DETERMINATION OF DETONATION PRODUCTS EQUATION OF STATE USING CYLINDER TEST

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Abstract. Contemporary research in the field of explosive applications implies utilization of „hydrocode“ simulations. Validity of these simulations strongly depends on used parameters in the equation of state for considered explosive compounds. A new analytical model for determination of Jones-Wilkins-Lee (JWL) equation of state parameters based on cylinder test has been proposed. The model relies on analysis of cylinder motion and detonation products expansion. Available cylinder test data for five explosive compositions are used for calculation of JWL parameters. Good compatibility between results of the model and the literature data is observed, justifying suggested analytical approach.

Keywords: explosive, detonation, cylinder test, JWL equation of state

1. Introduction

Modern approach to research in the field of explosive applications includes the use of so-called “hydrocodes” [1] – robust programs for numerical simulation of complex, high-energy physical-chemical processes involving the detonation, shock waves, large strains, high strain rates, etc. Validity of these simulations highly depends on the used equation of state of detonation products of explosive composition considered. There are a number of proposed equations that define the isentrope of gaseous detonation products [2], [3]: polytropic expansion law, Williamsburg, LJD (Lennard-Jones-Devonshire), BKW (Becker-Kistiakowsky-Wilson) and JWL (Jones-Wilkins-Lee). For simplicity, greater accuracy and availability of data for a significant number of explosive compositions, the most frequently used is the empirical JWL equation of state of detonation products, which has the form [4]:

$$p = A\mathrm{e}^{-R_1 V} + B\mathrm{e}^{-R_2 V} + CV^{-(1+\omega)} \tag{1}$$

where p is the pressure of detonation products, $V=\rho_0/\rho$ is expansion ratio of detonation products, while A, B, C, R_1, R_2 and ω are parameters determined by comparison with experimental results. The first term of the equation defines the behavior of detonation products at very high pressures and low expansion ratio, the second addend is related to the mean pressure, and the third term describes the isentrope in the domain of low pressure, i.e.

large expansion ratio. In this context, only the parameter ω has a physical meaning and approximately satisfies the relation:

$$\omega = \gamma - 1, \tag{2}$$

where γ is polytropic constant for detonation products at pressures close to atmospheric.
There are two ways to determine the JWL parameters of equation of state: (i) by use a thermo-chemical code, (ii) using some of the tests. The former method implies a semi-empirical program that can predict a chemical reaction using thermodynamics, and will not be considered here. The latter approach is based on detonation products expansion physics, it is more reliable and will be further investigated.
The most common source of experimental data to obtain parameters of JWL equation of state is the cylinder test [5], [6], [7] and [8]. Standard copper tube is filled with explosive of interest and the planar detonation wave (normal to the cylinder axis) is generated. As the detonation wave passed through observed section, the radial displacement of copper tube obscure the backlighting (provided e.g. by an argon light bomb) and the history of displacement is recorded by streak camera (Fig. 1).

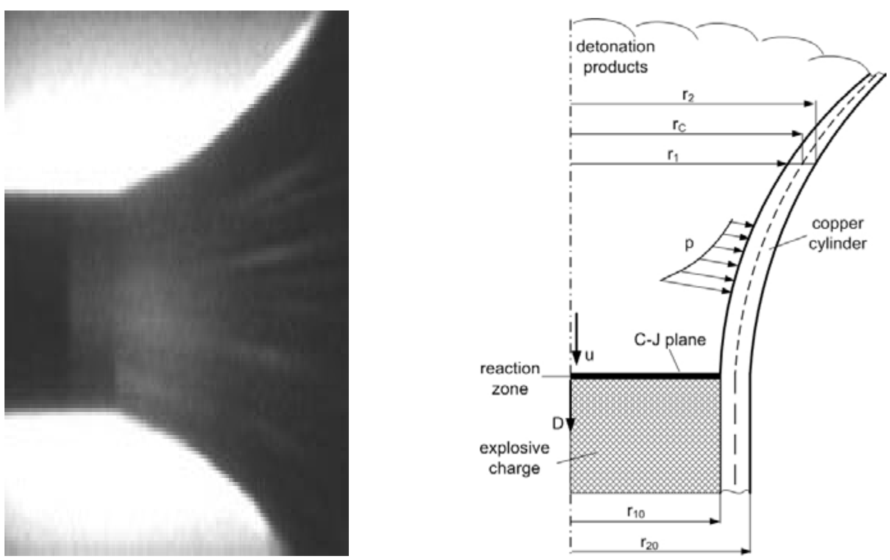

Figure 1. Cylinder test: a) streak camera record, b) motion of copper tube under the action of detonation products (geometry and notation)

