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PREDICTION OF DETONATION AND JWL EOS PARAMETERS OF ENERGETIC MATERIALS USING EXPLO5 COMPUTER CODE

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The thermochemical computer code EXPLO5 has been used for simple calculations of detonation properties and energy of an important class of organic explosives, namely nitro-aromatic energetic compounds such as cast TNT and mixtures, as well as new synthesized organic nitro-aromatic explosives. This procedure is based on the chemical-equilibrium steady-state model of detonation and it uses the Becker-Kistiakowsky-Wilson (BKW) equation of state for gaseous detonation products, the ideal gas and virial equations of state of gaseous combustion products, and the Murnaghan equation of state for the condensed products.The detonation products composition in the code is calculated by applying the Gibbs energy minimization method and is designed so that the users can choose between the explosive types of constants in the BKW-EOS.

The code calculates the parameters of state of the products along the shock adiabate, starting from a density of a given unreacted explosive (ρ_0) and then increasing it in an arbitrary chosen step up to the density of about $1.5{\cdot}\rho_0$. It determines the Chapman-Jouget (C-J) point as a point on the shock adiabate at which Velocity of Detonation (VOD) has a minimum value. The program also calculates the coefficient in the Jones-Wilkins-Lee (JWL) equation of state along the expansion isentrope by a built in JWL fitting program, and energy available for performing mechanical work.

In this paper, EXPLO5 is used to estimate the detonation parameters and JWL coefficients for TNT, NTO/TNT and Composition B explosive charges, comparison of these values to the literature values as well as those determined experimentally. The use of EXPLO5 is vitalin theefforts employed by the Landward Sciences group with respect to-the determination of the same parameters experimentally.

1. INTRODUCTION

The major goals of thermochemical codes and empirical codes is to provide insight to the understanding the energetic molecules thatare used in energetic applications. Of importance is the ability to predict theperformance of a compound before the laborious and expensive task of synthesis.

Nowadays many numerical methods and programs are being used for carrying out thermodynamic calculations of the detonation parameters of condensed explosives, for example a BKW Fortran (Mader, 1967), Ruby (Cowperthwaite and Zwisler, 1974) TIGER (Cowperthwaite and Zwisler, 1976), CHEETAH (Fried, 1996), EXPLO5(Sućeska , 2001), BARUT-X (Cengiz et al., 2007). These computer codes describe the detonation on the basis of the solution of Euler's hydrodynamic equation based on the description of an equation of state. Some of the well-known equations of stateincludes: the Becker-Kistiakowsky-Wilson equation of state (BKW-EOS) (Mader, 1967), the Jacobs-Cowperthwaite- Zwisler equation of state (JCZ-EOS)(Cowperthwaite and Zwisler , 1976), Kihara-Hikita-Tanaka (KHT-EOS) (Tanaka, 1985). Although the JCZ-EOS calculations have a strong theoretical basis, the BKW-EOS is the most widely used method for the prediction of detonation properties. (Kamlet and Jacobs, 1967)introduced empirical equations for the calculation of the detonation velocity and pressure of CHNO explosives at loading densities greater than 1.0 g/cm^3. To calculate the C-J detonation velocity and pressure usually requires the experimental solid state heat of formation as well as the (initial) loading density and the molecular formula of an explosive.

During synthesis, formulation and numerical modelling of the new energetic materials, the knowledge of the properties such as VOD, the detonation pressure, temperature, heat release and the density of the detonation products at the Chapman-Jouguet (C-J) point is important as it influences the energy released upon explosion and therefore dictatesthe performance of the material (Göbel, 2009). For chemists concerned with the new synthesis and formulations, knowledge of these detonation properties and their use in the thermochemical modelling is pivotal,in deciding on the feasibility of further investment in the research effort. Furthermore, thermochemical codes are used to provide insight to understand which molecules of the energetic compounds and /or detonation products are responsible for performance and sensitiveness of the high explosives.

The use of EXPLO5, a thermochemical computer code, for the calculation of detonation parameters of energetic materials including high explosives has been demonstrated by several researchers (Sućeska, 2001; Sućeska, 1991; Sućeska , 2004; Skare and Suceska, 1995). This code is based on the chemical-equilibrium steady-state model of detonation and it uses the Becker-Kistiakowsky-Wilson (BKW) equation of state for gaseous detonation products, the ideal gas and virial equations of state of gaseous combustion products, and the Murnaghan equation of states for condensed products. The detonation products composition in the code is calculated by applying the Gibbs energy minimization method and is designed so that the users can choose between the explosive types of constants in the BKW-EOS.

