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A Non-Ideal Detonation Model for Evaluating the Performance of Explosives in Rock Blasting

By

S. Esen

Metso Minerals Process Technology Asia-Pacific, Brisbane, Australia

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Summary

A new model to predict the non-ideal detonation behaviour of commercial explosives in rock blasting is presented. The model combines the slightly divergent flow theory, polytropic equation of state, simple pressure-dependent rate law and statistical expressions to model the effect of confinement on detonation. The model has been designated as DeNE, an acronym for the Detonics of Non-ideal Explosives. It is aimed at predicting the detonation state and subsequent rarefaction (Taylor) wave to provide the pressure history for different explosive, rock type and blasthole diameter combinations. It enables the prediction and comparison of the performance of commercial explosives in different blasting environments. The unconfined detonation velocity data has been obtained from the testing of six commercial explosives to calibrate DeNE. A detailed sensitivity analysis has been conducted to evaluate the model. The model has been validated using the results of hydrocodes as well as measured and published in-hole detonation velocity data.

Keywords: Non-ideal detonation; commercial explosives; rock blasting; detonation velocity.

1. Introduction

Although explosives have been used for rock blasting for over a century, plausible scientific theories on rock fragmentation by blasting have emerged only during the last few decades. However, the rock breakage process is still not fully understood and controlled to the level now demanded by blasting customers. Computer modelling as an engineering tool has been extended to blasting to carry out extensive computations in blast simulations. Nevertheless, the validity of these models is dependent on knowledge of the explosive/rock interaction process (Leiper and Plessis, 2001; Cundall et al., 2001; Cunningham, 2001). Therefore, the prediction of explosive performance is crucial to the understanding of the explosive/rock interaction process and of rock breakage.

There is now a very wide range of commercial explosive products available to the mining industry. Broadly speaking, they can be classified as being one of the following: nitroglycerin-based (dynamites), water gels/slurries, emulsions, ANFO, blends (mixtures of water-in-oil emulsions and ANFO) (Dowding and Aimone, 1992; Hopler, 1998). Modern commercial explosives range from pure ANFO to pure emulsions including blends of these. Their performance is dependent upon their detonation properties in addition to the rock type and blasthole diameter. The selection of a suitable explosive for a given geotechnical environment in order to produce the desired blasting result has become more important and vital to the economics of mining operations. This means that the ability to understand explosive behaviour has become even more important than it has been. A pre-requisite to achieving this goal is an improved understanding of detonation science.

The methods available for determining explosive performance range from simple calculations and field tests (e.g. ballistic mortar, brisance, Trauzl lead block test, Langefors' weight strength) to extremely complex computations which have theoretical studies of detonation as their underlying basis.

With the widespread use of blasting agents which do not detonate in small laboratory sample sizes, the usefulness of small-scale laboratory test methods for explosive strength has become very limited (Persson et al., 1993). The weight strength method is traditionally associated with the strength markings of different dynamite grades, and has little correlation with the effectiveness of an explosive in blasting. It has no meaningful relation to modern commercial products such as ANFO products, water gels, and emulsions. This method calculates the total thermodynamic energy and does not explain how much of this energy is useful in rock breaking. Therefore, the weight strength method is considered not to be a useful parameter for the rating of explosive performance (Tosun, 1991; Persson et al., 1993; Hopler, 1998).

Explosive performance modelling using theoretical analyses is divided into two types: ideal detonation modelling and non-ideal detonation modelling. The use of detonation theories to compute the detonation properties of explosives is potentially an effective method of predicting the performance of explosives and offers valuable insight into the realistic performance of commercial explosives.

Explosive performance has generally been computed from ideal detonation codes, which were developed primarily for military explosives. They have limited applications in predicting the performance of commercial explosives as the calculated detonation properties assume independence of charge diameter and confinement. Nevertheless, they represent the starting point for a blast model. Ideal detonation codes provide reasonable estimates of the maximum performance attainable from an explosive and a good insight into the thermodynamic behaviour of the detonation products (Braithwaite et al., 1996). They also provide some key input to non-ideal detonation models and allow the comparison of ideal and non-ideal performance. Ideal detonation theories are well established in the literature and there are a number of codes available (e.g. BKW, Cheetah, IDeX, TDS, Tigerwin, Vixen-i). A reliable ideal detonation code should use an intermolecular potential equation of state, since this addresses the fundamentals of detonation and eliminates the calibration required for empirical equation (Cundall et al., 2001).

It is well recognised that commercial explosives exhibit non-ideal detonation behaviour since their performance is influenced by blasthole diameter and confinement (e.g. Kirby and Leiper, 1985; Braithwaite et al., 1990; Persson et al., 1993; Byers

Brown, 2002; Esen, 2004b; Souers et al., 2004). Byers Brown (2002) noted the fact that although the basic physico-chemical nature of non-ideal detonation and the laws governing it in mathematical form have been known for over 50 years, there is as yet no established method of analyzing the problem so that it can be solved approximately with acceptable accuracy. Therefore, research into non-ideal detonation modelling is necessary to predict the performance of commercial explosives.