The original way of determining the parameters of JWL equation of state [4] implied the variation of their values in a hydrocode, until a satisfactory correspondence between numerical and experimental results is obtained. It was also proposed several different ways of determining the unknown parameters of equations of state without applying the hydrocodes, e.g. [9], [10] and [11].
The aim of this paper is to propose a new analytical model for simple and reliable determination of unknown parameters of JWL equation of state based on the results of the cylinder test.

2. Model

Presented analytical model is based on integration of energetic approach [12] and the concept of the cylinder motion due to the detonation products pressure [13]. These models are analyzed in detail in [14].

Approximation of measured cylinder displacement. The result of experiment is the curve obtained by high-speed photography that represents history of the cylinder outer surface displacement:

$$\Delta r_2 = r_2 - r_{20} = f(t)\,. \tag{3}$$

This function is usually represented in discrete form

$$\left(t_i,\ (\Delta r_2)_i\right),\ i = \overline{1,\ n}\ , \tag{4}$$

where n is total number of measured points from the camera record.
In order to calculate tube wall velocity and acceleration, it is necessary to approximate experimental results (4) with a proper function. Analysis of a large number of possible functions showed that the two functions very well describe the results of experiments. The first function [15] has the form:

$$F_1(t) = \frac{v_\infty t g(t)}{\dfrac{2v_\infty}{a_0} g'(0) + g(t)}\,, \tag{5}$$

where a_0 is initial cylinder acceleration, v_∞ is asymptotic radial cylinder velocity, and function $g(t)$ is defined as:

$$g(t) = \left(1+t\right)^\sigma - 1\,. \tag{6}$$

Using numerical optimization methods, parameters a_0, v_∞ and σ are determined providing minimum deviation of function (5) from experimental results (4) in the sense of the least square method.
Different function, based on the assumption of exponential drop of detonation products pressure, is proposed in [l3]:

$$F_2(t) = \sum_{i=1}^{2} a_i \left[b_i t - \left(1 - e^{-b_i t}\right)\right], \tag{7}$$

where a_i, b_i (i=1,2) are parameters to be optimized.
For each experimental result, parameters in functions (5) and (7) are determined, and the function with better approximation of experiment is used for further calculation, so we have:

$$\Delta r_2 = F(t)\,. \tag{8}$$

We will assume that the cylinder motion is defined by displacement of the central cylinder surface, defined by relation:

$$r_2^2 - r_c^2 = r_c^2 - r_1^2 = \frac{1}{2}\left(r_{20}^2 - r_{10}^2\right). \tag{9}$$

Central surface displacement $\Delta r_c = F_c(t)$ and displacement of internal surface Δr_1 are easily obtained from (8) and (9).

Cylinder velocity and acceleration. Kinematics of the system was determined as described in [13] and [16]. Differentiation of the optimized function of central surface displacement gives the values of "apparent" velocity and acceleration of the cylinder:

$$v_a = \frac{\mathrm{d}F_c(t)}{\mathrm{d}t}, \quad a_a = \frac{\mathrm{d}^2 F_c(t)}{\mathrm{d}t^2}. \tag{10}$$

Analysis of the motion of cylindrical liner shows that inclination centerline angle θ can be determined from relation:

$$v_a = D \tan\theta. \tag{11}$$

The real values of cylinder velocity and acceleration are:

$$v = 2D\sin\frac{\theta}{2}, \quad a = a_p \cos^3\theta. \tag{12}$$

Pressure of detonation products. Since the cylinder acceleration is determined, the pressure of detonation products can be determined from the equation of motion of an elementary cylinder part, taking into account the strength of the cylinder [17], considering that the circular stress is dominant:

$$p = \frac{\left(M + \frac{C}{2}\right)a}{2\pi r_1} + \sigma_f\left(\frac{r_2}{r_1} - 1\right). \tag{13}$$