The code calculates the thermodynamic parameters of the products along the shock adiabate, starting from a density of a given unreacted explosive (ρ_0) and then increasing it in an arbitrary chosen step up to the density of about 1.5·ρ_0. It is designed to enable the calculation of detonation parameters at the C-J point. The program also calculates the coefficient in Jones-Wilkins-Lee (JWL) equation of state along the expansion isentrope by a JWL fitting program built in, and energy available for performing mechanical work. The most common equation used in the calculation is in the form:

$$p = Ae^{-R_1V} + Be^{-R_2B} + CV^{-(1+\omega)}$$

where p is pressure, $V$is relative volume of the gaseous detonation products. $V = \rho_0/\rho$, where ρ is the density of gaseous products. A, B, C, R_1, R_2andω are the JWL coefficients.

In this work, EXPLO5 is used to estimate the detonation parameters and JWL coefficients for TNT, Comp-B and 50%:50% mixture of NTO:TNT explosive charges. The results are compared to the literature values and those determined experimentally in the same work. The use of EXPLO5 in this manner will help to validate our experimental efforts employed for the determination of the same parameters.

2. EXPERIMENTAL

OFHC copper tubes of 25.4mm diameter and the length of 300mm were filled with various explosive types which were varied from TNT, Comp-B to 50/50 TNT/ NTO as shown in Table 1. Ultra-high speed framing camera was used to capture the expansion of the copper tube in 32 frames and these frames were captured at different positions and time within the range of the frames and then used in a fitting routine to deduce the continuous motion of the tube wall.The test set-up and the use of the Cordin ultra-high-speed camera for capturing the results of the expanding copper tube is described by Izak Snyman 2016 (**USING AN ULTRA-HIGH SPEED CAMERA TO CAPTURE A TUBE EXPANSION TEST**, SABO 2016).

Table 1: Cylinder tests explosive charges variable parameters.

Cylinder explosive	Charge Mass(g)	ρ_0 (g/cm^3)
TNT	135	1.56
Comp-B	145	1.67
NTO/TNT	150	1.73

EXPLO5 was used to predict the detonation parameters and JWL coefficients for above mentioned explosive charges. The results are compared to the literature values and those determined experimentally.

3. RESULTS AND DISCUSSION

Table 2 shows charge types, densities and the sets of parameters which were used as inputs in EXPLO5 computer code calculations.

Table 2: Material models and parameter sets of explosive charges used as inputs in EXPLO5 code.

HE charge	Ratio	ρ_0	Molecular weight	Oxygen balance	Running mode	*Equation of State	Initial Temperature
type	%	(g/cm^3)		%			(K)
TNT	100	1.56	227.13	-73.96	Standard	BKW EOS	3600
Comp-B	100	1.67	221.34	-45.51	Standard	BKW EOS	3600
NTO/TNT	50:50	1.73	165.41	-49.28	Standard	BKW EOS	3600

co-volumes of the equation of state running mode are α = 0.5, β = 0.38, κ = 9.4, θ = 4120.

2.1 Calculation of detonation parameters along the shock adiabate by EXPLO5 code

The C-J point is determined as a point on the shock adiabate of detonation products at which detonation velocity, calculated using equation:

$$D = \sqrt{\frac{p - p_0}{V_0 - V}}$$

has its minimum ($V_0 = 1/\rho_0$ is a specific volume of explosive, p_0 is ambient pressure, and p and V are the values of pressure and specific volume of shock adiabate).

2.1.1. Velocity of Detonation predictions

The velocity of detonation calculated with the EXPLO5 program using the densities of TNT (1.56 g/cm^3), Comp-B (1.67 g/cm^3) and NTO/TNT (1.73 g/cm^3). Figure 1a shows the velocity of detonation outputs for TNT charge from EXPLO5. The minimum value of VOD is 6.65 km/s and it occurs at the specific volume of0.45 cm^3/g. Figure 1b shows the velocity of detonation outputs for Compo-B charge from EXPLO5. The minimum value of VOD is 7.74 km/s and it occurs at the specific volume of 0.49 cm^3/g. Figure 1c shows the velocity of detonation outputs for NTO/TNT charge from EXPLO5. The minimum value of VOD is 7.39 km/s and it occurs at the specific volume of 0.46 cm^3/g.