This paper summarises the detonation characteristics of commercial explosives, gives a brief review of existing non-ideal detonation models and presents a new non-ideal detonation model including sensitivity analysis and validation of the code.

2. Detonation Characteristics of Commercial Explosives

If we detonate a cylindrical column of explosive and measure the velocity of detonation (VoD), we will find that VoD decreases as the diameter of the column decreases. This effect is caused by a pressure fall at the side of the column. When the diameter is large the losses are small relative to the energy production at the wave front. If the column diameter is small the energy losses are larger relative to the energy generated at the wave front. The decrease in velocity continues until a diameter (the failure diameter) is reached where the energy losses are so great relative to the energy production that the detonation fails to propagate (Cooper, 1996). It is also widely recognised that increased confinement can have a similar effect to that of an increased charge diameter.

In a non-ideal situation, as represented in Fig. 1, the shock front is always curved, the flow of the reaction products diverges and reaction is never complete in the detonation zone. The detonation driving zone (DDZ) terminates at the sonic line and contributes to the support of the detonation process (Byers Brown, 2002). In this case, the detonation velocity may approach, but never exceeds, the ideal detonation velocity (Persson et al., 1993). It is widely recognised that the degree of non-ideality of an explosive can be judged by the difference in the ideal and the actual detonation velocities.

The flow behind the sonic line is supersonic, so that perturbations such as compression and rarefaction waves, which move at the local sound speed, can never catch up with the DDZ, and therefore cannot contribute to or diminish the speed of the detonation wave. The rarefaction (Taylor wave) which occurs in the supersonic, still reactive, the flow between the sonic line and the end of the reaction zone is of importance, especially with commercial explosives which may have slow energy-releasing reactions and can contribute substantially to the blast (Byers Brown, 2002).

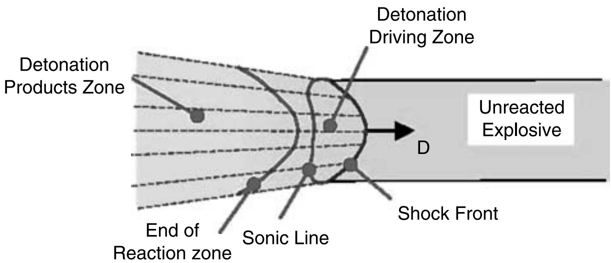

Fig. 1. Non-ideal (two-dimensional) detonation representation (Byers Brown, 2002)

3. A Brief Review of Existing Non-Ideal Detonation Models

Esen (2004a) has reviewed ten existing non-ideal detonation models and/or theories:

- Wood–Kirkwood axial perturbation theory (Wood and Kirkwood, 1954);
- Steady-state two-dimensional detonation (Bdzil, 1981);
- Chan's Theory (Chan, 1981);
- Slightly divergent flow theory (Kirby and Leiper, 1985);
- Time-dependent two-dimensional detonation (Bdzil and Stewart, 1989);
- Detonation shock dynamics (Bdzil and Stewart, 1989);
- Cowperthwaite's exact axial solution (Cowperthwaite, 1994);
- SveBeFo's model (Deng et al., 1995, 1999);
- Souers's and Esen's empirical models (Souers, 1997; Esen, 2001);
- Variational approach (Byers Brown, 1998).

The conclusions of this review are best summarised as follows:

a) None of the approaches are developed sufficiently to adequately model the non-ideal detonation behaviour of commercial explosives. This is in-line with the conclusions reached by Cundall et al. (2001).
b) The more fundamental the approach is, the better the reliability of the model, but the more difficult it is to implement in practice. It should be noted that fundamental approaches are potentially reliable provided that the corresponding inputs are correct. Therefore, applications of these approaches could be limited.
c) Kirby and Leiper's (1985) slightly divergent flow analysis bears some resemblance to reality and provides an acceptable representation of detonation in non-ideal commercial explosives. It is incorporated in the CPeX (Kirby, 1985) and Vixen-n (Cunningham, 2003) non-ideal detonation codes and is also used in this study.
d) It was noted that the confinement calculations in both CPeX and Vixen-n codes are not reliable and that the kinetic rate law is complex and includes a large number of adjustable parameters (Byers Brown, 2002). The calibration process including unconfined VoD data fitting by adjusting up to 16 rate parameters is lengthy and requires expertise (Byers Brown, 2002; Esen, 2003).
e) All methods require calibration of kinetic (rate law) parameters using experimental unconfined detonation velocity data. The calibration process in a number of models is lengthy and complex depending on the kinetic parameters used. They also need assumptions in choosing equations of state, rate laws and mixture rules in addition to the assumptions made in the theory.
f) There is no established method of analysing the effect of confinement on detonation analytically (Esen, 2004b).
g) It should also be recognised that some degree of empiricism is inevitable in non-ideal detonation modelling of commercial explosives due to the complexity of the problem with heterogeneous commercial explosives and uncertain field conditions including rock and explosive loading (Byers Brown, 2002).
h) A number of the models are proprietary and not readily available to the industry.