In equation (13), M and C are the cylinder and explosive charge mass per unit length, respectively:

$$M = \pi\rho_m\left(r_{20}^2 - r_{10}^2\right), \quad \mathrm{C} = \pi\rho_0 r_{10}^2, \tag{14}$$

where ρ_m and ρ_0 are densities of metal and explosive.
Flow stress of the cylinder σ_f is determined by empirical Johnson-Cook model [18]:

$$\sigma_f(\varepsilon, \dot{\varepsilon}, T) = \left[A + B\varepsilon^n\right]\left[1 + C\ln\dot{\varepsilon}^*\right]\left[1 - (T^*)^m\right]. \tag{15}$$

where ε is the equivalent plastic strain, $\dot{\varepsilon}$ is the plastic strain-rate and A, B, C, n, m are material constants. The normalized strain-rate and temperature in equation (15) are defined as:

$$\dot{\varepsilon}^* = \frac{\dot{\varepsilon}}{\dot{\varepsilon}_0}, \quad T^* = \frac{T - T_0}{T_m - T_0}, \tag{16}$$

where $\dot{\varepsilon}_0$ is the effective plastic strain-rate of the quasi-static test used to determine the yield and hardening parameters A, B and n; T_0 is a reference temperature, and T_m is a reference melt temperature. In the present analysis, the influence of thermal softening is neglected due to extremely short time nature of the process.

Detonation products expansion ratio. If it is assumed that the flow of detonation products is quasi-one-dimensional, the continuity equation applies in the form:

$$\rho_0 A_0 D = \rho A(D-u) \,, \tag{17}$$

where u, ρ and A are current values of velocity and density of detonation products, and the channel cross-section area. Using the equation of continuity and Bernoulli equation, we get [19]:

$$\left(\frac{M}{C}+\frac{1}{2}\right)\frac{v^2}{2} = \frac{p}{\rho_0}\frac{A}{A_0} - Du \,. \tag{18}$$

Combining relations (17) and (18), expansion ratio can be determined from

$$V = \frac{\rho_0}{\rho} = \frac{A}{A_0}\left[1 - \frac{A}{A_0}\frac{p}{\rho_0 D^2} + \frac{1}{2}\left(\frac{M}{C}+\frac{1}{2}\right)\left(\frac{v}{D}\right)^2\right], \tag{19}$$

where A/A_0 is the geometric expansion ratio:

$$\frac{A}{A_0} = \left(\frac{r_1}{r_{10}}\right)^2 . \tag{20}$$

Energy balance. Energy conservation law for the system consisting of explosive charge and metallic cylinder can be written in form:

$$\rho_0 DA\Delta t\left(U - Q + \frac{u^2}{2} + T_{\mathrm{kin}} + A_{\mathrm{def}}\right) = puA\Delta t \,. \tag{21}$$

In eq. (21) U is internal energy of detonation products per unit mass, Q – detonation heat per unit mass, u – velocity of detonation products in axial direction, T_{kin} – kinetic energy of radial motion of cylinder and gases (Gurney energy) per unit mass of explosive, and A_{def} – cylinder deformation work per unit mass of explosive charge. Eq. (21) can be simplified to the form:

$$E - E_0 + \frac{\rho_0 u^2}{2} + E_{\mathrm{kin}} + W_{\mathrm{def}} = p\frac{u}{D}, \tag{22}$$

where E=$\rho_0 U$, and E_0= $\rho_0 U$ are internal energy and detonation heat per unit volume of explosive charge, E_{kin}= $\rho_0 T_{\mathrm{kin}}$ and W_{def}= $\rho_0 A_{\mathrm{def}}$ are Gurney energy and deformation work per unit volume of explosive charge.
Detonation heat E_0 is readily obtained by thermo-chemical analysis or from the experiment. Detonation products mass velocity is determined by:

$$u = D\left(1 - V\frac{A_0}{A}\right). \tag{23}$$

Specific Gurney energy can be calculated from [17]:

$$E_{\text{kin}} = \frac{\rho_0 v_1^2}{2}\left[\frac{M}{C}\left(\frac{r_1}{w}\right)^2 \ln\left[1 + \left(\frac{w}{r_1^2}\right)^2\right] + \frac{1}{2}\right], \tag{24}$$

where v_1 is the internal cylinder surface velocity and w is defined as:

$$w^2 = r_{20}^2 - r_{10}^2. \tag{25}$$

Deformation work can be calculated from relation:

$$W_{\text{def}} = \frac{\sigma_y + \sigma_f}{2}\left[\left(\frac{r_{20}}{r_{10}}\right)^2 - 1\right]\ln\frac{r_1 + r_2}{r_{10} + r_{20}}, \tag{26}$$

where σ_f is the cylinder material yield stress.
Introducing the energy term:

$$E_1 = p\frac{u}{D} - \frac{\rho_0 u^2}{2}, \tag{27}$$

one can get energy equation (22) in the form:

$$E = E_0 + E_1 - E_{\text{kin}} - W_{\text{def}}, \tag{28}$$

that enables determination of the internal energy E of detonation products.

Internal energy of detonation products. Assuming adiabatic expansion of detonation products and having in mind Eq. (1), internal energy of gases is determined by:

$$E(V) = \int_V^\infty p\,\mathrm{d}V = \frac{A}{R_1}\mathrm{e}^{-R_1 V} + \frac{B}{R_2}\mathrm{e}^{-R_2 V} + \frac{C}{\omega}V^{-\omega}. \tag{29}$$

Since internal energy $E(V)$ is calculated from eq. (28), unknown JWL equation of state parameters A, B, C, R_1, R_2, and ω can be optimized in order to fit Eq. (29).
At the same time, the JWL parameters should satisfy three additional conditions:
(i) pressure at the Chapman-Jouget (CJ) state is equal to the experimentally determined value p_{CJ}:

$$A\mathrm{e}^{-R_1 V_{CJ}} + B\mathrm{e}^{-R_2 V_{CJ}} + C V_{CJ}^{-(1+\omega)} = p_{CJ}, \tag{30}$$

(ii) internal energy of detonation products at the CJ state is:

$$\frac{A}{R_1}\mathrm{e}^{-R_1 V} + \frac{B}{R_2}\mathrm{e}^{-R_2 V} + \frac{C}{\omega}V^{-\omega} = E_0 + \frac{\rho_0 u_{CJ}^2}{2}, \tag{31}$$

(iii) slope of the Rayleigh line is determined by:

$$AR_1 e^{-R_1 V_{CJ}} + BR_2 e^{-R_2 V_{CJ}} + C(1+\omega) V_{CJ}^{-(2+\omega)} = \rho_0 D^2 . \tag{32}$$

Algorithm for determination of JWL parameters. The procedure for determination of JWL equation of state parameters from the cylinder test is presented in flowchart (Fig. 2). Eq. (13) provides the initial detonation products pressure p_{initial}. This value is based on the second derivative of the fitting function $F_c(t)$ and therefore cannot be used as the definitive pressure of detonation products. Instead, p_{initial} is used for calculation of internal energy E, and then JWL parameters are optimized by fitting procedure, providing the new value for detonation product pressure p. Procedure is repeated with the new value of pressure until the difference between two pressures becomes small enough.

