(x) + T)^2}. \quad (21)$$

In accordance with [7], the expression for the thermal pressure will have the form

$$P_T = -\frac{A}{\theta(x)} \cdot \frac{d\theta(x)}{dx} \cdot \frac{T^2}{\theta(x) + T}. \quad (22)$$

Knowing that the equation is fair

$$P_T = (n(x) - 1) \frac{\rho_{0K}}{x} E_T, \quad (23)$$

we obtain the characteristic function  $\theta(x)$ , which is related to equation  $n(x)$

$$\frac{d \ln \theta(x)}{dx} = -\frac{n(x) - 1}{x}. \quad (24)$$

The dependence  $\theta(x)$  follows from expression (24) and (16)

$$\theta(x) = \theta_0 \cdot x^{1-n_0} \cdot \left( \frac{x^2 + B \cdot x_m^2}{x^2 + \frac{1}{B} \cdot x_m^2} \right), \quad (25)$$

where

$$B = \frac{2 + (n_m - n_0)}{2 - (n_m - n_0)}.$$

In addition, we make the condition that the isobar  $P = 10^{-4}$  GPa pass through a point characterizing the normal state ( $P = 10^{-4}$  GPa,  $T = 293$  K,  $\rho = \rho_0$ ,  $C_P = C_{P0}$ ), and also through the melting point at  $P = 10^{-4}$  GPa ( $T = T_m$ ,  $C_P = C_{Pm}$ ,  $\rho = \rho_m$ ). In describing the dependence  $C_P(T)$  for  $P = \text{const}$  must be expressed  $C_P$  in terms of  $T$  and  $x$ . To this end, we use the equation from [8]

$$C_P = C_V - \frac{T \cdot \left(\frac{\partial P}{\partial T}\right)_X^2}{\rho_{0K} \cdot \left(\frac{\partial P}{\partial x}\right)_T}. \quad (26)$$

Knowing that  $\left(\frac{\partial P_X}{\partial T}\right)_X = 0$ , we differentiate expression (23). The derivative  $\left(\frac{\partial P}{\partial T}\right)_X$  is written in the form

$$\left(\frac{\partial P_T}{\partial T}\right)_X = \frac{(n(x) - 1) \cdot \rho_{0K}}{x} \cdot C_V. \quad (27)$$

Since expression (19) is valid, the derivative  $\left(\frac{\partial P}{\partial x}\right)_T$  will have the form

$$\left(\frac{\partial P}{\partial x}\right)_T = \frac{dP_X}{dx} + \left(\frac{\partial P}{\partial x}\right)_T. \quad (28)$$

The equation of state of a substance is determined by the set of equations (15)–(17), (25) and contains 7 parameters:  $\rho_{0K}$ ,  $C_{0K}$ ,  $A$ ,  $n_0$ ,  $n_m$ ,  $x_m$  and  $\theta_0$ . The numerical values of these parameters are determined in such a way as to best describe the behavior of the Hugoniot adiabat state of matter at a point characterizing the normal state of  $P = 10^{-4}$  GPa,  $T = 293$  K,  $\rho_0 = \rho(P_0, T_0)$ ,  $C_{P0} = C_P(\rho_0, T_0)$ ,  $C_P = C_{P0}$  and at the melting point  $P = 10^{-4}$  GPa,  $T_1 = T_m$ ,  $\rho_1 = \rho_m(T_m, P_0)$ ,  $C_{P1} = C_P(T_m, P_0)$ .

### 3. Results of Calculations

Calculations are performed for several simple substances and complex chemical compounds. The selection of the basic parameters of the equation of state was carried out with the help of the original version of the Simplex-method [9]. For target function, we selected a sum of quadratic differences between calculation and experimental values of function for the thermal expansion of matter and the specific heat at constant pressure. For the materials considered, a satisfactory agreement with the experimental data was obtained. A comparison of the Hugoniot adiabats for simple substances is shown in Fig. 1, for complex chemical compounds – in Fig. 2, respectively. The value of the dimensionless pressure is determined by expression (29)

$$\Pi = \frac{P}{\rho_0 C_0^2}. \quad (29)$$

As comparative pressure values, the experimental values taken from [2] and the theoretical values determined from expression (15) are used.