The model developed in this study is aimed at addressing and where possible eliminating, the drawbacks *b*, *d*, *e* and *f* identified above while developing an alternative non-ideal detonation model. The approach followed in the development of this alternative model involves the use of an established theoretical model (slightly divergent flow analysis), experimental measurements and the statistical analysis of the experimental (detonation velocity and shock curvature) data.

4. Development of a Non-Ideal Detonation Model for Commercial Explosives

4.1 Description of the Non-Ideal Detonation Problem and Assumptions

Figure 2, which is a modified version of the corresponding figure in Braithwaite et al. (1990), illustrates the non-ideal detonation process. A cylindrical stick of explosive of diameter d (mm), which is initiated at one end, produces a detonation wave with a curvature of radius R_s (mm), and a constant velocity of propagation, D (km/s). The position of the sonic locus is determined by the energy release in the detonation zone mechanically driving the shock. The time taken to reach the CJ plane from the shock front is t_{CJ} (Fickett and Davis, 2000). The distance between the shock front and the sonic locus is x_{CJ}. Reaction is complete when the distance is x_{rz}. The detonation problem is modelled by differential/algebraic equations in order to determine the flow properties as a function of distance or time. The DDZ model solves the flow properties between $x=0$ and $x=x_{CJ}$ and the Taylor wave model determines the flow properties between $x=x_{CJ}$ and $x=x_{rz}$ and onwards.

The key simplifications and assumptions in the slightly divergent flow theory are:

- steady-state detonation;
- Lagrangian (shock frame formulation);
- cylindrical coordinates;
- pseudo-one-dimensional theory applies to the central stream-tube area;
- radial velocity on the central stream-tube is zero. The divergence term is considered in an approximate manner; and
- empirical relations are assumed for the shock front curvature and shape of the isobars.

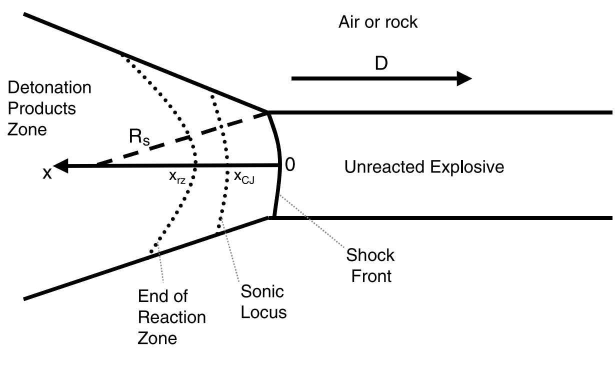

Fig. 2. Detonation front regime for non-ideal cylindrical explosive (Braithwaite et al., 1990)

4.2 Modelling the Reactive Flow in the Detonation Driving Zone

The critical platform for the non-ideal detonation model developed in this study comprises Kirby and Leiper's (1985) slightly divergent flow theory, the equation of state (EoS) (Braithwaite et al., 1989) and the reaction rate law (Howard et al., 1998). They have been proven independently and shown to apply to commercial explosives. The model includes a novel approach for the effect of confinement on detonation using statistical expressions.

The DDZ model employs the slightly divergent flow analysis, which requires the numerical solution of differential/algebraic equations involving the shock front and sonic locus. Kirby and Leiper (1985) gave the physical background and the general formulation of this problem. Braithwaite et al. (1990), Beardah and Thomas (1991, 1994), Zhang and Gladwell (1992, 1993) and Sturgeon et al. (2001) further described it in mathematical detail.

Following these researchers, Esen (2004a) has proposed a DDZ model consisting of nine ordinary differential equations (ODEs) for nine variables $(u, p, A, \lambda, \omega, E, v, \rho, x)$:

$$\dot{u} = \frac{uc^2(\sigma\dot{\lambda} - 2\omega)}{c^2 - u^2} \tag{1}$$

$$\dot{p} = -\rho u \dot{u} \tag{2}$$

$$\dot{A} = 2A\omega \tag{3}$$

$$\dot{\lambda} = R(\lambda, p) \tag{4}$$

$$\dot{\omega} = \frac{-\dot{u}}{R(x, x_{CJ}, d)} \tag{5}$$

$$\dot{E} = \dot{p}\frac{\partial E(p, v, \lambda)}{\partial p} + \dot{v}\frac{\partial E(p, v, \lambda)}{\partial v} + \dot{\lambda}\frac{\partial E(p, v, \lambda)}{\partial \lambda} \tag{6}$$