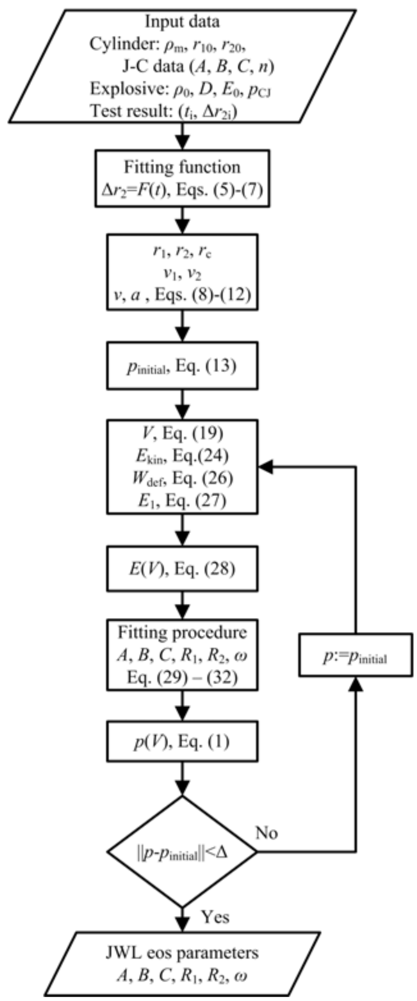

Figure 2. Algorithm for determination of JWL equation of state parameters from the cylinder test

3. Model results and comparison with experimental data

Presented model is applied to determination of the parameters of JWL equation of state for five explosives. Properties of the copper cylinder are listed in Table 1 [18] and [20]. Characteristics of tested explosives are given in Table 2 (all data are taken from [20], except for FH-5 [14]). Experimental cylinder test data (t_i, $(\Delta r_2)_i$) are also used from [20] and [14].

Table 1. Characteristics of copper cylinder

Density	Dimension		Flow stress parameters by Johnson-Cock model			
ρ_m (kg/m^3)	r_{10} (mm)	r_{20} (mm)	A (MPa)	B (MPa)	C	n
8940	12.70	15.30	89.63	291.6	0.025	0.31

Table 2. Detonation properties of examined explosive compositions

Explosive composition	Density	Detonation velocity	Pressure at CJ state	Detonation heat
	ρ_0 (kg/m^3)	D (m/s)	p_{CJ} (GPa)	E_0 (GPa)
TNT	1630	6930	21.0	7.0
Composition B (RDX/TNT-64/36)	1717	7980	29.5	8.5
PBX (HMX/NC/CEF-94/3/3)	1840	8800	37.0	10.2
HMX	1891	9110	42.0	10.5
FH-5 (RDX/W-95/5)*	1600	7930	24.96	8.7

* cylinder dimensions for FH-5 test: r_{10}=10.20 mm, r_{20}=12.70 mm

Model results for the cylinder test with TNT will be presented as a representative example. Experimentally determined cylinder displacement is fitted with analytical functions defined by Eq. (5) and (7). Exponential function (7) provided better agreement with experimental data in this case (Fig. 3).

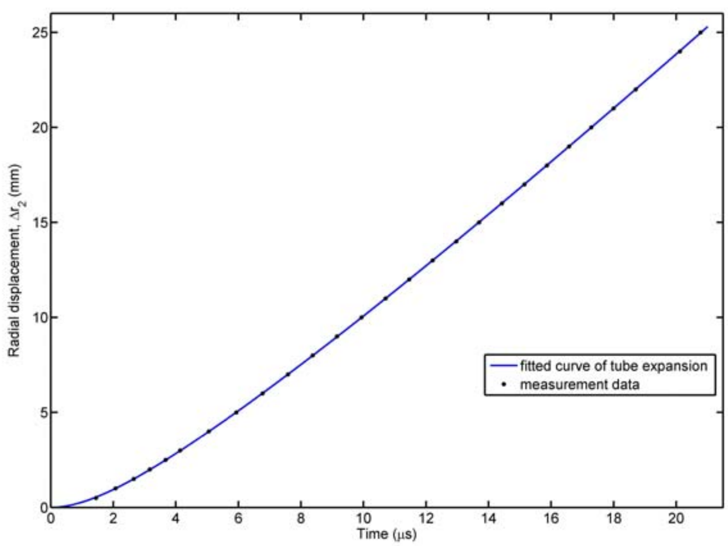

Figure 3. Experimental tube expansion data for TNT [20] fitted with analytical function (7)

Calculated evolution of internal and external cylinder radii is shown in Fig. 4.

