Full Paper

Propellants, Explosives, Pyrotechnics

DOI: 10.1002/prep.202000215

# Prediction of Cylinder Wall Velocity Profiles for ANFO Explosives Combining Thermochemical Calculation, Gurney Model, and Hydro-Code

**Muhamed Suceska,*[a] Chan Hay Yee Serene,[b] Zhang Qingling,[b] Mario Dobrilovic,[a] and Barbara Stimac[a]**

*Dedicated to Professor Thomas M. Klapötke on the Occasion of His 60th Birthday*

**Abstract:** Theoretical prediction of performance indicators of explosives plays an important role in the development of new explosives and explosive formulations. Of particular interest is the possibility to estimate the velocity of metal liner driven by an explosive charge. We present a theoretical model for estimation of metal cylinder wall velocity profiles of non-ideal ANFO explosives. The model is based on thermochemical calculations using EXPLO5 code, expressing the Gurney energy in terms of JWL equation of state, and using hydro-code simulation. The Wood-Kirkwood detonation theory, incorporated in EXPLO5, is applied for calculation of detonation parameters of non-ideal ANFO explosives. It was found that this approach enables prediction of cylinder wall velocity for ANFO explosives, with the error at $V/V_0 = 7$ expansion ratio not exceeding 100 m/s.

**Keywords:** Thermochemical calculation · ANFO · Cylinder test · Gurney energy · Wall velocity

## 1 Introduction

Detonation pressure, detonation velocity, and heat of detonation have been traditionally used as performance indicators of explosives. These parameters enable comparison of the effectiveness of different explosives, but they cannot answer the question of how fast an explosive can drive metal liner. In 1943, R. Gurney [1] proposed a simple and versatile semi-empirical model capable of predicting fragment velocity from an explosive confined in metal casing, and under various loading conditions and geometries.

The Gurney model is based on the assumptions that the energy of an explosive winds up as kinetic energy of detonation products and kinetic energy of cylinder wall. Furthermore, the model assumes there is no gradient in density of detonation products, and distribution of detonation product velocity is linear and dependent on the ratio of the mass of metal to the mass of explosive ($M_C/M_E$) and the Gurney constant. For circular cylindrical geometry, the Gurney formula is given as [1,2]

$$v_s = \frac{\sqrt{2E_G}}{\sqrt{(\mu + 0.5)}} \tag{1}$$

where $v_s$ is terminal velocity of driven metal, $\mu$ is the ratio of the mass of metal ($M_C$) to the mass of explosive ($M_E$), $\sqrt{2E_G}$ is the Gurney velocity (in m/s) and $E_G$ is the Gurney energy per unit mass.

A few remarks regarding the Gurney model should be highlighted. The model does not take into accounts axial expansion, "end losses" of gases in axial direction, shock reverberation in gas phase, reaction zone and its effects on energy delivery, and the cylinder wall yield strength [2,3]. Further, the Gurney energy is not constant but depends on the ratio of mass of metal and mass of explosive, geometry of the system [4], and the expansion ratio considered [5].

The usual way of determination of the Gurney energy is by measuring cylinder wall velocity in a standard copper cylinder expansion test [6,7,8]. The cylinder wall velocity at expansion ratio $V/V_0 = 7$ is typically taken as terminal cylinder wall velocity and it is used for the calculation of the Gurney energy and Gurney velocity from Eq. 1.

Many studies have been dedicated to the theoretical prediction of Gurney energy. The simplest approach is empirical and involves finding a correlation between easily measurable detonation parameters (e.g. detonation velocity) and the Gurney velocity [9–15]. Unfortunately, most of such empirical approaches are not accurate enough. It was

[a] *M. Suceska, M. Dobrilovic, B. Stimac*
*Faculty of Mining, Geology and Petroleum Engineering*
*Department of Mining Engineering and Geotechnics*
*University of Zagreb*
*Pierottijeva 6*
*10000 Zagreb*
**e-mail: muhamed.suceska@rgn.unizg.hr*
[b] *C. H. Y. Serene, Z. Qingling*
*Nanyang Technological University*
*Emerging nanoscience Research Institute*
*50 Nanyang Avenue*
*Singapore 639798*

  

shown in [15] that the Gurney velocity can be more accurately predicted from the detonation energy along the expansion isentrope, where detonation energy is calculated theoretically using thermochemical code EXPLO5 [15,16]. Our analysis, based on a large number of reported experimental data [15,16], as well as the work of Hardesty and Kennedy [17] and Danel and Kazandijan [5], has shown that experimental Gurney energy (which is obtained at $V/V_0 = 7$) agrees well with the detonation energy calculated by thermochemical code at $V/V_0 \approx 3$. Hardesty and Kennedy [17] attributed this energy difference to the fracturing of the cylinder wall after it is strained to the point of rupture, so the detonation products leak out between the fragments and do not contribute to the value of the Gurney energy at larger expansion ratios.

It is also noticed [16] that for the same expansion ratio experimental Gurney energies are about 10% lower than detonation energies calculated from EXPLO5's expansion isentrope. Danel and Kazandjian [5] have shown that, despite the discrepancy, using the results of thermochemical calculations along with the hydro-codes, gives good prediction of cylinder wall velocity. The authors concluded that this is an indication that the Gurney model does not give accurate prediction of the cylinder wall velocity.

Our aim in this paper is to test the possibility of theoretical evaluation of the Gurney energy and the cylinder wall velocity of ANFO explosives by combining thermochemical calculations, the Jones-Wilkins-Lee (JWL) model, the Gurney model, and hydro-code calculations. The Wood-Kirkwood non-ideal detonation model, incorporated in EXPLO5, is used for calculation of detonation properties and expansion isentrope of ANFO, while experimental cylinder wall velocities and hydro-codes are used to verify and validate the model.

## 2 Description of Model

### 2.1 EXPLO5's Kinetic Module

The Wood and Kirkwood (WK) slightly divergent detonation theory [18,19], incorporated in EXPLO5 thermochemical code, enables calculation of detonation properties of non-ideal explosives. The coupling of the WK theory and EXPLO5 code is described in [20,21].