$$\dot{v} = \frac{v}{u}(\dot{u} + 2\omega u) \tag{7}$$

$$\dot{\rho} = -\frac{(\dot{u} + 2\omega u)}{uv} \tag{8}$$

$$\dot{x} = u \tag{9}$$

in which

$$E = E(p, v, \lambda) \tag{10}$$

$$c^2 = v^2 \left[\frac{p + \left(\dfrac{\partial E}{\partial v}\right)_{p,\lambda}}{\left(\dfrac{\partial E}{\partial p}\right)_{v,\lambda}} \right] \tag{11}$$

$$\sigma = \frac{1}{\rho c^2}\left(\frac{-\left(\frac{\partial E}{\partial \lambda}\right)_{p,v}}{\left(\frac{\partial E}{\partial p}\right)_{\lambda,v}}\right) \tag{12}$$

$$R(x, x_{CJ}, d) = \frac{R_s^2(x_{CJ}, d) - xR_s(x_{CJ}, d) + \frac{\zeta x^2}{2}}{R_s(x_{CJ}, d) - \zeta x} \tag{13}$$

$$R_s = \alpha(d - \beta x_{CJ}) \tag{14}$$

where $^\bullet \equiv d/dt$ represents differentiation with respect to time; u (km/s) is the particle velocity relative to the shock front; p (GPa) is the pressure; A is the area of a stream-tube of fluid which has unit area at the shock front; $R(\lambda, p)$ is the reaction rate vector; λ is the extent of chemical reaction varying from 0 for the unreacted explosive (no reaction) to 1 for the detonation products (complete reaction); ω (μs^{-1}) is the divergence defined as the radial velocity of the stream-tube at unit distance from the axis of the cylinder; E (MJ/kg) is the specific internal energy; v (cm^3/g) is the specific volume; ρ (g/cm^3) is the fluid density; x (mm) is the distance downstream of the shock front, and $R(x, x_{CJ}, d)$ is the radius of curvature of an isobar at a distance x (mm) downstream of the shock front. $R_s(x_{CJ}, d)$ is the radius of the curvature of the shock front. c (km/s) is the local fluid sound speed; σ is the thermicity coefficient of the fluid, and x_{CJ} (mm) is the CJ distance (reaction zone length). ξ is a curvature parameter. α and β are experimentally determined parameters with values $\alpha = 3.75$ and $\beta = 6.33$, respectively (Esen, 2004a).

4.2.1 The Choice of the Reactive Equation of State and Rate Law

The solution of the DDZ problem depends on the choice of the equation of state and rate law. A computationally convenient EoS has been adopted in this study. The unreacted or explosive phase is described by a simple polytropic EoS and the reacted or product phase is described by a polytropic EoS with a density-dependent index. The reasons for these choices are purely computational. The choices are believed to simplify the overall algorithms employed in modelling the non-ideal detonation for commercial explosives. For this research, the EoS of a condensed phase explosive is that considered in Braithwaite et al. (1989). The reactive EoS is (Braithwaite et al., 1989)

$$E = pv\left(\frac{1-\lambda}{\gamma_x - 1} + \frac{\lambda}{\gamma_p - 1}\right) - \lambda q + (1 - \lambda)E_t \tag{15}$$

in which

$$\gamma_p = \gamma_0 + \gamma_1 \frac{\rho}{\rho_0} + \gamma_2 \frac{\rho^2}{\rho_0^2} \quad \text{or} \quad \gamma_p = \gamma_0 + \gamma_1 \frac{v_0}{v} + \gamma_2 \frac{v_0^2}{v^2} \tag{16}$$

where the subscript 0 represents the initial state; subscript p represents the product phase; γ is the adiabatic gamma coefficient; q is the heat of reaction; E_t is the turbulent stored energy; and ρ_0 is the unreacted explosive porous density. The γ_i constants are determined by requiring that the correct values for $(\partial np/\partial nv)_s$ are returned at the C–J state and at infinite expansion. These are taken from an ideal detonation code. γ_0 is set equal to the ideal gas value (Kirby and Leiper, 1985).

The simple polytropic EoS has been applied successfully to commercial explosives and the results appear to demonstrate the applicability of the EoS in modelling the detonics of commercial explosives (Kirby and Leiper, 1985; Braithwaite et al., 1989, 1990; Zhang and Gladwell, 1992, 1993). CPeX and Vixen-n non-ideal detonation codes employ this EoS. The results have shown the applicability of this EoS to commercial explosives.

A pressure-dependent rate law, which is similar to that of Howard et al. (1998) is used in this study:

$$\dot{\lambda} = k(1 - \lambda)\left(\frac{p}{P_{\mathrm{ref}}}\right)^2 \tag{17}$$

where k is the rate constant, and P_{ref} is the reference pressure with a value 1 GPa.