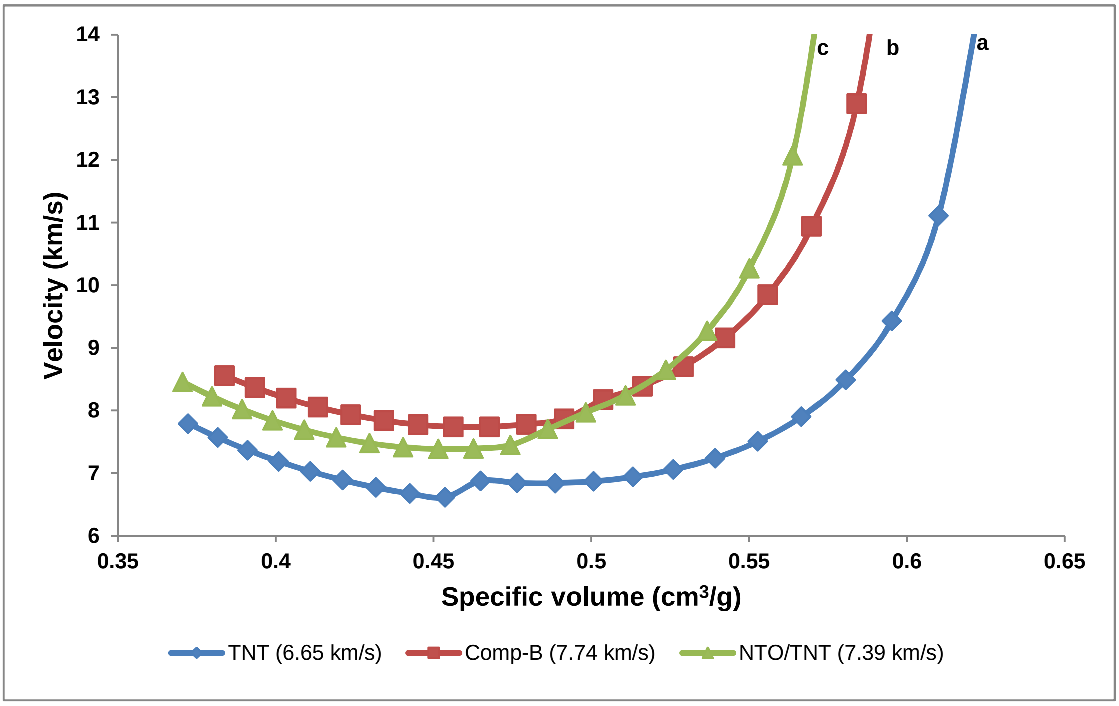

Figure 1: Change of detonation velocity of a. TNT, b. Comp-B and c. NTO/TNTwith specific volume of detonation products.

2.1.2. Detonation pressure predictions

Figure 2a shows C-J point detonation pressure outputs of TNT charge at 20.88 Gpa and occurs at specific volume of 0.45 cm^3/g. Figure 2b shows C-J point detonation pressure output of Compo-B charge at 23.89 Gpa and occurs at the specific volume of 0.49 cm^3/g. Figure 2c shows C-J point detonation pressure output of NTO/TNT charge at 21.5 Gpa and occurs at the specific volume of 0.46 cm^3/g.