Briefly, the WK flow equations consider both rate of chemical reactions and rate of radial expansion of products and enable prediction of detonation velocity of explosives as a function of explosive charge diameter. The theory is coupled with EXPLO5 in such a way that a separate subroutine integrates the WK flow equations, while thermochemical module of EXPLO5 calculate fraction of reacted explosive ($\lambda$), concentration of reaction products, and the energy of unreacted and reacted fractions of explosive for each $p,V,\lambda$ state along the reaction path. Therefore, consumption of explosives is kinetically controlled (determined by specified reaction rate equation), while concentration of reaction products is thermodynamically controlled and determined by the state of instantaneous chemical equilibrium between the products at a given $p$, $v$, $T$, and $\lambda$ state. The mixture of unreacted explosive and reaction products is treated by assuming pressure and thermal equilibrium between all phases of the mixture. The self-sustaining steady-state detonation velocity is obtained by varying detonation velocity until two WK conditions are satisfied simultaneously: a) the flow is sonic (i.e. $D\text{-}u_p = C$) and b) the release of energy by chemical reactions is balanced by energy loss by the radial flow. In addition to the initial condition, the WK detonation model requires:

- equations of state of unreacted explosive and detonation products
- thermodynamic functions of unreacted explosive and products as a function of temperature
- reaction rate model
- rate of radial expansion

The state of gas-phase products is described by the modified Becker-Kistiakowsky-Wilson (BKW-M) equation of state incorporated in EXPLO5. This equation has been shown to predict accurately pressures at lower densities of explosives [22]. The state of the unreacted ANFO and condensed detonation products is described by Murnaghan equation of state [23]:

$$p = \frac{1}{\kappa n}\left[\left(\frac{V_0}{V}\right)^n - 1\right] \tag{2}$$

where $V_0$ is the molar volume of a product when $p = 0$, $\kappa$ is the inverse of the bulk modules and $n$ is pressure derivative of the bulk modulus. The values of $\kappa = 1.46\ \mathrm{GPa}^{-1}$ and $n = 4.6$ are used (derived from ANFO's shock Hugoniot: $U_s = C + s\ u_p$, where $C = 920\ \mathrm{m\,s}^{-1}$, $s = 1.4$, $n = 4\mathrm{s}^{-1}$; $\kappa = 1/(\rho_0 C^2)$) [23].

The rate of radial expansion along the centre streamline ($\omega_r$), required by the WK model, is calculated by equation [19]:

$$\omega_r = (D - u)/R_c \tag{3}$$

where $R_c$ is radius of shock front curvature and $u$ is particle velocity in the shock frame.

The rate of ANFO decomposition is described by a single-step pressure-dependent reaction rate model [24].

$$\frac{d\lambda}{dt} = k(1-\lambda)^c p^d \tag{4}$$

where $\lambda$ is the mass fraction of reacted explosive (conversion), $k$ is the rate constant, $p$ is pressure, and $c$ and $d$ are rate constants. We found [25] that $k = 0.045\ \mu\mathrm{s}^{-1}\ \mathrm{GPa}^{-1.4}$, $c = 1$, and $d = 1.4$ the best describe dependence of detonation velocity of ANFO on inverse charge radius.

Thermodynamic functions of reaction products and unreacted ANFO are derived from the enthalpy, where the en-

  

thalpy dependence on temperature is described by a four-degree polynomial. For unreacted ANFO we derived polynomial coefficients from the heat capacity data reported in [26, 27] for pure ammonium nitrate.

The main output of the described model is self-sustaining detonation velocity for the specified charge radius. In addition, the calculation gives fraction of reacted explosive and concentration of detonation products at the sonic point, detonation parameters ($D$, $p$, $u_p$, $C_0$, $Q_v$, $T$, etc.), time- and spatial distribution of thermodynamic and flow parameters within detonation driving zone, as well as the width and duration of detonation driving zone.

### 2.2 Evaluation of Gurney Energy

Once the sonic point is determined, the expansion isentrope is calculated starting from the sonic point, down to the atmospheric pressure and the room temperature. Given that a part of ANFO remains unreacted at the sonic point, the expansion isentrope is calculated assuming reacted fraction remains unchanged during the expansion, while reaction products formed are allowed to react with each other above equilibrium freezing temperature (taken to be 2250 K). This is a necessary simplification of the real expansion process because thermochemical codes are not able to take into account time-dependence of reacted fraction during the expansion. Certainly, this assumption will affect the results, however, it is realistic to expect that the impact on the cylinder test results is not significant, due to the following reasons. More than 95 % of the terminal Gurney energy (and wall velocity) is attained in the first 55 μs, i.e. $V/V_0 > 4$ [28], while explosive completely reacts in a time much longer than the recording time in the cylinder test (recording time is about 100 μs [28] while time to complete consumption may be much above 200 μs (depending on charge size and confinement characteristics [29]). According to the pressure-based reaction rate model (Eq. 4), reaction rate decreases with pressure decrease and conversion increase. Thus, when expansion starts the rate of ANFO decomposition becomes slower, approaching zero at $\lambda \rightarrow 1$. The approximate calculation showed that for ANFO having $D = 3.9\ \mathrm{km\,s^{-1}}$, fraction that reacts between the sonic point ($t \sim 10$ μs) and $V/V_0 = 7$ ($t \sim 100$ μs) equals about 5%. Reactions that occur beyond $V/V_0 = 7$ do not contribute cylinder test results at all.

From the calculated pressure and internal energy *vs.* volume data along the isentrope, the detonation energy is calculated by applying the Jones-Wilkins-Lee (JWL) model [7, 30, 31]. The JWL model assumes pressure *vs.* volume along the isentrope to be described by equation [7]:

$$p = Ae^{-R_1 V_r} + Be^{-R_2 V_r} + CV_r^{-(1+\omega)} \tag{5}$$

where $V_r = V/V_0$ (or $\rho_0/\rho$) is the relative volume (or expansion ratio), $A$, $B$, $C$, $R_1$, $R_2$, and $\omega$ are the JWL coefficients. Integration of the above equation yields the internal energy of the detonation products along the expansion isentrope ($E_s$):

$$E_s(V_r) = -\int_{\infty}^{V_d} p\mathrm{d}V_r = \frac{A}{R_1}e^{-R_1 V_r} + \frac{B}{R_2}e^{-R_2 V_r} + \frac{C}{\omega}V_r^{-\omega} \tag{6}$$

The detonation energy at any relative volume ($E_d(V_r)$) is given by equation [29]:

$$E_d(V_r) = E_0 + E_s(V_r) \tag{7}$$

where $E_0$ is detonation energy at infinite volume and it is defined as the difference between internal energy at the sonic point ($E_s(CJ)$) and the compression energy ($E_c$) from an initial volume of explosive to the sonic point ($E_0 = -E_s(CJ) - E_c$).