The above reaction rate form has been implemented in the Kinetic Cheetah code, which is based on the Wood and Kirkwood model. Howard et al. (1998) inferred effective kinetic rates proportional to p^2 for a variety of ideal and non-ideal explosives and their composites. They found that this choice, while simpler than most reactive flow rate laws, is adequate to model steady-state detonation over the range of materials and diameters studied. Furthermore, a similar rate form has been applied successfully to ANFO type explosives by Bdzil et al. (2002) and Sharpe (2003). This rate law is computationally convenient and simplifies the overall algorithms employed in modelling the non-ideal detonation for commercial explosives.

4.2.2 Initial Conditions

The initial conditions ($t = 0$) are (Esen, 2004a):

$$u = u_s(D) \tag{18}$$

$$p = p_s(D) \tag{19}$$

$$A = 1 \tag{20}$$

$$\lambda = 0 \tag{21}$$

$$\omega = \frac{D - u_s(D)}{R_s(x_{CJ}, d)} \tag{22}$$

$$E = \frac{p_s(v_o - v_s)}{2} \tag{23}$$

$$v = v_s(D) \tag{24}$$

$$\rho = \rho_s(D) \tag{25}$$

$$x = 0 \tag{26}$$

where the subscript s represents for the shock state. Equations 18, 19, 23, 24 and 25 can be obtained from the shock jump equations given in Appendix A.

4.2.3 Method of Solution of the DDZ Problem

Equation (1) exhibits a singularity whenever $u = c$ and $2\omega = \sigma \dot{\lambda}$. Thus, Eq. (1) cannot be solved when $t = t_{CJ}$. However, at all points $t \in [0, t_{CJ})$, Eq. (1) has a solution. In order to solve the singularity problem, the root search problem was transformed into a minimisation. A figure of merit function Y is defined to be

$$Y(D) = \min(\eta^2 + t^2\psi^2) \quad 0 < t < t_{\max} \tag{27}$$

where

$$\eta = c^2 - u^2 \tag{28}$$

and

$$\psi \equiv \sigma \dot{\lambda} - 2\omega \tag{29}$$

We have $Y = 0$ when $\eta = \psi = 0$ holds. ψ is multiplied by t in Y to yield a unitless function. Although the implementation of the specialised minimiser is somewhat cumbersome, the underlying principle is simple: we need to find minima of $Y(D)$ that are very close to 0. The Bulirsch-Stoer extrapolation method is used as the numerical solution technique for ODEs. It is a variable-order technique that is based on a modified version of the midpoint method (Schilling and Harris, 2000).

4.2.4 The Effect of Confinement on Detonation

The solution of the DDZ model requires the determination of the two key flow parameters for a given confinement (rock) type: the confined VoD and the radius of the curvature of the shock front. These parameters are predicted using statistical relations in the absence of analytical models. This should permit acceptable representations of the non-ideal detonation problem for commercial explosives used in rock blasting operations.

Within the scope of a research and development project on explosives and blasting techniques carried out in Turkey (Bilgin et al., 1999), numerous in-hole VoD measurements were conducted at several mines in addition to unconfined tests. Confined VoD data was presented by Bilgin and Esen (1999, 2000), Bilgin et al. (2000) and Esen et al. (2000). Eight commercial explosives were tested at varying degrees of confinement and blasthole diameters of 32–241 mm.

Based on the experimental in-hole VoD measurements, the following empirical model was developed to determine the confined VoD (Esen, 2004a):

$$D_c = D_u\left(1 + \left(\frac{D_{CJ} - D_u}{D_{CJ}}\right)\left(\frac{M}{1 + aM^b}\right)\right) \tag{30}$$

where

$$M = \frac{\rho_r v_p}{\rho_o D_u} \tag{31}$$

and a and b are constants with values 4.563 and 0.688, respectively; D_c is the confined VoD (km/s); D_u is the unconfined VoD of an explosive at a given charge diameter (km/s); D_{CJ} is the ideal VoD (km/s); ρ_r is the rock density (g/cm^3);

v_p is the P-wave velocity of the intact rock (km/s); and ρ_0 is the density of the unreacted explosive (g/cm^3).

The above model requires the prediction of the unconfined VoD at a given charge diameter. In order to characterise a commercial explosive, a number of unconfined tests should be carried out at a wide range of charge diameters. The following equation has been shown to be the most capable of modelling the unconfined detonation velocity data of explosives with varying non-ideality (Esen, 2004b):

$$\frac{D_u}{D_{CJ}} = \frac{1}{1 + m\left(\frac{1}{d}\right) + n\left(\frac{1}{d}\right)^2} \tag{32}$$

where m and n are fitting constant; d is the charge diameter (mm); and D_{CJ} is the ideal detonation velocity determined by the Vixen-i ideal detonation code (km/s). This model allows the determination of the unconfined VoD at a given charge diameter.

The effect of confinement on the shock curvature has not been solved analytically in the literature. On the other hand, there are limited measured confined shock curvature data in the literature, which have been presented by Forbes and Lemar (1998) and Souers (2002). However, these measurements were conducted in metal tubes (brass and copper) and involved mainly the use of high explosives. To date similar measurements have not been conducted in rock.