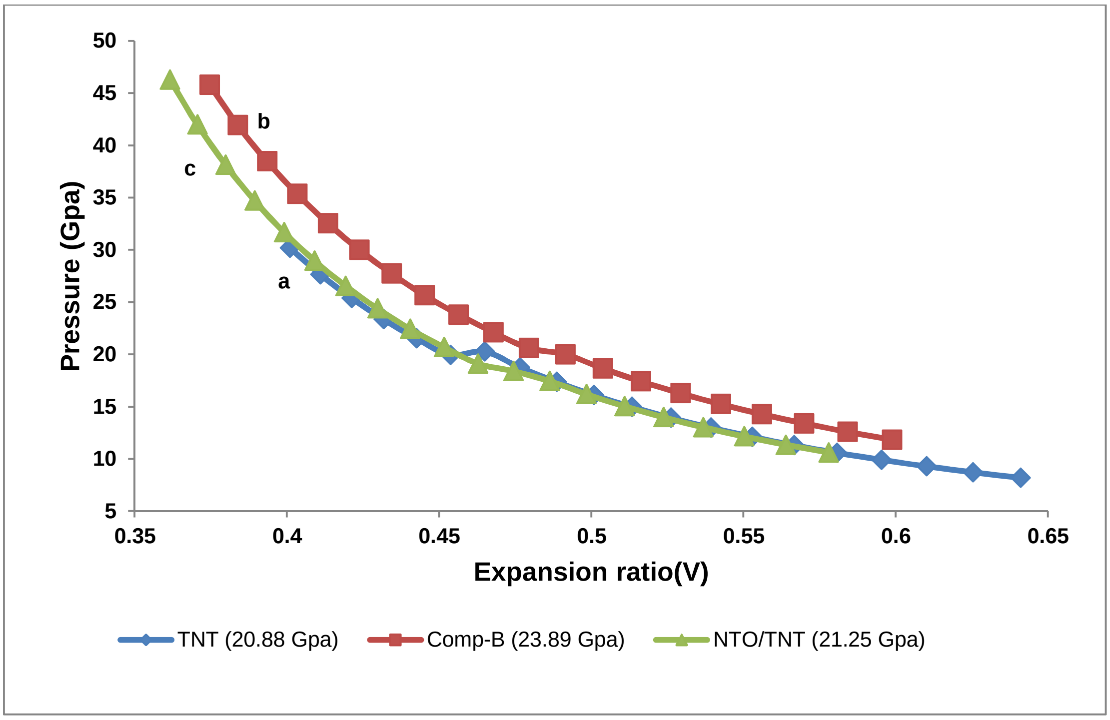

Figure 2: **Change in the detonation pressure of a. TNT, b. Comp-B and c. NTO/TNT with the specific volume of detonation products.**

2.2. Calculation of JWL equation of state parametersalong expansion isentrope by EXPLO5 code: Comparisons with the cylinder test results.

The parameters throughout expansion isentrope are calculated by running EXPLO5 code in the way that enables to halt all chemical reactions and freeze the BKW detonation products composition at 1800K.
In this section the JWL coefficients are evaluated from EXPLO5 code results in the following way:

- The code calculates detonation parameters, i.e. parameters at the CJ point,
- It then calculates the parameters throughout the expansion isentrope of the detonation products isentrope (p; v; T; g; etc.), starting from the CJ point up to a selected relative volume.
- Finally, by the non-linear fitting of the so-calculated p-v values, the JWL coefficients are obtained.
- Once the JWL coefficients are evaluated, the energy on expansion isentrope and the detonation energy are calculated.

2.2.1. Calculations of the JWL parameters

The expansion isentrope for the detonation products of TNT, Comp-B and NTO/TNT from the pressure at the CJ point to the atmospheric one was calculated. This value of the "frozen" temperature results from the theoretical and experimental data presented below.The coefficients of the JWL isentrope were determined on the basis of the values of pressure and the specific volume along the isentrope obtained from thermochemical calculations. The expansion isentropes calculated by the use the thermochemical codes at theoretical maximum density are compared in Figure 3 with the JWL curves.

