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Overview / Przegląd

Using thermochemical code EXPLO5 to predict the performance parameters of explosives
Zastosowanie programu termochemicznego EXPLO5 do predykcji parametrów użytkowych materiałów wybuchowych

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Abstract: *Thanks to the development of more powerful computers and efficient numerical techniques, numerical modelling has become a compulsory tool in solving various problems in the field of energetic materials. In cases where measuring techniques are still unable to measure a given parameter, numerical modelling may be the only option of obtaining a value. In addition, numerical modelling helps us to better understand some phenomena, particularly in understanding the influence of input parameters on output results, as well as saving time and money. The thermochemical equilibrium code EXPLO5 is such a tool which enables theoretical prediction of performance of high explosives, propellants and pyrotechnic compositions. The code is used by more than 80 research laboratories worldwide.*

Streszczenie: *Ciągły rozwój coraz bardziej wydajnych komputerów oraz technik obliczeń numerycznych powoduje, że stosowanie modelowania numerycznego staje się koniecznością przy rozwiązywaniu różnorodnych problemów w obszarze materiałów wysokoenergetycznych. Tendencja ta jest szczególnie wyraźna w przypadkach, w których metody pomiarowe nadal nie umożliwiają zmierzenia wartości badanego parametru, tzn. gdy tylko modelowanie numeryczne daje możliwość określenia jego wartości liczbowej. Ponadto, modelowanie numeryczne umożliwia nam lepsze poznanie niektórych zjawisk, np. lepsze zrozumienie wpływu warunków początkowych danego procesu na jego wyniki końcowe. Dodatkowym atutem stosowania modelowania numerycznego jest oszczędność czasu i pieniędzy. Tego typu narzędziem jest EXPLO5, program do opisu równowagi termochemicznej. Umożliwia on, na drodze analizy teoretycznej, dokonanie predykcji efektów działania materiałów wybuchowych kruszących, paliw rakietowych i mieszanin pirotechnicznych. Program ten jest używany w ponad 80 laboratoriach badawczych w całym świecie.*

Keywords: *explosives, performance, detonation, kinetic detonation, JWL coefficients, Gurney* energy, detonation *energy*
Słowa kluczowe*: materiały wybuchowe, efekt działania, detonacja, detonacja kinetyczna, współczynniki JWL, energia Gurney'a, energia detonacji*

1. Theoretical background and application

Thermochemical codes solve thermodynamic equations between detonation products species to determine the chemical equilibrium at specified volume, pressure, and temperature. When coupled with the Chapman-Jouguet (C-J) detonation theory, they can predict detonation velocity, pressure, energy, heat, temperature, etc. of explosives.

EXPLO5 calculates the equilibrium composition of detonation products applying the free energy minimization technique. It uses the Becker-Kistiakowsky-Wilson (BKW) and EXP-6 equations of state (optionally) for gaseous detonation products, and the Murnaghan equation of state for condensed products. EXPLO5 is designed to enable calculation of chemical equilibrium composition and thermodynamic parameters of state along the shock adiabat of detonation products, the C-J state and the detonation parameters at the C-J state, as well as the parameters of state along the expansion isentrope. The program has a non-linear curve fitting program built in to fit relative volume-pressure data along the expansion isentrope in accordance with the Jones-Wilkins-Lee (JWL) model, enabling calculation of the energy available for performing mechanical work and the Gurney velocity. Recently the Wood-Kirkwood detonation theory has been incorporated into EXPLO5, which allows for modelling of time-dependent phenomena (e.g. partial detonation, detonation reaction zone profile, etc.) [1].

EXPLO5 can handle a wide variety of different molecules and their mixtures (containing up to 48 different chemical elements: C, H, N, O, Al, Cl, Si, F, B, Ba, Ca, Na, P, Li, K, S, Mg, Mn, Zr, Mo, Cu, Fe, Ni, Pb, Sb, Hg, Be, Ti, I, Xe, U, W, Sr, Cr, Br, Co, Ag, Zn, Sn, Bi, Cs, Hf, Ge, Nb, Ta, Yb, Y, and V). EXPLO5's Database includes around 700 of the most frequently used reactants and more than 1000 possible products. Users can manipulate the database (add or remove compounds, modified data, etc.). EXPLO5's graphical user interface is intuitive and easy to use. It allows the user to run detonation calculations with only one edit window, e.g. Figure 1 shows the graphical user interface for version V6.05.03 [1].