In the absence of analytical models and/or experimental measurements, the following simple empirical relationship proposed by Braithwaite (2003) is used to predict the radius of the confined shock curvature (Rs_c):

$$\frac{Rs_c}{Rs_u} = 1 + \frac{\rho_r v_p}{\rho_0 D_c} \tag{33}$$

where Rs_u is the radius of the unconfined shock curvature given by Eq. (14).

The DDZ model presented above has been coded in the C++ programming language using an ODE solver included in the numerical library provided by Schilling and Harris (2000). The code is named DeNE (Detonics of Non-ideal Explosives). The input parameters are the ideal detonation data (unreacted explosive density, ideal detonation velocity, heat of reaction, ideal (expanded) gas gamma and ideal CJ gamma), unreacted explosive properties (Mass fraction of liquid-MFL, solid and liquid densities, Hugoniot parameters-C_o and s), unconfined VoD versus charge diameter data, blasthole diameter and intact rock properties (density and P-wave velocity). The code outputs the detonation properties (detonation velocity, detonation pressure, extent of chemical reaction, specific internal energy, density, specific volume, particle velocity, sound speed, stream tube area, divergence, distance and time downstream of the shock front) at the DDZ which are also input to the Taylor wave model (Esen, 2004a).

4.3 A Mathematical Model for the Taylor Expansion Wave

The DDZ model described in Section 4.2 determines the detonation state between the shock front and the sonic locus (see Fig. 2). According to the detonation analysis carried out for ANFO by Sharpe (2003), the reaction taking place at the DDZ is approximately 73–95% complete depending on the charge diameter and confinement.

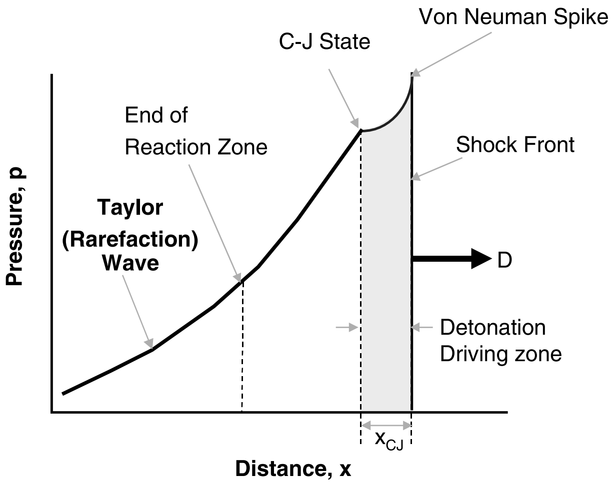

Fig. 3. Profile of the Taylor expansion wave (Esen, 2004a)

Lower figures are obtained for smaller charge diameters and/or confinement. This suggests that commercial explosives do not react completely at the DDZ. Thus, the flow between the sonic locus and the end of the reaction zone is still reactive. Since the reaction is complete at the end of the reaction zone, the flow is non-reactive from this end to an arbitrary end pressure and isentropic expansion takes place from that zone onwards.

The rarefaction wave which brings the product gases from the sonic locus (C–J state) to an arbitrary end pressure is called the Taylor (rarefaction) wave (Cooper, 1996). This is shown in Fig. 3.

The gamma law is preferred in this study to estimate the isentrope over the range from the sonic locus to the pressure to which the expansion ends. This model is computationally convenient. The flow behind the Taylor wave is considered complex and calculations should include the non-steady processes (Braithwaite et al., 2003). However, these fundamental studies are still in development stage. It is believed that the gamma law should suffice to predict the isentrope following the sonic locus. The model should be viewed as a model, which provides only a first approximation for the flow analysis.

The gamma law is described by the following relation (Zukas and Walters, 1998; Fickett and Davis, 2000)

$$p = p_{CJ}\left(\frac{v_{CJ}}{v}\right)^{\gamma} \tag{34}$$

where the subscript *CJ* is for the C–J state. p_{CJ}, v_{CJ} and γ are obtained from the DDZ model.

The work done by the expansion of the reaction products (*W*) is defined as the work of the products expanding from volume at the C–J point (v_{CJ}) to a volume v minus the energy of compression of the explosive (E_c):

$$W(v) = -E_c + \int_{v_{CJ}}^{v} p dv \tag{35}$$

where

$$E_c = \frac{1}{2}\rho_0 D^2 \left(1 - \frac{v_{CJ}}{v_0}\right)^2$$

After integration using relations 34 and 35, the following expression is obtained for the expansion work:

$$W = -E_c + \frac{p_{CJ} v_{CJ}}{\gamma - 1}\left[1 - \left(\frac{v_{CJ}}{v}\right)^{\gamma-1}\right] \tag{36}$$

The end pressure specified in the code is 20 MPa which is the minimum pressure value that detonation products (explosion gases) do useful work in blasting (Hagan and Duval, 1993). It is believed that the gamma law should suffice to predict the isentrope following the sonic locus. The Taylor wave model used in this study should be viewed as a model which provides only a first approximation for the flow analysis.