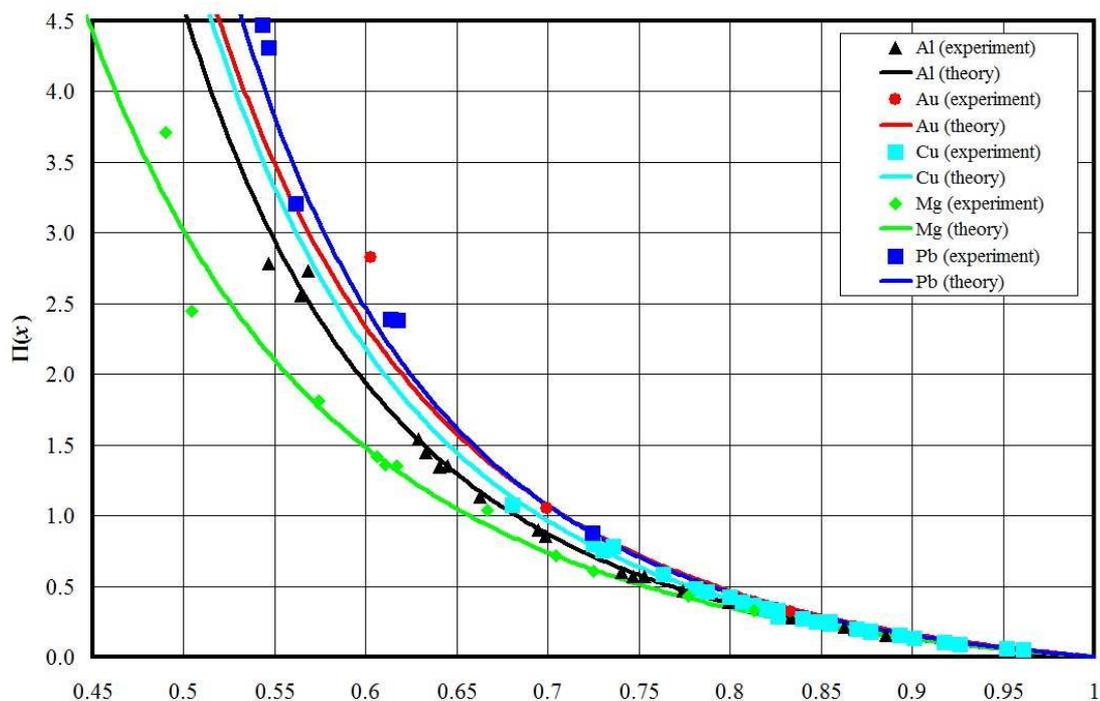


Fig. 1. Comparison of experimental and theoretical Hugoniot adiabats of simple substances