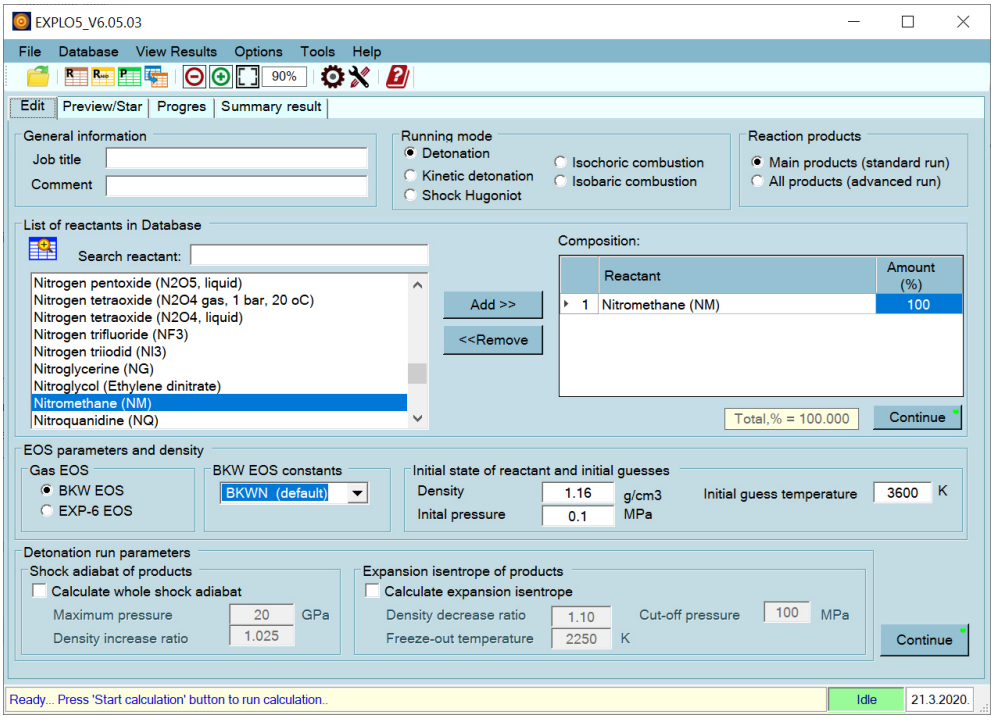


Figure 1. EXPLO5's user interface [1]

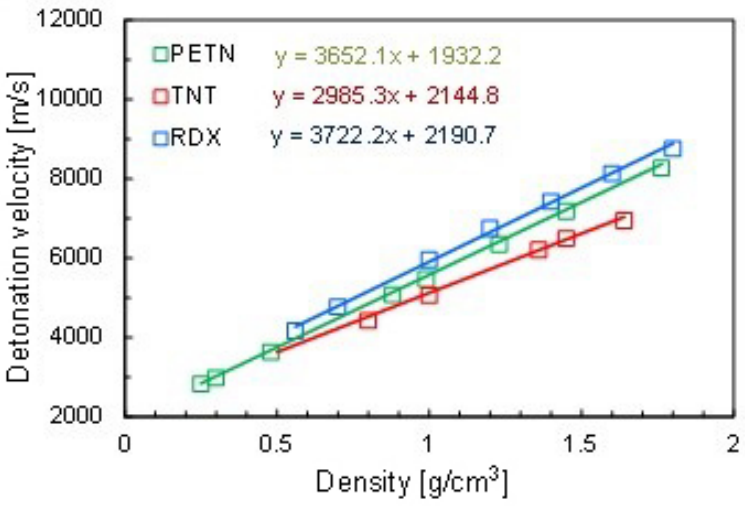
2. Composition of detonation products

Standard EXPLO5 detonation runs include calculation of detonation parameters for a specified explosive (or mixture of reactants) at a specified density. Optionally, a detonation run may also include calculation of parameters of state along the expansion isentrope of detonation products, from which the detonation energy and the Gurney velocity and energy may be derived. The standard run is used by those interested in predicting detonation properties of new explosives and formulations (e.g. synthesis chemists), while the second option is used when more details on explosive energy output – including its capability to drive surrounding material, is required. The main output results of a standard detonation run are given in Table 1 and Figure 2. In Table 1:

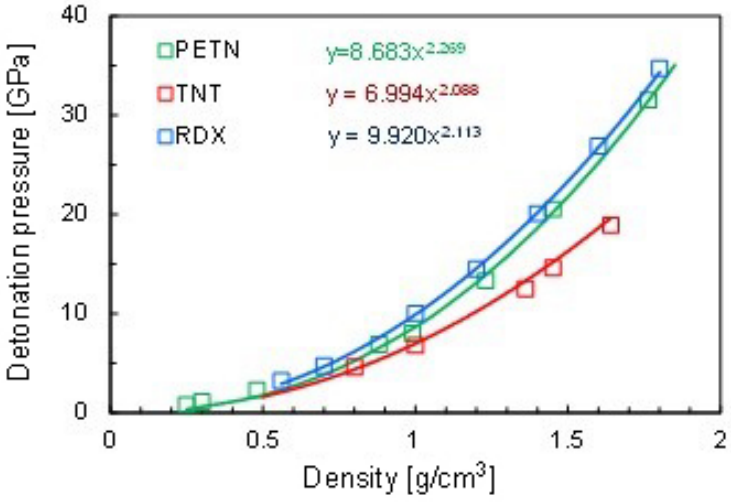
– calculations carried out using BKW EOS for gas phase products,
– products whose concentrations are less than 0.001 mol/mol of explosive are not shown

Table 1. Calculated detonation parameters and concentration of detonation products for some typical high explosives

Input parameters	Unit	RDX	PETN	TNT	
General formula	–	$C_3H_6N_6O_6$	$C_5H_8N_4O_{12}$	$C_7H_5N_3O_6$	
Density	[g/cm^3]	1.80	1.763	1.64	1.45
Enthalpy of formation	[kJ/kg]	316.6	–1688.1	–261.3	–261.3
Oxygen balance	[%]	–21.61	–10.12	–73.96	–73.96
Parameters at the CJ point					
Detonation velocity	[m/s]	8802	8375	6753	6458
Detonation pressure	[GPa]	33.94	30.52	18.11	15.14
Particle velocity	[m/s]	2142	2067	1635	1616
Detonation heat	[kJ/kg]	–5739	–6010	–4397	–4392
Detonation temperature	[K]	3753	3979	3184	3249
Concentration of products at the CJ point [mol/mol of explosive]					
N_2(g)	–	2.97191	1.99390	1.46827	1.45599
H_2O(g)		1.67173	2.61674	1.69145	1.73242
CH_2O_2(g)		1.22894	1.35752	0.61825	0.44832
CO_2(g)		0.71230	3.02349	1.02229	0.92164
C(solid, graphite)		–	–	–	4.02338
C(solid, diamond)		0.60129	–	4.29137	–
CO(g)		0.44543	0.61739	1.02695	1.52663
NH_3(g)		0.04759	0.00924	0.05137	0.06553
H_2(g)		0.01685	0.01065	0.05675	0.11025
HCN(g)		0.00815	0.00145	0.01199	0.02231
CH_4(g)		0.00250	–	0.01886	0.03645
C_2H_4(g)		–	–	–	0.00571



(a)



(b)

Figure 2. Dependence of calculated detonation velocity on (a) detonation pressure (b) density of explosives (squares represent experimental data points, the solid line EXPLO5 calculations); experimental data are taken from [2] and [3]

Figure 2 illustrates the effect of density of explosives on detonation velocity and detonation pressure. The almost linear increase of detonation velocity with density is consistent with experimentally obtained measurements, as well as pressure increase with (approximately) density squared. The effect of oxygen balance and density of the explosive on the composition of detonation products can be seen in Table 1. For instance, at a density of 1.64 g/cm^3, TNT produces diamond, while at 1.45 g/cm^3 it produces graphite. This is due to the fact that the phase state and concentration of products is determined by pressure and temperature.

When it comes to the accuracy of prediction of detonation parameters of explosives, it should be noted that numerous validations of EXPLO5 calculations carried out so far, on a broad range of densities and compositions, confirmed that it predicts detonation velocity for ideal high explosives, with a standard deviation of 1.8-2.3% (depending on the equation of state used and set of explosives used for the validation). Calculated detonation pressure varies somewhat more significantly – the standard deviation is 5.6-7.2% [1].