5. Unconfined and Confined VoD Data Collection

A series of unconfined and confined (in-hole) VoD tests for a wide range of charge diameters and explosive types were conducted to provide both input and validation data for the non-ideal detonation model developed in this study.

One of the key inputs to the non-ideal detonation model is unconfined VoD versus charge diameter data for an explosive product being considered. This requires a series of unconfined VoD measurements for a range of charge diameters of interest. All non-ideal detonation models require experimental unconfined VoD data to calibrate kinetic (rate law) parameters for each explosive type. In-hole or rock confined VoD on the other hand, provides data to validate the predicted VoDs and also gives good insight into the product's performance under specific field conditions.

Six commercial explosives were tested to obtain a wide range of unconfined VoD versus charge diameter data. These explosives were used in this study because they exhibit various levels of non-ideality. Furthermore, they are widely used in surface mining operations. The commercial product names and manufacturers are not explicitly given to protect the supplier's intellectual property. Thus, they are coded as shown in Table 1.

A continuous VoD recording system manufactured by MREL in Canada, Microtrap (2003), was used in both unconfined and confined tests. The system uses continuous resistance wire technique.

Table 1. Commercial explosives tested as part of the study

Explosive code	Explosive type	Explosive description	Cup density (g/cm^3)
Blend1	Blend	65% Emulsion and 35% ANFO – gas sensitised	1.050
Blend2	Blend	65% Emulsion and 35% ANFO – gas sensitised	1.120
Blend3	Blend	80% Emulsion and 20% ANFO – microballoon sensitised	1.290
Heavy ANFO1	Heavy ANFO	30% Emulsion and 70% ANFO	1.050
ANFO1	ANFO	94% Ammonium nitrate and 6% fuel oil	0.828
ANFO2	ANFO	94% Ammonium nitrate and 6% fuel oil	0.750

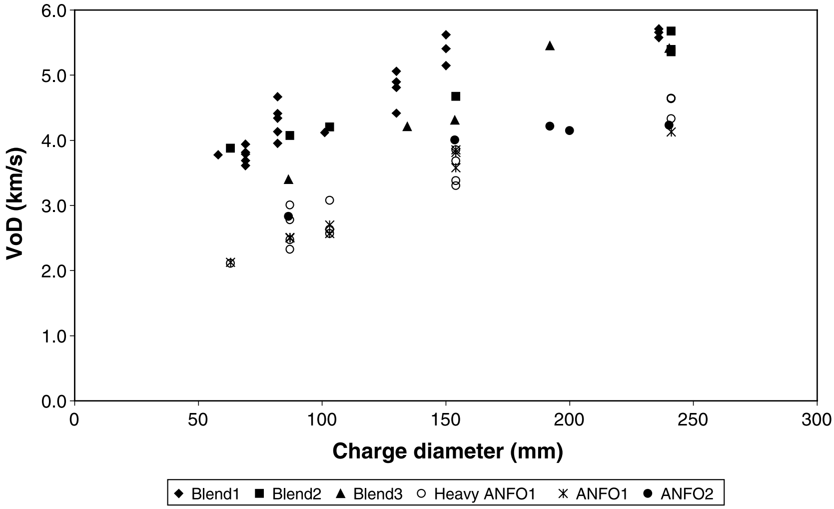

Fig. 4. Unconfined VoD versus charge diameter (Esen, 2004a)

Figure 4 shows a plot of unconfined VoD versus charge diameter for the explosives listed in Table 1. A total of 77 unconfined VoD tests were conducted to obtain the required data. The variations in the unconfined VoDs for Blend1, Blend2, Heavy ANFO1 and ANFO1 are found to be in the ranges of 66–273, 175, 179–305 and 7–150 m/s, respectively (Esen, 2004a). These observations are consistent with experiences documented by Smith (2000), indicating that the uncertainty in VoD measurements is in the order of 200 m/s. The major factors affecting the variations in unconfined VoD are (Esen, 2004a):

- variability in product mix for the small masses loaded directly from the bulk explosive vehicle;
- variability in the in-pipe density; and
- possible unstable behaviour of the bulk explosive in smaller diameter which could be approaching the critical diameter.

In-hole VoD data were obtained for four commercial explosives, namely Blend1, Blend2, Blend3 and ANFO2 (Table 1). They were recorded from single and multiple blastholes in production blasts in different rock types and blasthole diameters. A total of eight in-hole VoD tests which resulted in 15 successful VoD data for four commercial explosives were collected from four mines. The variation in the confined VoD ranges from 121 to 370 m/s (Esen, 2004a). The main possible causes are (Esen, 2004a):

- explosive type and diameter of the explosive charge;
- density gradient along the explosive column; and
- rock type (confinement) and presence of the discontinuities intersecting the blasthole.