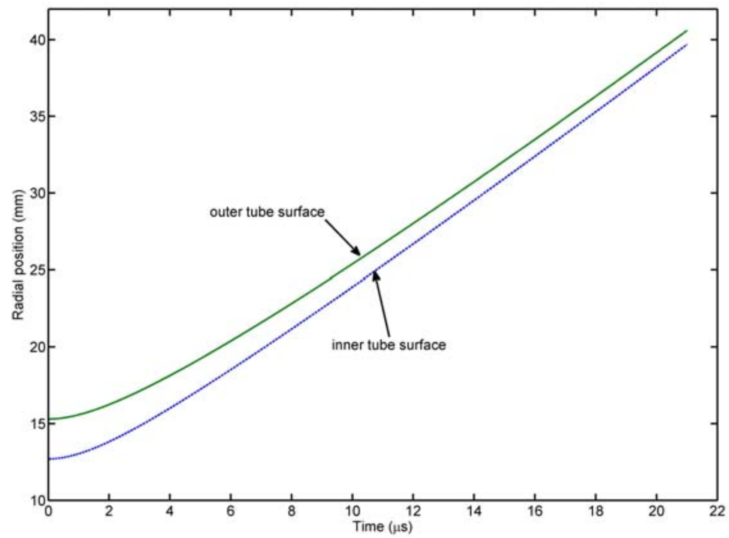

Figure 4. Computed radial position of inner and outer cylinder surface for TNT cylinder test

Velocity histories for both inner and outer tube surface are presented in Fig. 5. The Gurney limit velocity is also indicated (for TNT, literature data [20] v_G=2440 m/s is used), showing good accordance with calculated external cylinder surface velocity.

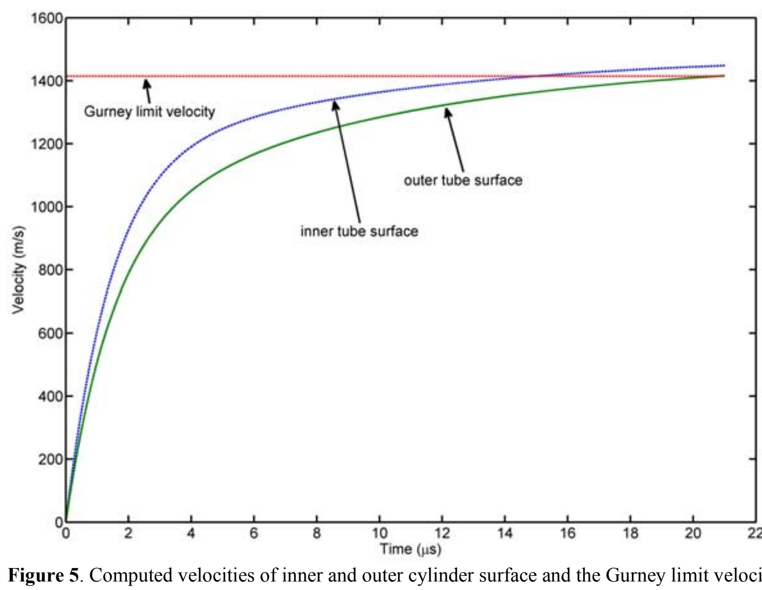

Figure 5. Computed velocities of inner and outer cylinder surface and the Gurney limit velocity

Determined expansion ratio V is compared to the geometric expansion ratio (Fig. 6):

$$V_g = \frac{A}{A_0} = \left(\frac{r_1}{r_{10}}\right)^2 . \tag{33}$$

Significant deviation is noted, especially for very low and very high expansions. This means that simple calculation of expansion ratio by Eq. (33) is not sufficiently accurate.

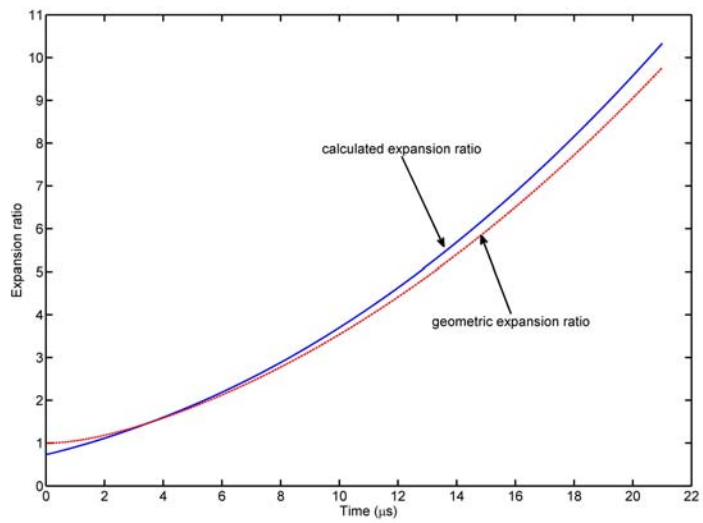

Figure 6. Detonation products expansion ratio from the model compared with simple geometric expansion ratio