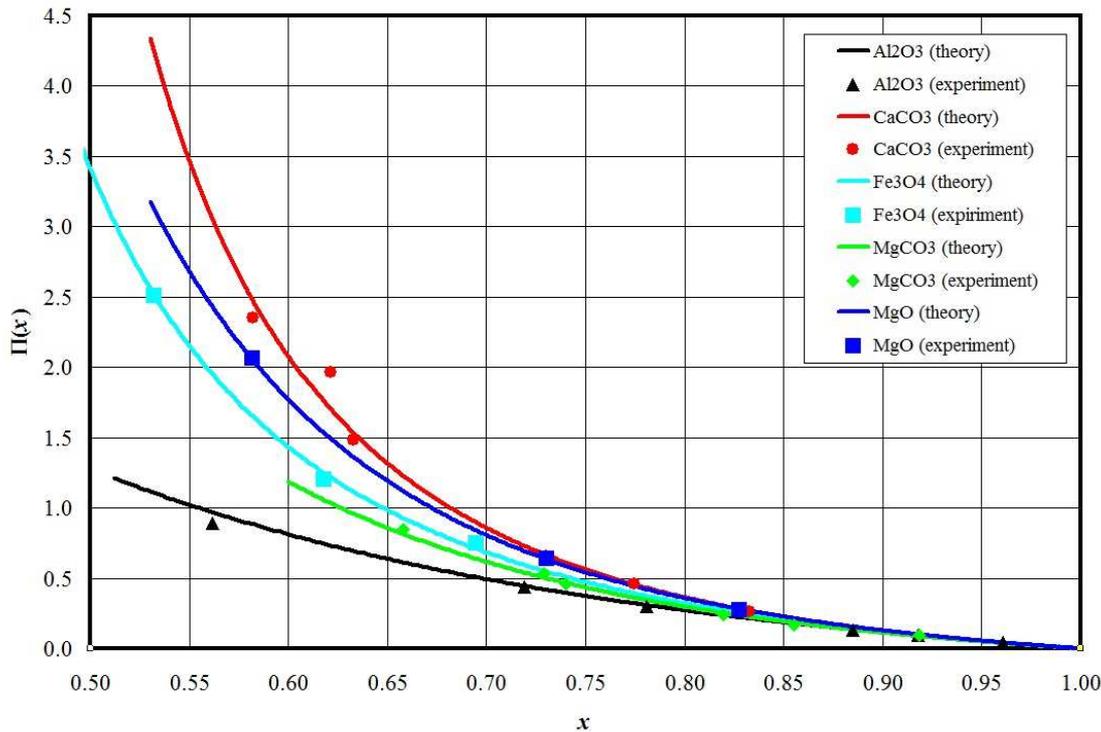


Fig. 2. Comparison of experimental and theoretical Hugoniot adiabats of complex compounds

The temperature dependence of the heat capacity for simple substances is shown in Fig. 3, for complex chemical compounds – in Fig. 4, respectively. The experimental values of the heat capacity are taken from the reference books [10–14].