3. Detonation energy and JWL coefficients

Hot detonation products push on their surroundings and this is the work they are doing, or energy they are transferring. The work process is assumed to be isentropic and the expansion is represented by the expansion isentrope in the *p-V* diagram (Figure 3). EXPLO5 is designed to calculate thermodynamic parameters along the isentrope and assumes that the state of equilibrium in the products stabilises above 2250 K, while below this temperature all product concentrations are stopped and equilibrium chemistry ceased, with only *PdV* energy released afterwards. Once the expansion isentrope is calculated, detonation energy (i.e. energy available for performing mechanical work) is calculated applying the so-called JWL model [4]. The model assumes that the detonating explosive compresses instantly from room temperature and pressure, along the Rayleigh line to the C-J point where it expands along the isentrope given by the JWL equation of state [4]:

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

where $V_r=V/V_0$ (or ρ_0/ρ) is the relative volume (or expansion ratio), *A, B, C,* R_1, R_2 and ω are the JWL coefficients. By integrating Equation 1 one obtains the internal energy of the detonation products along the expansion isentrope (E_s):

$$E_s(V_r) = -\int_{\infty}^{V_r} p\, dV_r = \frac{A}{R_1} e^{-R_1 V_r} + \frac{B}{R_2} e^{-R_2 V_r} + \frac{C}{\omega} V_r^{-\omega} \tag{2}$$

The energy of the detonation products at any relative volume ($E_d(V_r)$) is given by Equation 3:

$$E_d(V_r) = -\{[E_s(CJ) - E_s(V_r)] - E_c\} \tag{3}$$

where E_c is the energy of shock compression of detonation products from initial volume to the CJ state. Since at infinite volume the energy of the products equals zero, the detonation energy at infinite volume (E_0) is:

$$E_0 = E_d(V_r \to \infty) = -[E_s(CJ) - E_c] \tag{4}$$

Once the expansion isentrope is calculated, the program uses a built-in subroutine to determine the JWL coefficients and to calculate detonation energy as a function of relative volume (Figure 3). Detonation energies calculated by EXPLO5 agree very well with the energies derived experimentally using the cylinder test (the difference for standard high explosives is up to 5%).

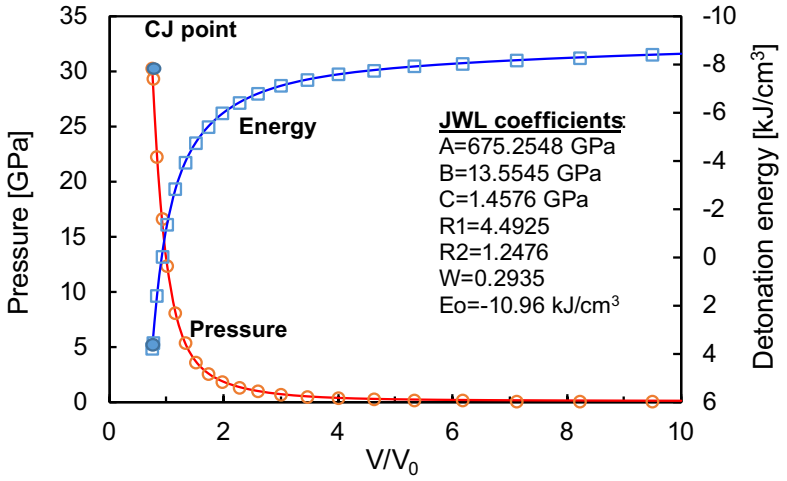


Figure 3. Expansion isentrope (red line and ○) and detonation energy (blue line and □) of PETN having a density 1.763 g/cm^3, as a function of relative volume

4. Gurney velocity and cylinder wall velocity

The question of how fast an explosive can drive its surrounding material is of major interest in the application and safety of explosives. In 1943, Gurney [5] proposed a semi-empirical model which relates linear velocity (v_s) and the ratio of the mass of metal to the mass of explosive (M_C/M_E) and the Gurney energy (E_G). For a circular geometry this relationship takes the form:

$$\frac{v_s}{\sqrt{2E_G}} = \left(\frac{M_C}{M_E} + \frac{1}{2}\right)^{-0.5} \tag{5}$$

where is called the Gurney velocity (v_G).

The Gurney velocity is typically derived from the cylinder expansion test by measuring terminal cylinder wall velocity (typically at an expansion ratio corresponding to 7 relative volumes). However, it can also be predicted by EXPLO5 calculations using two approaches. The first approach consists of correlation between the Gurney velocity and some easily measurable detonation parameter, usually detonation velocity (D) [6]:

$$\sqrt{2E_G} = D/A \tag{6}$$

where A is constant (usually between 2.95 and 3). This approach, however, predicts the Gurney velocity with a significant error (RMSE = 6.6%).