The Gurney assumption on uniformity of density of detonation products implies uniformity in pressure, and thus constant entropy during the expansion. This enables Gurney energy to be expressed in terms of JWL equation, as a function of volume expansion [3]. Assuming the internal energy of detonation products transfers entirely to the Gurney energy (kinetic energy of gas and cylinder wall), the Gurney energy and detonation energy at the same expansion ratio can be equated:

$$E_G(V_r) = E_d(V_r) \tag{8}$$

The cylinder wall velocity at any expansion ratio ($v_s(_{Vr})$) is then calculated by equation:

$$v_s(V_r) = \frac{\sqrt{2E_G(V_r)}}{\sqrt{\left(\frac{M_C}{M_E} + \frac{1}{2}\right)}} \tag{9}$$

### 2.3 Hydro-Code Simulation

To evaluate the accuracy of the JWL coefficients derived by EXPLO5 numerical simulations are carried out in hydro-code AUTODYN, using 2D axisymmetric Lagrangian formulation. The calculations are done by applying programmed burned model that requires the JWL parameters, detonation velocity, and pressure as input parameters. All required parameters are calculated by EXPLO5, which means no experimental parameters are used. The explosive element size (axial × radial) was 1 × 1 mm for all calculations, while the copper cylinder wall elements were 0.5 × 0.5 mm, except for tests where wall thickness was above 5 mm in which case, 1x1 mm element size was used. The initiation line was set at the front end of charge, and wall velocity is registered by gauges located midway across the thickness of the cylinder wall. The Johnson-Cook strength model and the Johnson-

  

Cook damage model are used for the copper cylinder [32]. The copper is modeled using material parameters given in [33]

## 3 Experimental Section

### 3.1 Results and Discussion

Our previous studies have shown that at the same expansion ratio, detonation energies calculated by EXPLO5 code are systematically ~10% higher than the Gurney energies derived from experimental cylinder wall velocities [15, 16]. Similar results are reported also by Hardesty and Kennedy [17] and by Danel and Kazandijan [5] who used different thermochemical codes. Danel and Kazandijan showed that such discrepancy is not due to an inadequate equation of state incorporated in thermochemical codes because thermochemical calculations along with hydrocode calculations give good prediction of the cylinder wall velocity. This difference in energies indicates that the Gurney model does not give accurate prediction of the cylinder wall velocity.

Although our focus in this paper is on ANFO explosives, validation of the described model was first done on several standard ideal explosives. The validation included calculation of expansion isentrope, evaluation of the JWL coefficients, calculation of the Gurney energy, and calculation of the wall velocity by hydro-code AUTODYN

### 3.2 Validation of Model

#### *3.2.1 Ideal Explosives*

Four ideal explosives (PETN, HMX, TNT, and Comp B), for which reliable experimentally derived JWL coefficients have been reported in literature [6, 7, 34, 35], are chosen for analysis. Since the analysis gave similar results for all four tested explosives, only PETN results will be shown here. Pressure-volume data obtained using literature reported JWL coefficients given in Table 1 are compared with those obtained using EXPLO5's JWL coefficients (Figure 1).

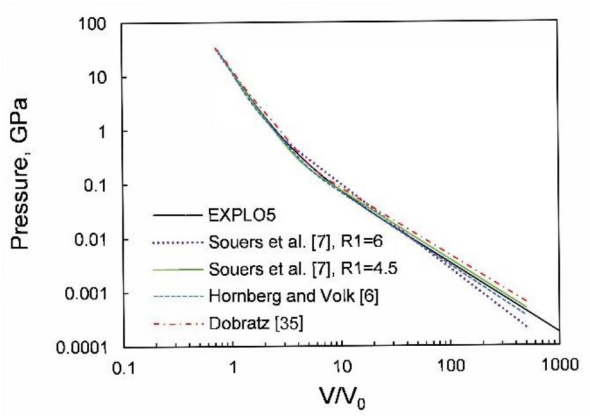


**Figure 1.** Comparison of PETN pressure-relative volume profiles calculated by different sets of JWL coefficients.

Table 1 shows that EXPLO5's calculated JWL coefficients are close to Souers et al.'s newer set of coefficients ($R_1 =$ 4.5), while Figure 1 shows that calculated pressure-volume data are similar for all five tested sets. Calculated $p_{CJ}$ ranges from 31.5 to 33.5 (i.e. 6%), while at larger expansion ratios, the difference expressed in percentages is larger (e.g. at $V/V_0 = 100$ pressure ranges between 0.0027 and 0.0043 GPa, i.e. ~60%). All studied sets of JWL coefficients predict similar detonation energy-volume profiles (difference between them is 3% relative to the mean value), Figure 2. At the same time, all sets result in 6–12% higher detonation energy than experimental Gurney energy at the same relative volume. EXPLO5's JWL coefficients predict 10% higher detonation energy over the entire range of expansion ratios. The exception is the JWL coefficients of Hornberg and Volk which predict lower detonation energy which matches experimental Gurney energy.

Some authors [17] explained the differences in calculated energy by thermochemical code and experimental Gurney energy by energy losses (cylinder wall fragmentation and products leaking, "end losses" due to axial ex-

**Table 1.** PETN JWL coefficients from different sources.

| Parameter | EXPLO5 This work | Souers *et al.* [7] | Souers *et al.* [7] | Hornberg and Volk [6] | Dobratz [35] |
|---|---|---|---|---|---|
| $\rho_0$, g cm$^{-3}$ | 1.763 | 1.763 | 1.763 | 1.763 | 1.77 |
| $A$, GPa | 689.716 | 1032.158 | 622.045 | 670.36 | 617.05 |
| $B$, GPa | 14.1912 | 90.57 | 21.465 | 10.4 | 16.926 |
| $C$, GPa | 1.34038 | 3.7274 | 1.4966 | 1.564 | 0.69 |
| $R_1$ | 4.53585 | 6.00 | 4.50 | 4.44191 | 4.40 |
| $R_2$ | 1.17541 | 2.60 | 1.50 | 1.19107 | 1.20 |
| $\omega$ | 0.29739 | 0.57 | 0.29 | 0.35 | 0.25 |
| $D$, km s$^{-1}$ | 8.384 | 8.274 | 8.283 | 8.30 | 8.30 |
| $p_{CJ}$, GPa | 31.5 | 31.5 | 33.1 | 32 | 33.5 |
| $E_0$, kJ cm$^{-3}$ | 10.95 | 10.8 | 11.2 | 10.1 | 10.1 |