Specific energy balance as a function of expansion ratio is given in Fig. 7. The known specific detonation energy E_0, and computed values of kinetic energy E_{kin}, deformation work W_{def} and specific energy E_1 enable determination of specific internal energy $E(V)$.

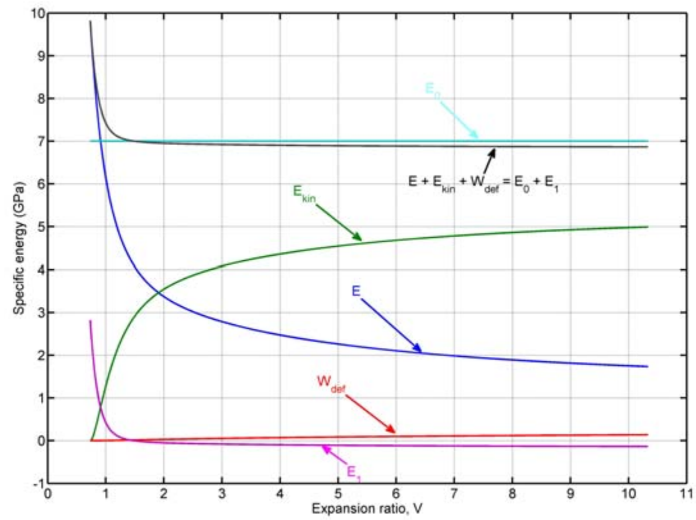

Figure 7. Balance of specific energies involved in the process of detonation product expansion in cylinder test

Specific internal energy of detonation products $E(V)$ obtained by the proposed model is compared with the literature curve (Fig. 8). Good agreement between model and literature curve can be noted.

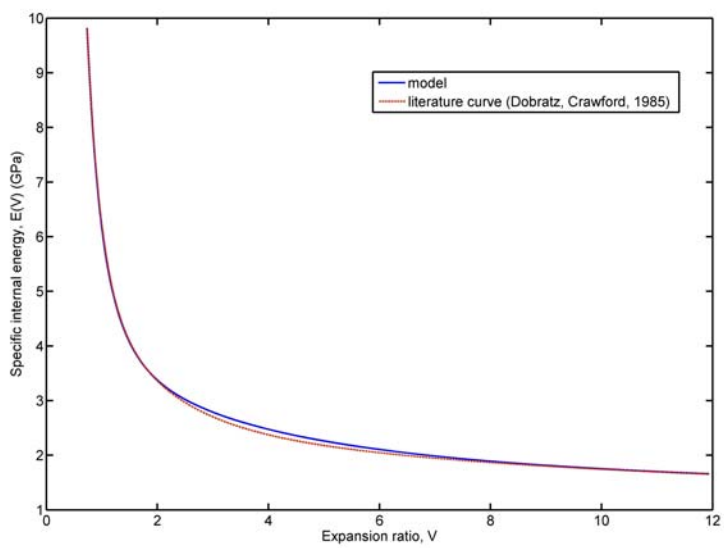

Figure 8. Comparison of calculated specific internal energy of detonation products with literature data

Fig. 9 shows the contribution of the three terms of JWL equation of state to the specific internal energy, after the fitting procedure. It is confirmed that the third term in Eq. (29) is equal to the whole internal energy for large expansions (V>6), and the first term can be neglected for small expansion (V<2.5)