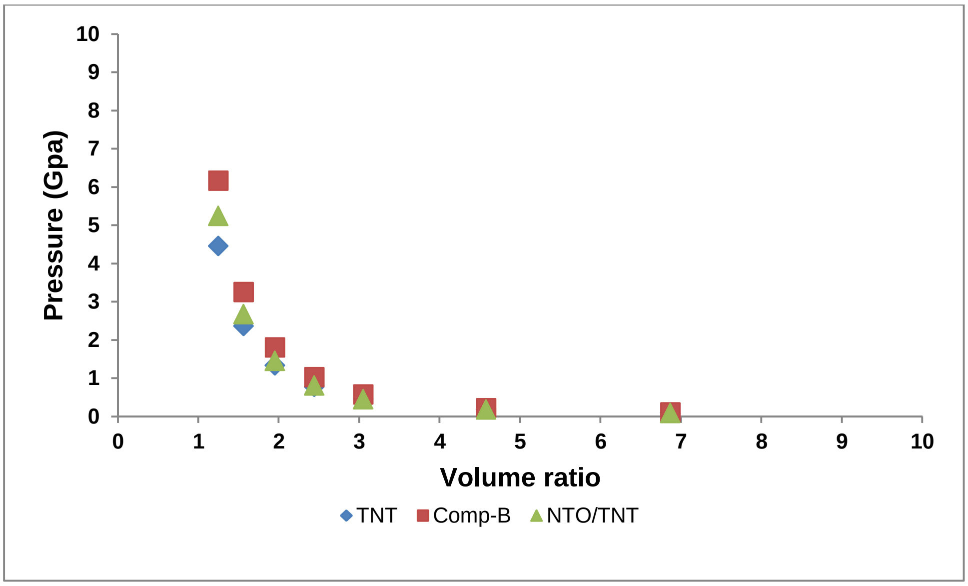

Figure 3: **p-V curves obtained from EXPLO5data at theoretical maximum density for each explosive charge.**

Figure 4 compares the p-V curves of gaseous products of TNT obtained by EXPLO5 to those obtained by the copper tube data analysis at the calculated/experimental density of 1.56 g/cm^3.

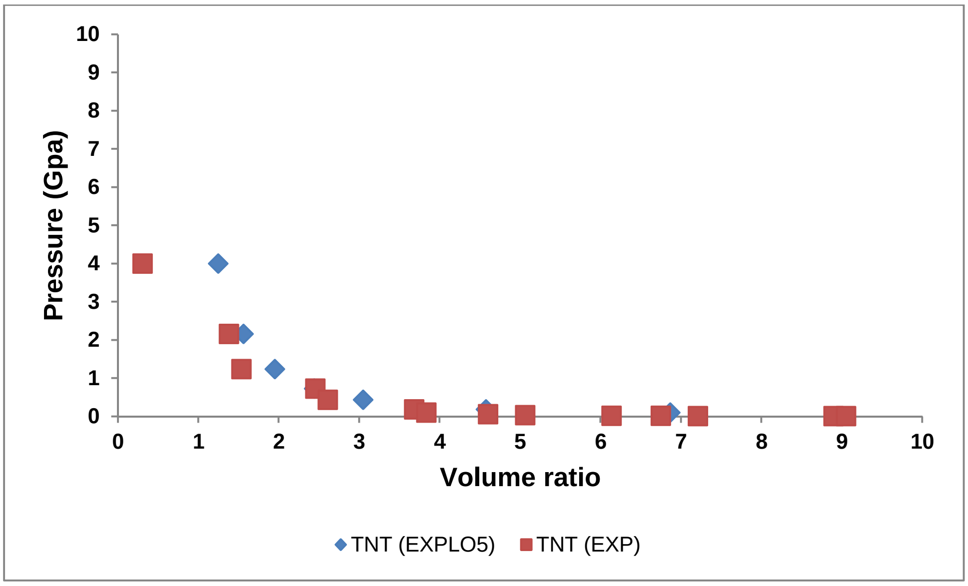

Figure 4: **Comparison of p-V curves for TNT obtained by EXPLO5 and tube test data at a density of 1.56 g/cm^3.**

Figure 5 compares the p-V curves of gaseous products obtained by EXPLO5 to those obtained by the copper tube data analysis at the calculated/experimental density of 1.67 g/cm³.