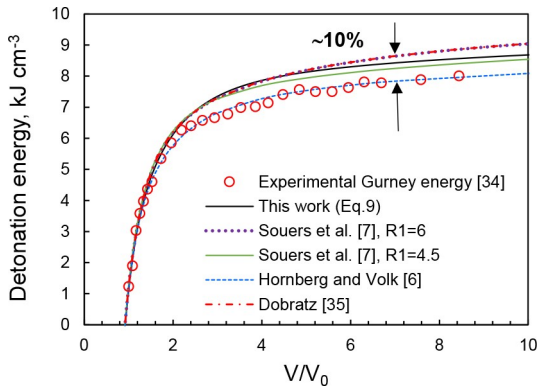


**Figure 2.** Comparison of calculated detonation energies and experimental Gurney energy for PETN.

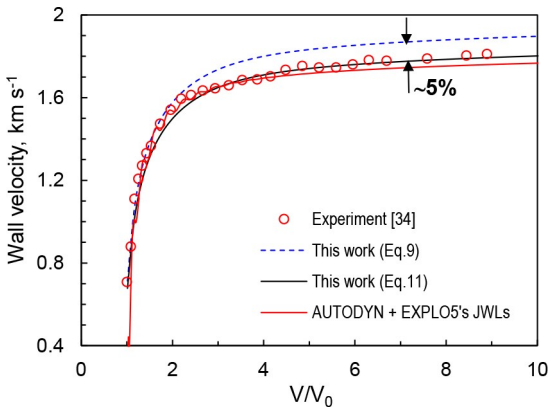


**Figure 3.** Comparison of PETN cylinder wall velocities calculated by AUTODYN using EXPLO5's JWL coefficients and by modified Gurney equation.

pansion, the wall yield strength, etc.), which are not considered in the Gurney model. Souers and Minich [36] gave a detailed analysis of cylinder test corrections. They listed five types of corrections that must be considered, with the wall thinning and work hardening being most important. Unlike the Gurney model, hydro-codes are capable of taking into account the strength of material. A rudimentary calculation on PETN using AUTODYN hydro-code, with and without inclusion of the material strength indicated a 6% difference in calculated Gurney energy. This partly explains the energy difference between the Gurney model and hydro-code calculations. The results reported in [16], as well as the results shown in Figure 2, suggest that the overall energy losses accounts for about 10% of the total energy. The easiest way to take into account energy losses is to reduce calculated detonation energy in the Gurney equation (Eq. 9) by a factor ($k_f$):

$$E_G^*(V_r) = k_f \cdot E_d(V_r) \tag{10}$$

where $k_f = 0.9$. Thus, the wall velocity should be calculated by modified Gurney equation:

$$v_s^*(V_r)^* = \frac{\sqrt{2E_G^*(V_r)}}{\sqrt{\left(\frac{M_C}{M_E} + \frac{1}{2}\right)}} \tag{11}$$

A standard way of evaluating JWL coefficients from cylinder test results is by hydro-code simulations. We used here the hydro-code AUTODYN to validate the capabilities of EXPLO5's JWL coefficients so as to reproduce experimental wall velocity-relative volume data. As shown in Figure 3, AUTODYN simulation with EXPLO5's JWL coefficients slightly underestimates the cylinder wall velocity of PETN (about 2.5% at $V/V_0 = 7$). Other sets of JWL coefficients given in Table 1 give similar results with the exception being Hornberg and Volk's set which gives about 10% lower wall velocity than experimental.

Figure 3 also shows that the wall velocities calculated by Eq. 11 closely match experimental data, whereas wall velocities calculated by Eq. 9 are higher than experimental by ~5%. AUTODYN and modified Gurney equation (Eq. 11) give very similar values of wall velocities over the entire range of relative volumes.

### 3.2.2 ANFO Explosives

Experimental cylinder test results for ANFO explosives reported by Nyberg *et al.* [28], Helm *et al.* [37], Sanchidrian *et al.* [38], and Davis and Hill [39] are used to test applicability of the model on ANFO explosives. Charge diameters in these experiments varied from 50.8 mm to 292.1 mm and $M_C/M_E$ ratio from 2.14 to 5.04 (Table 2).

Detonation parameters and the JWL coefficients for the ANFO explosives to be studied are calculated by EXPLO5's kinetic module as follows. The standard mode of calculation of detonation parameters by EXPLO5's kinetic module, i.e. the WK theory incorporated in the module, involves unconfined charges for which the relationship between charge diameter ($d_i$) and shock front curvature radius ($R_C$) can be determined experimentally or predicted by empirical equations [40–43]. However, if a reliable relationship between confined charge detonation velocity and shock front curvature radius is available, the kinetic module can calculate detonation parameters of confined explosives charges too [44]. In the absence of a reliable relationship between confined charge detonation velocity and shock front curvature radius, the radius of shock curvature was calculated iteratively by varying the shock curvature radius until calculated detonation velocity closely matches experimental for a given cylinder test configuration (Table 2).

Once the sonic point and the parameters at the sonic point are determined, the equilibrium expansion isentrope, and the JWL coefficients are calculated as described in Sec-

  