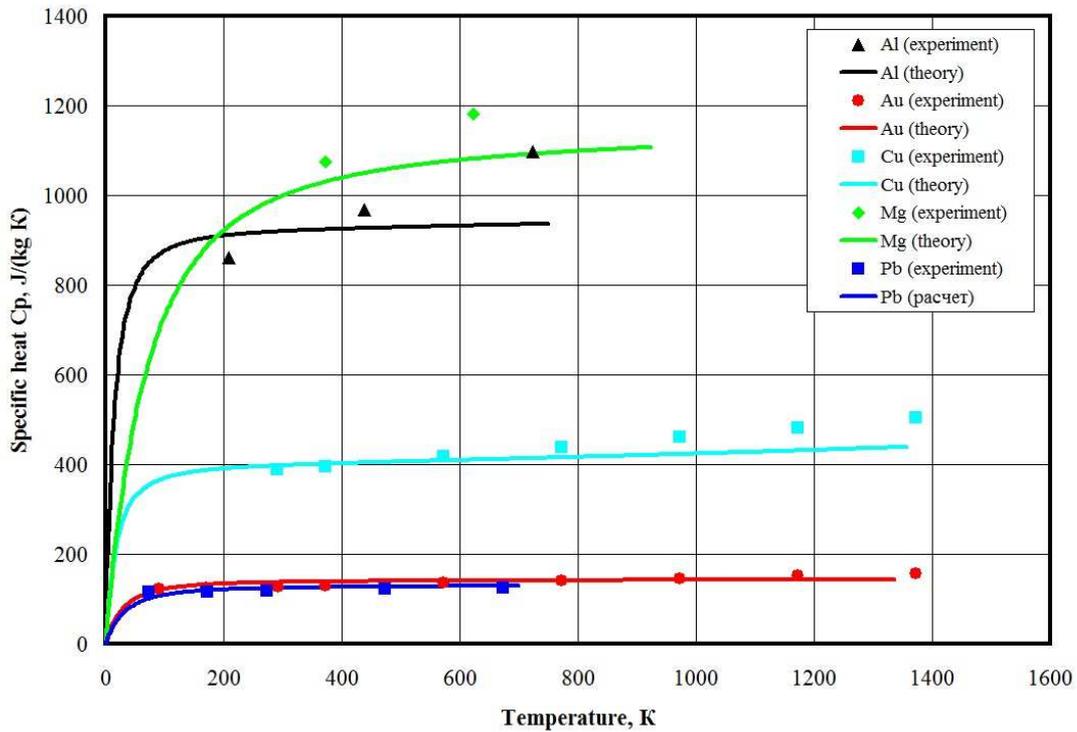


Fig. 3. Comparison of experimental and theoretical specific heat of simple substances

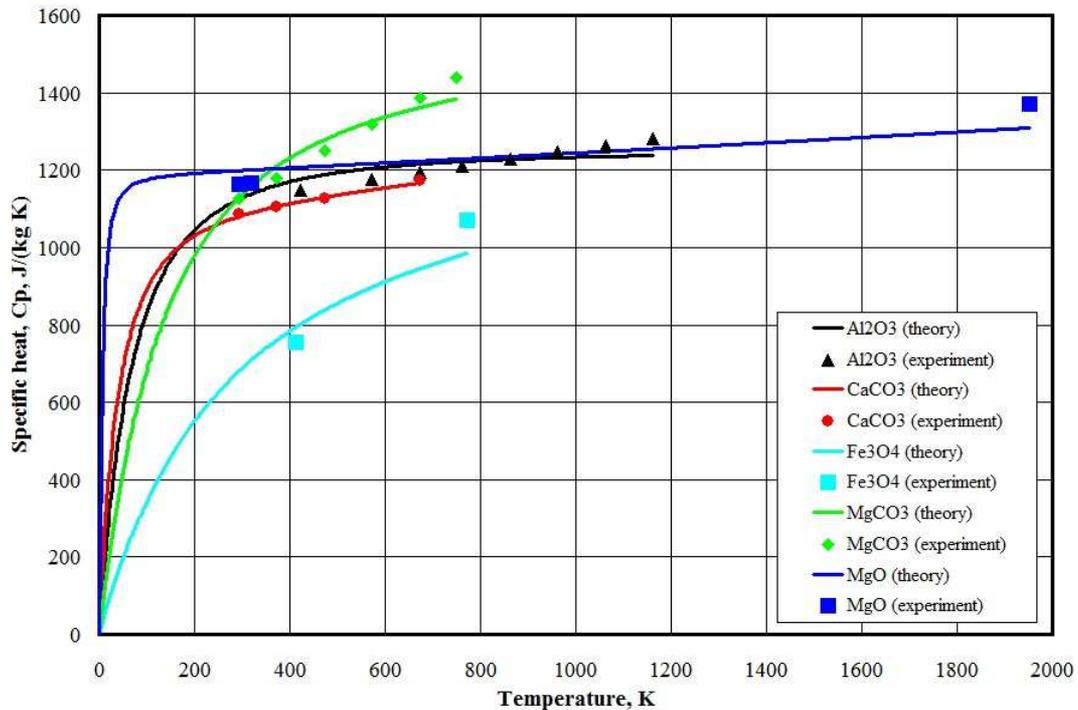


Fig. 4. Comparison of experimental and theoretical specific heat of complex compounds

Tables 1 and 2 are shown the results of calculations of the selection of the main parameters of the EOS. The values indicated in the tables  $n_0$  are adjustable parameters and in the area where  $n < 1$  it is not applied.