The second approach takes the internal energy states obtained during the expansion of the detonation products as a measure of energy output from an explosive. According to the Gurney theory, the Gurney energy corresponds to the difference between the internal energy at the C-J state and the internal energy remaining in the detonation products at a stage in their isentropic expansion. This difference corresponds to the amount of internal energy converted to kinetic energy and may serve as a measure of the energy available for driving metal.

Our analysis [6], as well as that of Hardesty and Kennedy [7] and Danel and Kazandijan [8], has shown that for the same products expansion ratio, the experimentally obtained Gurney energy is less than the calculated detonation energy. This is attributed to energy loses due to cylinder fracturing and leaking of products,

leaking of products through cylinder openings, and wall compression/thinning of the cylinder wall. This was confirmed for a series of explosives which for the same expansion ratio difference between the Gurney energy and detonation energy is 8-10%, depending on the equation of state of gas phase products used (Figure 4). In addition, it was found that the detonation energy at an expansion ratio V/V_0 = 2.9, correlates very well with the experimentally determined Gurney energies at an expansion ratio V/V_0 = 7. Based on this finding, terminal Gurney velocity (V/V_0 = 7) is calculated by EXPLO5 from detonation energy at V/V_0 = 2.9 ($v_G = \sqrt{2E_d}$). This allows prediction of the Gurney velocity of an explosive (ideal and non-ideal) with an error of less than 5% (Figure 5).

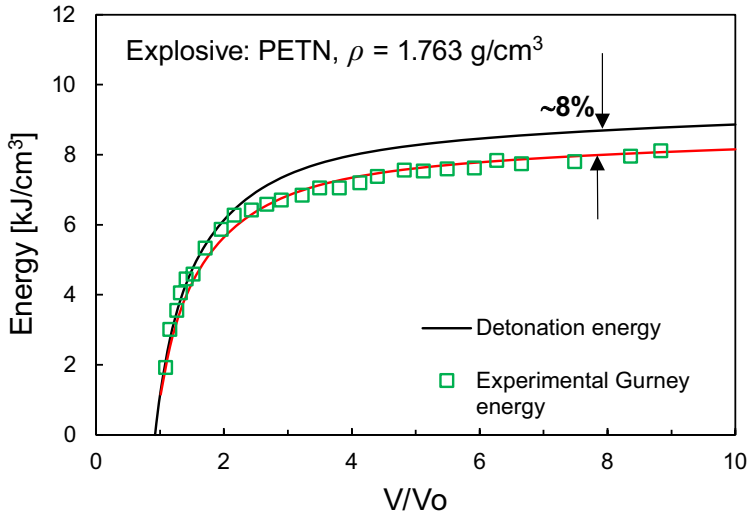


Figure 4. Detonation and Gurney energies of PETN vs. relative volume

Note: a) BKW EOS used; b) Gurney energy calculated from experimental copper cylinder wall velocities using Equation 5 (cylinder inner radius is 2.54 mm, wall thickness 2.6 mm)

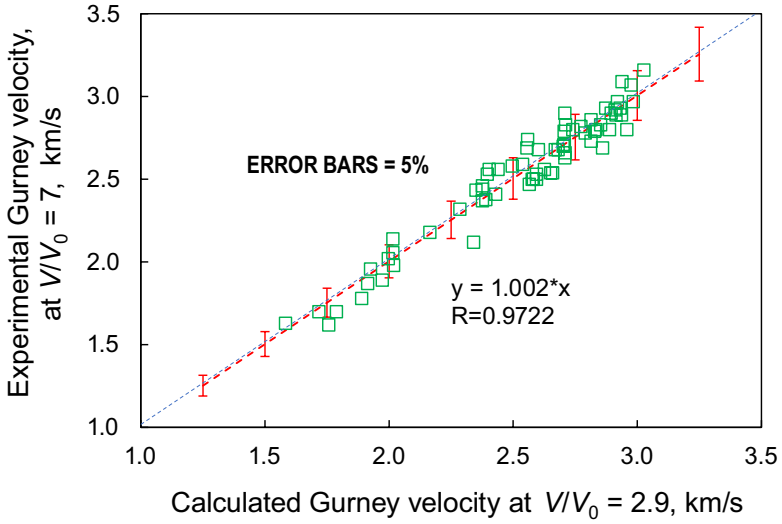


Figure 5. Comparison of experimental Gurney velocity at V/V_0 = 7 and calculated from detonation energy at V/V_0 = *2.9 for* 24 explosives (72 data points); experimental data taken from [9]