**Table 2.** ANFO explosives, cylinder test dimension, and calculated detonation parameters.

| ANFO name/ denotation | $\rho_0$, g cm$^{-3}$ | Cylinder dimensions | | | | Ref. | EXPLO5 calculation results | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | $d_i$, mm | $w$, mm | $M_C/M_E$ | $D_{exper.}$, Km s$^{-1}$ | | $R_C$, mm | $D$, Km s$^{-1}$ | $p_{CJ}$, GPa | $Q_v$, kJ kg$^{-1}$ | $D_{id}$, Km s$^{-1}$ | $D/D_{id}$ | $\lambda_{CJ}$ |
| Lambrit | 0.776 | 100 | 5 | 2.41 | 4.08 | [27,37] | 500 | 4.03 | 3.36 | 3.82 | 4.63 | 0.88 | 0.981 |
| Nagolita | 0.902 | 100 | 5 | 2.14 | 4.43 | [27,37] | 270 | 4.31 | 4.26 | 3.77 | 5.15 | 0.84 | 0.968 |
| A-U-100 | 0.830 | 100 | 5 | 2.26 | 3.88 | [37] | 250 | 3.89 | 3.24 | 3.76 | 4.83 | 0.80 | 0.965 |
| Prilit A | 0.850 | 100 | 5 | 2.24 | 3.85 | [27,37] | 210 | 3.85 | 3.23 | 3.85 | 4.93 | 0.78 | 0.957 |
| A-U-50 | 0.830 | 50 | 2.5 | 2.26 | 3.23 | [37] | 139 | 3.25 | 2.20 | 3.58 | 4.83 | 0.67 | 0.919 |
| D&H-101 | 0.931 | 101.6 | 10.2 | 4.22 | 4.17 | [38] | 185 | 4.17 | 4.06 | 3.73 | 5.27 | 0.79 | 0.957 |
| H-292.1 | 0.82 | 292.1 | 29.9 | 4.93 | 4.45 | [36] | 850 | 4.42 | 4.23 | 3.85 | 4.81 | 0.92 | 0.989 |
| H-101.6 | 0.78 | 101.6 | 10.2 | 5.04 | 3.89 | [36] | 380 | 3.91 | 3.16 | 3.79 | 4.65 | 0.84 | 0.972 |
| H-50.8 | 0.80 | 50.8 | 5.1 | 4.91 | 3.25 | [36] | 160 | 3.24 | 2.15 | 3.61 | 4.73 | 0.68 | 0.927 |

Legend: $D_{id}$ is detonation velocity at infinite diameter, $d_i$ – inner cylinder diameter, $w$- wall thickness

tion 2.2. The results of calculations are given in Tables 2 and 3.

The JWL coefficients of ANFO explosives calculated by EXPLO5 are validated by comparing calculated pressure-volume profiles, detonation energy-volume, and the wall velocity-volume profiles with those obtained using literature reported JWL coefficients derived from cylinder test experiments. For further validation, we compared calculated cylinder wall velocities of studied ANFOs with those obtained experimentally.

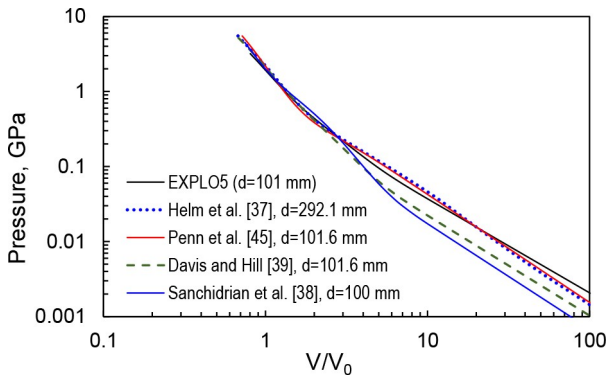


**Figure 4.** Pressure-volume profiles of ANFO calculated by different sets of JWL coefficients.

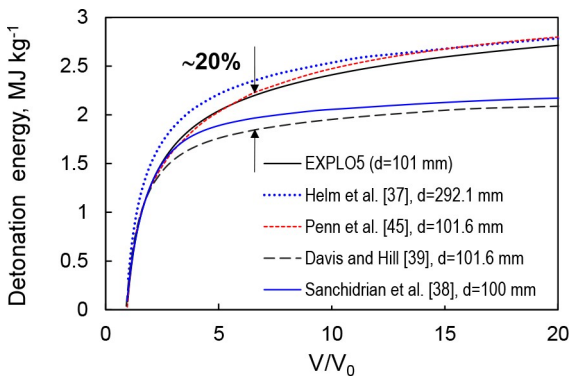


**Figure 5.** Detonation energies of ANFO calculated by different sets of JWL coefficients.

Figure 4 shows pressure-volume profiles for 101 mm ANFO charges, calculated by different JWL coefficients derived from cylinder test experiments and by EXPLO5's calculated JWL coefficients (Table 3).

The pressure-volume profile predicted by EXPLO5's JWL coefficients is quite close to those obtained by Helm *et al.* for 292.1 mm charge, and Penn *et al.* for 101.6 mm charge, but deviates significantly from those of Davis and Hill's and Sanchidrian *et al.* above $V/V_0 > 3.5$. The detonation energies calculated using different JWL sets of coefficients differ up to 20 % at $V/V_0 = 7$ (Figure 5).

Such large difference can be partly attributed to differences in the approach in deriving the JWL coefficients, and partly to differences in properties of ammonium nitrate and fuel oil used by different authors, density, detonation velocity, and $M_C/M_E$ ratio. Therefore, this comparison may not be entirely correct, but it illustrates the complexity in evaluation of JWL coefficients in the case of highly non-ideal explosives such as ANFO.

In evaluation of JWL coefficients from cylinder test data, some authors take the detonation energy such that it agrees with the measured detonation heat at 0.1 MPa. However, according to Eq. 6, lower integration limit should be $V \rightarrow \infty$ and accordingly, the energy should be that at infinite volume [7]. This will add about 0.5 kJ cm$^{-3}$ to the energy at 0.1 MPa, which is a significant correction. We derived JWL coefficients a lower limit of $V \rightarrow \infty$, and this is why our $E_0$(p = 0.1 MPa) agrees with detonation heat, while $E_0(V \rightarrow \infty)$ is about 0.4–0.5 kJ cm$^{-3}$ larger. Generally, our model gives significantly higher values of detonation energies at infinite volume than reported by Sanchidrian *et al.* [38].

The JWL coefficients calculated by EXPLO5 (Table 3) are validated through AUTODYN simulations, comparing calculated cylinder wall velocities with experimental for tested ANFOs. In addition, the Gurney equation (Eq. 9) and modified Gurney equation (Eq. 11), are also validated by compar-

  