**Table 1**

The results of the selection of the basic parameters of the equation of state  
for simple substances

Values	Al (Aluminium)	Au (Aurum)	Mg (Magnium)	Pb (Plumbum)	Cu (Cuprum)
$n_0$	1.62	1.515	1.291	1.719	1.49
$n_m$	1.933	2.564	1.944	2.027	2.997
$x_m$	1.908	2.485	2.613	1.66	2.484
$\rho_{0K}, g/cm^3$	2.908	19.668	1.833	11.501	9.014
$C_{0K}, km/s$	5.642	3.402	4.724	2.102	3.904
$A \cdot 10^6, kJ/g$	920	141	1106	128	395
$\theta_0, K$	15.012	8.004	43.141	39.168	1.466

**Table 2**

The results of the selection of the basic parameters of the equation of state  
for complex compounds

Values	Al <sub>2</sub> O <sub>3</sub> (Corundum)	CaCO <sub>3</sub> (Calcite)	Fe <sub>3</sub> O <sub>4</sub> (Magnetite)	MgCO <sub>3</sub> (Magnesite)	MgO (Periclase)
$n_0$	0.554	1.1617	0.518	0.897	1.073
$n_m$	1.242	2.375	2.353	2.120	2.220
$x_m$	1.522	0.621	1.041	1.415	0.852
$\rho_{0K}, g/cm^3$	3.969	2.755	5.294	3.183	3.501
$C_{0K}, km/s$	8.757	3.813	4.722	6.482	5.972
$A \cdot 10^6, kJ/g$	1251	1092	1064	1440	1184
$\theta_0, K$	50.912	33.174	18.762	42.445	4.003

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## References

1. Zababakhin E.I. *Some Questions of Dynamics of Gas Explosion*. Snezhinck, RFYaTs-VNIIEF, 1977. (in Russian).
2. Trunin R.F., Gudarenko L.F., Zhernokletov M.V., Simakov G.V. *The Experimental Data on Shock Compression and Adiabatic Expansion of Materials*. Sarov, RFYaTs-VNIIEF, 2001. (in Russian).
3. Zharkov V.I., Kalinin V.A. *The Equation of the Solids State at High Pressures and Temperatures*. Moscow, Nauka Publ., 1968. (in Russian).

4. Kuropatenko V.F. The Equation of the Components State of Low-temperature Plasma. *Encyclopedia of Low-temperature Plasma*. Series B, vol. VII, part 2. Moscow, Yanus-K, 2008. pp. 436–450. (in Russian).
5. Kuropatenko V.F. Equation of State of Detonation Products of Condensed Explosives. *Numerical Methods of Continuum Mechanics*, 1977, vol. 8, no. 6, pp. 68–71. (in Russian).
6. Kuropatenko V.F. Equation of State of Detonation Products of Dense Explosives. *Combustion, Explosion and Shock Waves*, 1989, no. 6, pp. 112–117. (in Russian).
7. Kuropatenko V.F. Modeling the Response of Substances to Dynamic Impact. *Russian Journal of Physical Chemistry B: Focus on Physics*, 2002, vol. 21, no. 10, pp. 46–54. (in Russian).
8. Kuropatenko V.F. *Models of Continuum Mechanics*. Chelyabinsk, Chelyabinsk State University, 2007. (in Russian).
9. Kuropatenko V.F., Filatov S.Yu. FK-EOS. *Official Bulletin of Computer Programs of Rospatent*, Moscow, FIPS, 2016, no. 2016613028, issued 2016-03-15. (in Russian).
10. *Physical and Chemical Properties of Elements*. Kiev, Naukova dumka, 1965. (in Russian).
11. Samsonov G.V., Vinnitskiy I.M. *Refractory Compounds. Guide*. Moscow, Metallurgiya, 1969. (in Russian).
12. Kikoin I.I. *Tables of Physical Quantities*. Moscow, Atomizdat, 1976. (in Russian).
13. Samsonov G.V. (Ed.) *Physical and Chemical Properties of Oxides*. Moscow, Metallurgiya Publ., 1969. (in Russian).
14. Ryabin V.A., Ostroumov M.A., Svit T.F. *Thermodynamic Properties of Substances*. Leningrad, Khimiya, 1977. (in Russian).