Due to energy loses, cylinder wall velocities at the different expansion ratios predicted using calculated detonation energies and assuming the entire energy of products transfers to kinetic energy on the wall, are higher than those obtained experimentally by the cylinder expansion test. However, taking 8-10% energy loses (as follows from previous discussion on Figure 4) wall velocity can be predicted with satisfactory accuracy (Figure 6).

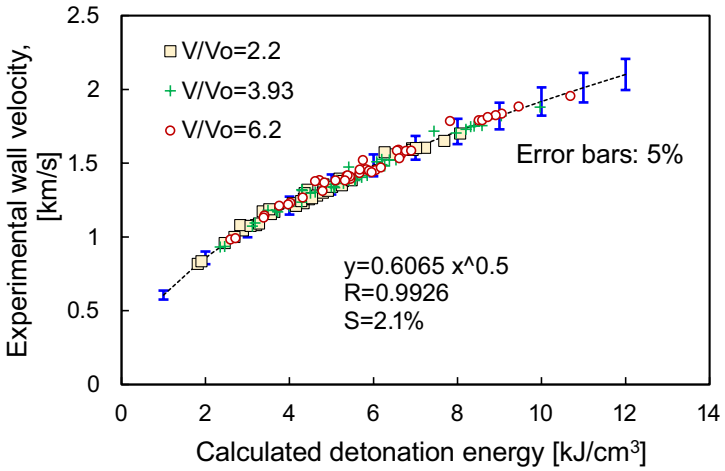


Figure 6. Relationship between cylinder wall velocity and detonation energy (43 different explosive formulations, 123 data points at 3 different expansion ratios); experimental data taken from [11-13]

Another approach of cylinder wall velocity estimation by EXPLO5, is based on an analytical relationship between cylinder wall velocity and detonation energy (Figure 7) in the form of Equation 7, taken from [10]. Equation 7 is applicable to the standard cylinder expansion test configuration (inner radius = 25.4 mm, wall thickness = 2.6 mm).

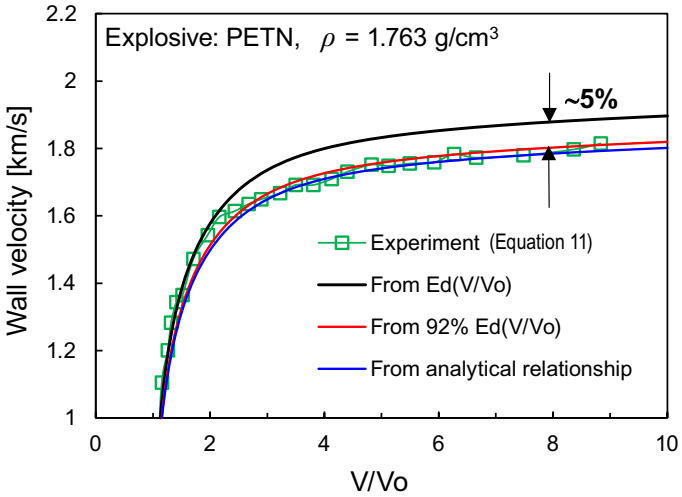


Figure 7. Experimental and predicted wall velocities of PETN vs. relative volume

$$v_s = 0.606\sqrt{\rho_0 E_d} \tag{7}$$

5. Kinetic detonation

Detonation of non-ideal explosives (e.g. ammonium-nitrate based, polymer bonded and metalized explosives, etc.) is poorly modelled by the C-J theory. Such explosives are characterized by a slower reaction rate, wider reaction zone, and consequently significant expansion of detonation products before the sonic point is reached. In addition, they show the strong dependence of detonation velocity on charge diameter and the existence and characteristic of charge confinement.

Incorporation of the Wood-Kirkwood (W-K) detonation theory in EXPLO5 enables modelling of detonation in non-ideal explosives. The theory considers cylindrical explosive charge of infinite length and solves Euler hydrodynamic flow equations along the axis of the cylinder. It treats radial expansion as a first order disturbance to a perfect one-dimensional flow along the axis and predicts detonation velocity as a function of the rate of chemical reactions and rate of radial expansion. Taking radial expansion as zero, the W-K flow equations become identical to the Zeldovich-von Neumann-Doering (ZND) theory, so the model can calculate time-dependent phenomena for ideal and non-ideal explosives [1].