**Table 3.** Calculated JWL coefficients and cylinder wall velocities for studied ANFOs.

| Parameter | Units | H-50.8 | H-101.6 | H-292.1 | Lambrit | Nagolita | Prilit A | A-50 | A-U-100 | D&H-101 |
|---|---|---|---|---|---|---|---|---|---|---|
| $\rho_0$ | g cm$^{-3}$ | 0.80 | 0.78 | 0.82 | 0.78 | 0.90 | 0.85 | 0.83 | 0.83 | 0.93 |
| *A* | GPa | 24.512991 | 41.967938 | 69.317046 | 45.710002 | 62.394852 | 42.057219 | 25.769962 | 42.063696 | 57.590155 |
| *B* | GPa | 0.572033 | 1.054352 | 1.732784 | 1.169164 | 1.430255 | 0.985142 | 0.587096 | 1.010185 | 1.285092 |
| *C* | GPa | 0.577346 | 0.663351 | 0.736988 | 0.683685 | 0.717596 | 0.666875 | 0.577889 | 0.676896 | 0.704957 |
| $R_1$ | | 3.243235 | 3.878952 | 4.323103 | 3.993251 | 3.859844 | 3.600482 | 3.199617 | 3.666969 | 3.671929 |
| $R_2$ | | 0.807274 | 1.004439 | 1.127025 | 1.044354 | 0.972008 | 0.908969 | 0.789569 | 0.935652 | 0.916147 |
| $\omega$ | | 0.212806 | 0.252286 | 0.275304 | 0.260953 | 0.256020 | 0.241440 | 0.208514 | 0.248145 | 0.246373 |
| *D* | Km s$^{-1}$ | 3.24 | 3.91 | 4.52 | 4.03 | 4.31 | 3.85 | 3.25 | 3.89 | 4.17 |
| $p_{CJ}$ | GPa | 2.15 | 3.17 | 4.44 | 3.36 | 4.26 | 3.23 | 2.20 | 3.24 | 4.06 |
| $E_0$ ($V\rightarrow\infty$) | kJ cm$^{-3}$ | −3.347 | −3.351 | −3.547 | −3.349 | −3.833 | −3.606 | −3.449 | −3.542 | −3.929 |
| $E_0$($p=0.1$ *MPa*) | kJ cm$^{-3}$ | −2.754 | −2.904 | −3.165 | −2.928 | −3.374 | −3.108 | −2.828 | −3.070 | −3.433 |
| $Q_d$ | kJ cm$^{-3}$ | −2,890 | −2,955 | −3,161 | −2,965 | −3,397 | −3,169 | −2,974 | −3,122 | −3,471 |
| $v_s(7)$, experiment | Km s$^{-1}$ | 0.820 | 0.875 | 0.893 | 1.182 | 1.225 | 1.114 | 1.074 | 1.124 | 0.888 |
| $v_s(7)$, AUTODYN | Km s$^{-1}$ | 0.811 | 0.845 | 0.884 | 1.190 | 1.298 | 1.189 | 1.149 | 1.222 | 0.943 |
| $v_s(7)$, Eq. 11 | Km s$^{-1}$ | 0.804 | 0.849 | 0.886 | 1.184 | 1.269 | 1.202 | 1.121 | 1.202 | 0.941 |

Legend: $v_s(7)$ is terminal cylinder wall velocity, at $V/V_0=7$.

ing calculated wall velocities with experimental. The results of comparison are given in Figure 6 and Figure 7.

It can be noticed that both AUTODYN and Eq. 11 reproduce Helm *et al.* experimental wall velocity profiles very well (maximum difference at $V/V_0=7$ does not exceed 30 m s$^{-1}$, i.e. 3%). Agreement with Nyberg *et al.* and Sanchidrian *et al.* experimental wall velocities at $V/V_0=7$ is poorer; difference is up to 75 m s$^{-1}$ (about 6%) for Nagolita and Lambrit, and 75–98 m s$^{-1}$ (6–9%) for A-U-110, A-U-50, and Prilit A. However, agreement at lower expansion ratios (up to 3.5) is satisfactory in all cases. It is also interesting to note that experimental pressure-volume curves for A-U-110, A-U-50, Prilit A, and D&H are "flat" above $V/V_0>4$. Wall velocity

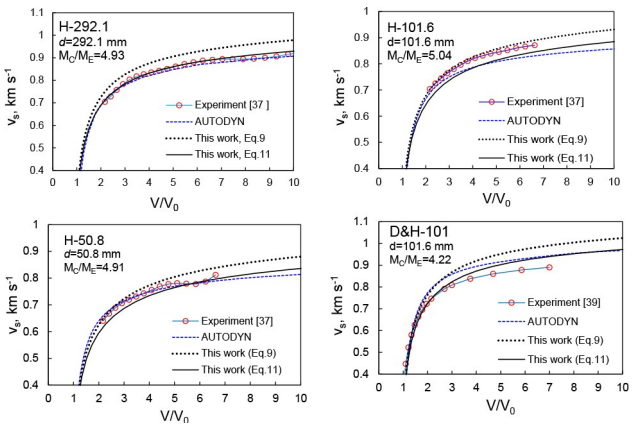


**Figure 6.** Comparison of calculated and Helm *et al.* and Davis and Hill's experimental wall velocity profiles.

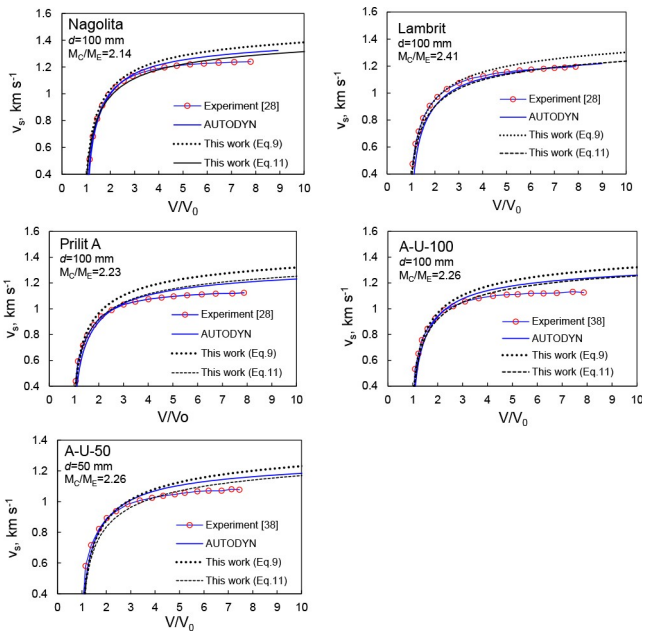


**Figure 7.** Comparison of calculated and Nyberg *et al.* and Sanchidrian *et al.* experimental wall velocity profiles.

for these ANFOs increases ~70–80 m s$^{-1}$ between $V/V_0 = 3$ and $V/V_0 = 7$, while in the case of Helm *et al.*'s experiments, both AUTODYN and Eq. 11, show an increase of wall velocity of 130–140 m s$^{-1}$ (12.5 %) between $V/V_0 = 3$ and $V/V_0 = 7$. Considering that decomposition of ANFO and generation of energy continues during the expansion, similar continuous increase in wall velocity should be expected in all experiments conducted under similar conditions (charge diameter and $M_C/M_E$ ratio). It is important to emphasize that AUTODYN and the modified Gurney equation (Eq. 11) predict very similar wall velocity-relative volume profiles for all studied ANFOs – the difference between them is less than 2.5 %.