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## МОДЕЛИРОВАНИЕ УДАРНОГО СЖАТИЯ И ТЕПЛОВОГО РАСШИРЕНИЯ ДЛЯ ПРОСТЫХ ВЕЩЕСТВ И СЛОЖНЫХ ХИМИЧЕСКИХ СОЕДИНЕНИЙ

*С.Ю. Филатов*

При изучении поведения сплошных сред, которые подвергаются воздействию динамических нагрузок, применяется математическое моделирование физических процессов с использованием современной вычислительной техники. Система уравнений механики сплошной среды представляет собой законы сохранения массы, импульса и энергии. Данная система уравнений замыкается уравнением состояния, которое построено для конкретного вещества или сложного химического соединения. В настоящей работе предложен способ построения уравнений состояния в области небольших давлений и температур. Основные параметры уравнения состояния подобраны для простых веществ и сложных химических соединений при помощи оригинальной версии симплекса-метода. Метод использует линейные зависимости скорости ударной волны от скорости вещества и данные по тепловому расширению при постоянном давлении. В качестве целевой функции выбрана сумма квадратичных разностей между расчетными и экспериментальными величинами теплового расширения вещества, а также теплоемкости при постоянном давлении. Для рассмотренных материалов получено удовлетворительное совпадение с экспериментом.

*Ключевые слова:* уравнение состояния вещества; симплекс-метод; тепловое расширение; ударное сжатие.

### Литература

1. Забабахин, Е.И. Некоторые вопросы газодинамики взрыва / Е.И. Забабахин. – Снежинск: РФЯЦ-ВНИИФ, 1977.
2. Трунин, Р.Ф. Экспериментальные данные по ударно-волновому сжатию и адиабатическому расширению веществ / Р.Ф. Трунин, Л.Ф. Гударенко, М.В. Жерноклетов, Г.В. Симаков. – Саров: РФЯЦ-ВНИИЭФ, 2001.
3. Жарков, В.И. Уравнение состояния твердых тел при высоких давлениях и температурах / В.И. Жарков, В.А. Калинин. – М: Наука, 1968.
4. Куропатенко, В.Ф. Уравнение состояния компонентов низкотемпературной плазмы / В.Ф. Куропатенко // Энциклопедия низкотемпературной плазмы. Серия Б. Т. VII, ч. 2. – М: Янус-К, 2008. – С. 436–450.
5. Куропатенко, В.Ф. Уравнение состояния продуктов детонации конденсированных ВВ / В.Ф. Куропатенко // Численные методы механики сплошных сред. – 1977. – Т. 8, № 6. – С. 68–71.
6. Куропатенко, В.Ф. Уравнение состояния продуктов детонации плотных ВВ / В.Ф. Куропатенко // Физика горения и взрыва. – 1989. – № 6. – С. 112–117.
7. Куропатенко, В.Ф. Моделирование отклика веществ на динамическое воздействие / В.Ф. Куропатенко // Химическая физика. – 2002. – Т. 21, № 10. – С. 46–54.

8. Куропатенко, В.Ф. Модели механики сплошных сред / В.Ф. Курпатенко. – Челябинск: Челябинский государственный университет, 2007.
9. Куропатенко, В.Ф. FK-EOS: Свидетельство о государственной регистрации Пр-ЭВМ № 2016613028 / В.Ф. Куропатенко, С.Ю. Филатов. – 2016613028; зарегистр. 15.03.2016, Роспатент.
10. Самсонов, Г.В. Физико-химические свойства элементов / Г.В. Самсонов. – Киев: Наукова думка, 1965.
11. Самсонов, Г.В. Тугоплавкие соединения / Г.В. Самсонов, И.М. Виноцкий. – М: Металлургия, 1969.
12. Кикоин, И.И. Таблицы физических величин / И.И. Кикоин. – М: Атомиздат, 1976.
13. Самсонов, Г.В. Физико-химические свойства окислов / Г.В. Самсонов. – М: Металлургия, 1969.
14. Рябин, В.А. Термодинамические свойства веществ / В.А. Рябин, М.А. Остроумов, Т.Ф. Свит. – Л: Химия, 1977.

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