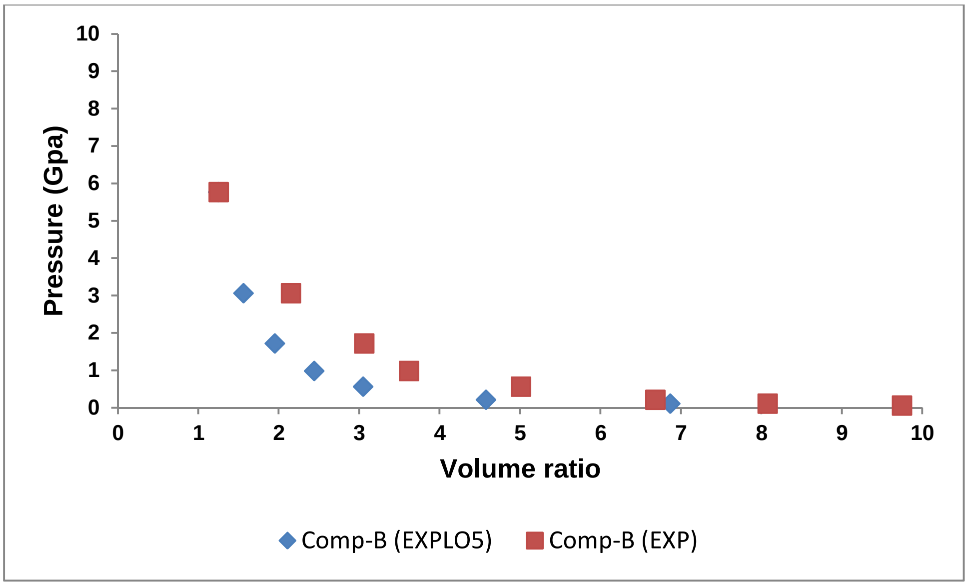

Figure 5: Comparison of p-V curves for Comp-B obtained by EXPLO5 and tube test data at a density of 1.67 g/cm³

The values of the JWL coefficients determined by EXPLO5, cylinder test results and those obtained from the literature are given in Table 3. The experimental JWL parameters of NTO/TNT are not reported her due to problems associated with initiation and low order detonation in the cylinder test experiment.

Table 3: Sets of the JWL coefficients calculated by EXPLO 5 code for explosives detonation products together with literature values

SOURCE	ρ_0 (g/cm³)	p_{CJ} (GPa)	D (km/s)	E_0 (kJ/cm³)	A (GPa)	B (GPa)	C (GPa	R_1	R_2	ω
TNT										
EXPLO5	1.56	20.9	6.65	6.66	317	8.9	1.4	4.4	1.4	0.42
Exp.	*1.56	18.2	6.83	7.0	350	1.8	1.8	4.7	1.0	0.34
(Elek et al. , 2015)	1.63	21.0	6.93	7.0	366	2.7	1.2	4.1	0.9	0.31
Dobratz, 1985	1.63	-	-	-	371	3.2	1.1	4.2	0.9	0.30

SOURCE	ρ_0 (g/cm^3)	p_{CJ} (GPa)	D (km/s)	E_0 (kJ/cm^3)	A (GPa)	B (GPa)	C (GPa	R_1	R_2	ω
Comp-B										
EXPLO5	1.67	23.9	7.74	8.7	432	13.2	1.68	4.3	1.3	0.47
Exp.	#1.67	24.3	7.63	6.1	540	7.0	1.08	4.2	1.1	0.34
(Elek et al. , 2015)	1.72	29.5	7.98	8.5	497	3.4	1.08	4.1	0.7	0.35
Dobratz, 1985	1.71	29.8	7.90	8.5	524	7.7	1.1	4.2	1.1	0.34
NTO/TNT										
EXPLO5	1.73	21.3	7.39	7.32	487.4	13.2	1.5	4.5	1.5	0.47
Exp.	1.73	22.9	7.28	-	-	-	-	-	-	-
(Smith, 1999)	1.74	23.1	7.34	-	-	-	-	-	-	-
(Cliff , 2000)	1.71	22.6	7.37	-	-	-	-	-	-	-

* the density for the TNT cast in the cylinder test was 6% lower than in those used by the references.

#the density for the Comp-B cast in the cylinder test was 4% lower than in those used by the references.

4. CONCLUSIONS

The results shows that there is a good indications that we can use the framing camera recording for evaluating the JWL constants, provided that we assume a specific functional form for the expansion of the copper cylinder. However our experimental procedure is work in progress.

Table 3 shows that there is generally good agreement in detonation velocity and pressure valuesof test explosives whencompared to those by EXPLO5and literature values.

It is also evident from Table 3 that the JWL's coefficients derived from EXPLO5 code deviate considerably compared to those derived from cylinder test data. For instance higher values for the constantω are obtained with EXPLO5 compared to the cylinder test values and those obtained from the literature.Such results are the consequence of p-v profile obtained by EXPLO5 code calculation i.e. for greater relative volumes EXPLO5 gives lower pressure values on the expansion isentrope and for lower relative volumes values it gives higher pressure values.It was also suggested and reported bySućeska, Muhamed,1999 that In order to bring the JWL's coefficients values into the usual range, and also to check the influence of fitting procedure on the results, two more fitting procedures must be tested: (a) fitting with fixed values of ω; (b) fitting with detonation energy as a known input parameter. The author concluded that theresults of first procedure gives the values of the JWL coefficients which are closer to the cylinder derived values.

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