Comparing available chemical energy of ANFOs (heat of detonation of reacted fraction of ANFO) and the Gurney energy at $V/V_0 = 7$ (terminal wall velocity), the conclusion is that only 45—60 % of available energy is converted to the Gurney energy. For comparison, in the case of PETN, 75 % of available energy is converted to Gurney energy.

## 4 Conclusions

The results presented here have demonstrated that combining thermochemical calculations and expressing Gurney energy in terms of JWL equation of state, provide a way to predict cylinder wall velocity of ANFO explosives.

The JWL coefficients derived by thermochemical calculations overestimate the Gurney energy (Eq. 8) of studied ideal explosives about 10 % and cylinder wall velocity (Eq. 9) by about 5% (Figures 2 and 3). However, when the same JWL coefficients are used along with AUTODYN hydro-code then good predictions of the wall velocity is obtained. This result confirms the validity of the JWL coefficients calculated by EXPLO5 but also indicates that the Gurney model does not predict correctly cylinder wall velocity. The same has been noted also by Danel and Kazandijan [5] and, in our opinion, is not related to an inadequate equation of state but to the fact that the Gurney model does not take into account energy losses that happen during the cylinder expansion tests (e.g. fracturing of cylinder wall and leaking of gas products, axial expansion of products, wall thinning and hardening, etc. [17, 36]). This is the reason why the detonation energies calculated by thermochemical codes are always higher than experimentally determined Gurney energies at the same expansion ratio.

We took the energy loses into account in a simple way so that we reduced theoretically calculated detonation energy by a factor $k_f = 0.9$ and expressed the Gurney energy as: $E_G(V/V_0) = k_f[E_d(V/V_0)]$. The modified Gurney energy agree much better with the Gurney energy obtained by cylinder tests and gives good prediction of cylinder wall velocity. The wall velocity profile of ANFO explosives calculated using modified Gurney energy agree very well with those obtained by AUTODYN simulation with a difference of less than 2.5 % over the entire range of expansion ratios.

The JWL coefficients derived by EXPLO5 calculations along with hydro-code AUTODYN predict the terminal wall velocities for ANFO explosives with an error of less than 6 % (75 m s$^{-1}$) for most the explosives studied, and 9 % (98 m s$^{-1}$) for some of them. The JWL coefficients derived by EXPLO5 calculations along with hydro-code AUTODYN predict the terminal wall velocities for ANFO explosives with an error of less than 6 % (75 m s$^{-1}$) for most the explosives studied, and 9 % (98 m s$^{-1}$) for some of them. The proposed model does not need the cylinder test data to derive the JWL coefficients for non-ideal explosives, however, it requires experimental $D$-$R_0$ and $R_c$-$R_0$ data to calibrate reaction rate model and radial expansion model.

## *Acknowledgements*

This research was supported by the Croatian Science Foundation (HRZZ), Croatia, under the projects IP-2019-04-1618 and I-2243-2017 and the Faculty of Mining, Geology and Petroleum Engineering, Zagreb, Croatia.

## References

[1] R. W. Gurney, *Initial Velocities of Fragments from Bombs, Shells, Grenades*, Report BRL 405, Army Ballistic Research Laboratories, Aberdeen Proving Ground, MD, USA, **1973**.
[2] J. E. Kennedy, Chapter 7: The Gurney model of explosive output for driving metal in: J. A. Zukas, W. Walters, *Explosive Effects and Applications*, Springer-Verlag, New York, **1998**, p. 221.
[3] P. J. Miller, K. E. Alexander, Determining JWL equation of state parameters using the Gurney equation approximation, *9th Symposium (International) on Detonation*, Portland, Oregon, USA, **1989**, p. 498.
[4] D. Mathieu, Prediction of Gurney parameters based on an analytic description of the expanding products, *J. Energ. Mater.* **2015**, *33*, 102–115.
[5] J. F. Danel, L. Kazandijan, A few remarks about the Gurney energy of condensed explosives, *Propellants Explos. Pyrotech.*, **2004**, *29/5*, 314–316.
[6] H. Hornberg, F. Volk, The Cylinder Test in the Context of Physical Detonation Measurement Methods, *Propellants Explos. Pyrotech.* **1989**, *24*, 199–211.
[7] P. C. Souers, B. Wu, L. C. Haselman, *Detonation equation of state at LLNL*, Report: UCRL-ID-119262, Lawrence Livermore National Laboratory, Livermore, **1995**.
[8] M. Suceska, *Test Methods for Explosives*, Springer-Verlag, New-York, **1995**.
[9] A. Koch, N. Arnold, M. Estermann, M. A simple relation between the detonation velocity of an explosive and its Gurney energy, *Propellants Explos. Pyrotech.* **2002**, *27*, 365–368.
[10] P. Locking, Gurney velocity relationship, *29th International Symposium on Ballistics*, Edinburgh, Scotland, **2016**, p.1291–1299.
[11] P. Locking, Accuracy of empirical Gurney velocity prediction models, *30th International Symposium on Ballistics*, Long Beach, California, USA, **2017**, p. 1415–1426.
[12] P. M. Locking, Accuracy of empirical predictions of an explosive's adiabatic exponent, *31st International Symposium on Ballistics*, Hyderabad, India, **2019**, p.1875–1887.

  