The main output result of kinetic detonation calculation is a self-sustaining detonation velocity as a function of unconfined explosive charge diameter (Figure 8). As seen in Figure 8, the calculation can satisfactorily reproduce experimental data for highly non-ideal ammonium nitrate-fuel oil (ANFO) explosive, provided that accurate radial expansion data and a properly calibrated reaction rate model are available.

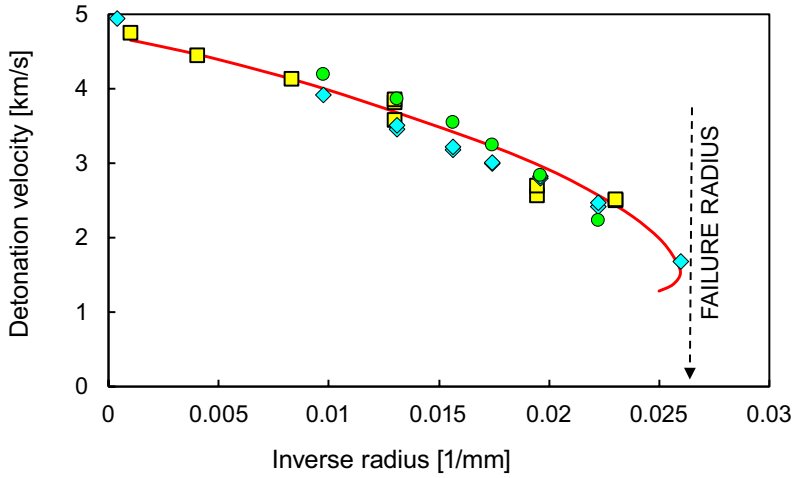


Figure 8. Experimental (●, ◆, and ■) and predicted (solid line) detonation velocities of ANFO as a function of inverse unconfined charge radius (charge density is 0.8 g/cm^3); experimental data taken from [14-16]

In addition, kinetic detonation gives a structure of the shock wave behind the shock front, starting from the von Neumann spike (VNS) down to the sonic point. This includes values of thermodynamic and flow variables along the reaction path. Figure 9 shows pressure and the reacted fraction of explosive profiles between the VNS and the sonic point for an ANFO charge.

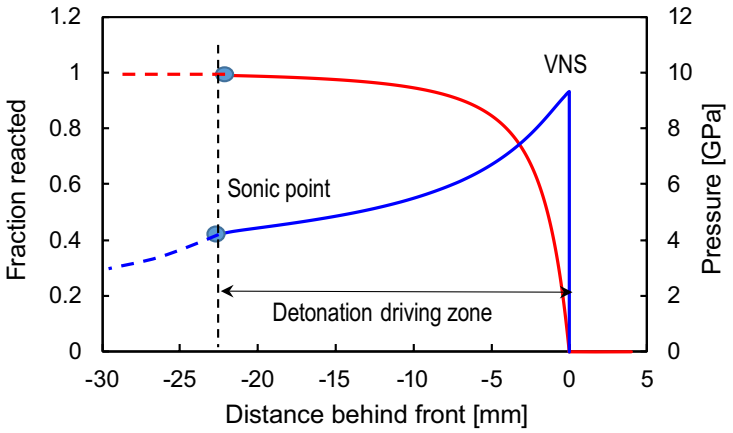


Figure 9. Calculated profiles of pressure and reacted fraction of explosive within the detonation driving zone of ANFO (confined charge, charge diameter 292 mm, detonation velocity equals 4.45 km/s)

6. Conclusions

- Thermochemical code EXPLO5 can be widely used in predicting the performance parameters of various explosive molecules and their mixtures knowing the general formula, enthalpy of formation and density.
- When it comes to high explosives, EXPLO5 can accurately predict the concentration of detonation products and detonation parameters (*D, p, Q, T*, etc.) which serve for the estimation of performance of explosives.
- Furthermore, EXPLO5 can estimate detonation energy (energy available to perform mechanical work), the Gurney energy, and velocity, as well as velocity of cylinder wall in standard copper cylinder expansion test configuration.

Acknowledgement

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