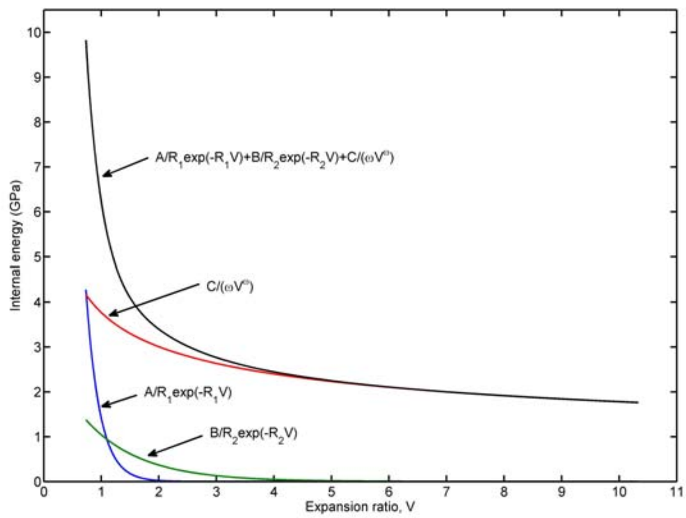

Figure 9. Specific internal energy of TNT detonation products as the sum of three term of JWL model

After the fitting procedure, obtained parameters are used to determine detonation products pressure curve that is compared with the literature data [20] (Fig. 10). Very good compatibility of these results is evident.

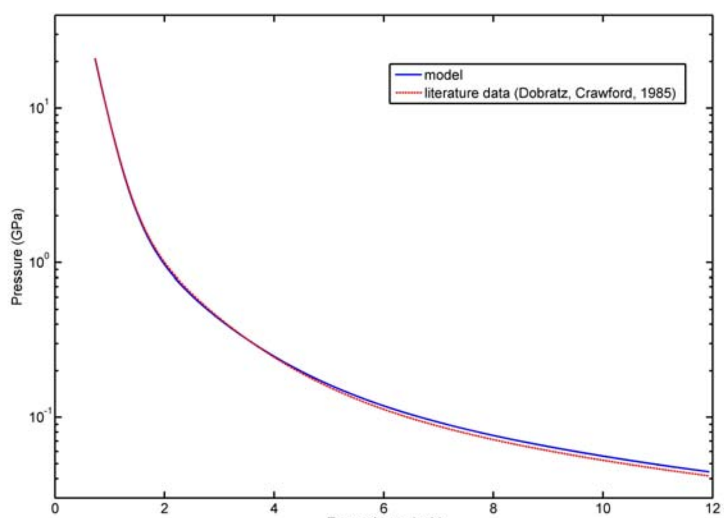

Figure 10. Comparison of p-V curves for TNT detonation products obtained by presented model and [20]

Calculated JWL parameters for all considered explosive compositions are presented in Table 3, along with literature data. Good agreement of model and literature *p-V* curves has been obtained.

Table 3. JWL parameters for five explosives – comparison of model results and literature data

Explosive	Method	R_1	R_2	ω	*A* (GPa)	*B* (GPa)	*C* (GPa)
TNT	model	4.1245	0.9436	0.3135	366.42	2.6983	1.1480
	lit. [20]	4.15	0.95	0.3	371.21	3.2306	1.0453
Comp B	model	4.0489	0.7833	0.3460	497.08	3.4246	1.1260
	lit. [20]	4.2	1.1	0.34	524.23	7.6783	1.0082
HMX	model	4.2018	1.1078	0.3072	768.74	1.2131	7.8843
	lit. [20]	4.2	1.0	0.30	778.28	7.0714	0.6430
PBX-9404	model	4.5403	1.3255	0.3007	832.26	1.7768	9.9479
	lit. [20]	4.60	1.30	0.38	852.40	18.020	1.2070
FH-5	model	4.2750	0.3175	0.2178	573.43	0.96006	0.82373

4. Conclusion

The paper considers problem of determination of detonation products JWL equation of state parameters from the cylinder test data. To solve this problem, a new analytical model has been proposed. The model is based on: (i) fitting the experimental data with analytical function, (ii) cylinder kinematics, (iii) cylinder motion dynamics, (iv) detonation products expansion analysis, (iv) energy balance, and (v) final fitting of detonation products internal energy. Computer program based on the model has been developed. Cylinder test data for five explosive compositions are used for calculation of JWL parameters. Extensive analysis indicates good compatibility between results of the model and the literature data.

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