[13] M. H. Keshavarz, New method for prediction of the Gurney energy of high explosives, *Propellants Explos. Pyrotech.* **2008**, *33*, 316–320.
[14] M. H. Keshavarz, S. Abolfazl, The simplest method for calculating energy output and Gurney velocity of explosives, *J. of Hazard. Mater.* **2006**, *131*, 1–5.
[15] B. Stimac, V. Bohanek, M. Dobrilovic, M. Suceska, Prediction of Gurney velocity based on EXPLO5 code calculation results, *23rd Seminar on New Trends in Research of Energetic Materials (NTREM)*, University of Pardubice, **2020**, p.693–704.
[16] M. Suceska, M. Dobrilovic, V. Bohanek, B. Stimac, Estimation of explosive energy output by EXPLO5 thermochemical code, *Z. Anorg. Allg. Chem.* **2020**, DOI: 10.1002/zaac.202000219 (in press).
[17] D. R. Hardesty, J. E. Kennedy, Thermochemical estimation of explosive energy output, *Combust. Flame* **1997**, *28*, 45–49.
[18] W. W. Wood, J. Kirkwood, Diameter effect in condensed explosives: the relationship between velocity and radius of curvature of the detonation wave, *J. Chem. Phys.* **1954**, *22*, 1920–1924.
[19] I. J. Kirby, G. A. Leiper, A small divergent detonation theory for in termolecular explosives, *8th International Symposium on Detonation*, Office of Naval Research, Arlington, USA, **1985**, p.176.
[20] M. Suceska, *EXPLO5 User's Guide*, OZM Research s.r.o., Hrochův Týnec, **2020**.
[21] B. Stimac, H. Y. Chan, M. Kunzel, M. Suceska, Numerical Modelling of Detonation Reaction Zone of Nitromethane by EXPLO5 Code and Wood and Kirkwood Theory, *Cent. Eur. J. Energ. Mater.* **2020**, *17*, 239–261.
[22] M. Suceska, H. Y. Chan, A. How-Ghee, Can the Accuracy of BKW EOS be Improved, *15th International Detonation Symposium*, San Francisco, USA, **2014**, p. 1247.
[23] S. Esen, P. C. Souers, P. Vitello, Prediction of non-ideal detonation performance of commercial explosives using the DeNE and JWL++ codes, *Int. J. Numer. Methods. Eng.* **2005**, *64*, 1889–1914.
[24] G. J. Sharpe, M. Braithwaite, Steady non-ideal detonations in in cylindrical sticks of explosives, *J. Eng. Math.* **2005**, 53, 39–58.
[25] B. Štimac, V. Škrlec, M. Dobrilović, M. Sućeska, Numerical modelling of non-ideal detonation in ANFO explosives applying Wood-Kirkwood theory coupled with EXPLO5 thermochemical code, *Defence Technology* **2020**, DOI: https://doi.org/10.1016/j.dt.2020.09.014 (in press).
[26] C. C. Stephenson, D. R. Bentz, D. A. Stevenson, The Heat Capacity of Ammonium Nitrate from 15 to 315 °K, *Journal of the American Chemical Society* **1955**, *77:8*, 2161–2169.
[27] M. Nagatani, T. Seiyama, M. Sakiyama, H. Suga, S. Seki, Heat Capacities and Thermodynamic Properties of Ammonium Nitrate Crystal: Phase Transitions between Stable and Metastable Phases, *Bull. Chem. Soc. Jpn.* **1967**, *40*, 1833–1844.
[28] U. Nyberg, I. Arvantidis, M. Olsson, F. Ouchterlony, Large size cylinder expansion tests on ANFO and gassed bulk emulsion explosives. In: *Explosives and blasting technique*, Balkema Publishers, Rotterdam **2003**, p.181.
[29] A. Minchinton, On the Influence of Fundamental Detonics on Blasting Practice, *11th International Symposium on Rock Fragmentation by Blasting*, Sydney **2015**, p. 41–53.
[30] P. C. Souers, J. W. Kury, Comparison of cylinder data and code calculations for homogeneous explosives, *Propellants Explos. Pyrotech.* **1993**, *18*, 175–183.
[31] M. Suceska, Evaluation of detonation energy from EXPLO5 computer code results , *Propellants, Explos. Pyrotech.* **1999**, *24*, 280–285.
[32] *AUTODYN, Explicit Software for Nonlinear Dynamics*, Theory manual, Revision 4.3, Century Dynamics, **2005**.
[33] P. M. Elek, V. V. Dzingalasevic, S. S. Jaramaz, D. M. Mickovic, Determination of detonation products equation of state from cylinder test: Analytical model and numerical analysis, *Thermal Science* **2015**, *19/11*, 35–48.
[34] G. I. Kerley, *Prediction of Explosive Cylinder Tests Using Equations of State from the PANDA Code*, Report: SAND93-2131, Sandia National Laboratories, Albuquerque, **1993**.
[35] B. M. Dobratz, *Properties of chemical explosives and explosive simulants*, Report UCRL-51319, Lawrence Livermore Laboratory, Livermore, **1972**.
[36] P. C. Souers, R. Minich, Cylinder Test Correction for Copper Work Hardening and Spall, *Propellants Explos. Pyrotech.* **2010**, *35*, 1–9.
[37] F. Helm, M. Finger, B. Heyes, E. Lee, H. Chueng, J. Walton, *High explosive characterization for the dice throw event*, Report UCRL-52042, Lawrence Livermore national Laboratory, Livermore, **1976**.
[38] J. A. Sanchidrian, R. Castedo, L. M. Lopez, P. Segarra, A. P. Santos, Determination of the JWL Constants for ANFO and Emulsion Explosives from Cylinder Test Data, *Cent. Eur. J. Energ. Mater.* **2015**, 12, 177–194.
[39] L. L. Davis, L. G. Hill, ANFO cylinder test, *12th Conference of the American Physical Society Topical Group on Shock Compression of Condensed Matter,* Atlanta, Georgia (USA), June 24 – 29, **2001**, AIP Conference Proceedings 620, p. 165.
[40] D. Kennedy, The Challenge of Non-ideal Detonation, *Journal de Physique* **1995**, *5*, 191–207.
[41] R. A. Catanach, L. G. Hill, Diameter effect curve and detonation front curvature measurements for ANFO, *12th Conference of the American Physical Society Topical Group on Shock Compression of Condensed Matter,* Atlanta, Georgia (USA), June 24 – 29, **2001**, AIP Conference Proceedings 620, p. 906.
[42] P. C. Souers, *A Library of Prompt Detonation Reaction Zone Data*, Report No: UCRL-ID-130055 Rev1, Lawrence Livermore National Laboratory, Livermore, **1998**.
[43] S. I. Jackson, M. Short, C. B. Kiyanda, Precursor detonation wave development in ANFO due to aluminum confinement, *14th International Detonation Symposium*, Idaho, USA, **2010**, p.750–749.
[44] S. Esen, A Non-Ideal Detonation Model for Evaluating the Performance of Explosives in Rock Blasting, *Rock Mechanics for Rock Engineering* **2008**, *41*, 467–497.
[45] L. Penn, F. Helm, M. Finger, E. Lee, *Determination of equation-of-state for four types of explosive*, Report: UCRL-51892, Lawrence Livermore National Laboratory, Livermore, **1975**.

Manuscript received: August 26, 2020
Revised manuscript received: September 15, 2020

  