The variations in unconfined and in-hole VoDs are ±305 and ±370 m/s, respectively, and are expected to impact on the predictions of any non-ideal detonation model including the model developed in this study. This, in fact, justifies the need to solve the non-ideal detonation problem for commercial explosives using the hybrid

Table 2. Intact rock properties

Rock	Density (g/cm^3)	P-wave velocity (m/s)	S-wave velocity (m/s)	Dynamic Young's modulus (GPa)	Dynamic Poisson's ratio
Kimberlite	2.264	2521	1381	11.0	0.28
Monzonite (Cadia Extension)	2.693	5023	2655	49.6	0.31
Fresh Volcanics (North Wall)	2.654	4480	2447	40.9	0.29
Monzonite (610 and 625 m Level)	2.706	4658	2490	43.7	0.30
East Porphyry	2.520	2430	1320	11.3	0.29
Metasediments	2.670	3310	1845	23.2	0.28
Kimberlite (TKB)	2.520	3945	1919	25.0	0.35
Hematite	4.220	5830	–	142.0	–
Breccia	2.750	6320	2584	51.4	0.30
Sandstone	2.500	4326	2101	29.7	0.35
Overburden	1.900	2598	1683	12.3	0.13
Overburden	1.900	2430	1683	9.0	0.29
Copper ore	2.970	5455	2619	55.0	0.35
Andesite	2.500	5660	3334	68.6	0.23

approach given the variations in the key explosive performance drivers such as explosive quality, explosive density, unconfined VoD and rock parameters.

The data collected in this study should provide the necessary input to the proposed model. Measured and published in-hole VoD data is presented in Section 6.2.3 to validate the model. Intact rock properties collected in this study are given in Table 2.

6. Sensitivity Analysis and Validation of the Model

6.1 Sensitivity Analysis of the DeNE Code

A detailed sensitivity analysis is reported in this section. The objective of the sensitivity analysis was to evaluate the model and investigate how the non-ideal detonation code responds to variations in its inputs. The sensitivity analysis has been conducted for the key identified input parameters in the DeNE code, which included uncertainties. It is aimed to assess the influences or relative importance of each input factor on the output variables (e.g. VoD, pressure and extent of reaction) and hence deal with uncertainties in the input parameters.

6.1.1 Parameters Included in the Sensitivity Analysis

The inputs of the DeNE were given in Section 4.2. The definition of these parameters and their relevance to the sensitivity analysis are given below:

- Ideal detonation parameters: These parameters are determined using the Vixen-i ideal detonation code. They have to be assumed accurate (Braithwaite, 2004) and thus are not included in the sensitivity analysis.
- *MFL*: The mass fraction of liquid is fundamental to the description of the nature of the explosive. It is 1.0 for emulsion and 0 for ANFO. The fuel oil component (usually 6%) of ANFO is not liquid explosive, so *MFL* for ANFO is 0, not 0.06. However with emulsion with 5% Al, the Al reaction is a solid reaction, so *MFL* is

0.95. The value for a 35% prill doped emulsion will be 0.65. Although *MFL* is a well-defined parameter, it is included in the sensitivity analysis as it may potentially provide information on the effect of solid components on the explosive's (particularly emulsion explosives) performance.

- Solid density: Density of the solid. Due to the uncertainty in the variable and its impact on the different explosive systems, it is included in the analysis.
- Liquid density: Density of the liquid. It is the base density of an emulsion prior to any gassing. For an emulsion, the base density is well defined. In general, liquid density for emulsions varies between 1.33 and 1.39 g/cm^3. Although it is a well-defined parameter, it is included in the sensitivity analysis as it may potentially provide information on the effect of the change in the base density on the explosive's (particularly emulsion explosives) performance.
- Hugoniot parameters: They are obtained from the $U-u$ (shock velocity–particle velocity) relation. Due to the uncertainty in these variables, they are included in the analysis.
- Blasthole diameter: It is a fixed operational parameter. Thus, it is not included in the analysis.
- Confinement parameters: Due to the uncertainty in the variables, they are included in the analysis.

In summary, the parameters included in the sensitivity analysis are: *MFL*, solid and liquid densities (ρ_S, ρ_L), Hugoniot (C_0, s) and confinement parameters (ρ_r, v_p). Having carried out this analysis, the study is further expanded with a view to explore the potential impact of the following on the explosive performance:

- blasthole diameter, explosive and rock types;
- Taylor wave model; and
- variations in the unconfined VoD of the explosive.

A set of different explosives with varying non-ideality was chosen to undertake this study. These explosives included the ANFO1 (Table 1), Blend1 (Table 1) and Lee's (1990) pure emulsion. These explosives were selected to carry out the analysis for a wide range of explosives ranging from pure ANFO to pure emulsion including blends

Table 3. Input parameters for the simulated explosives

Parameter	ANFO1	Blend1	Lee's (1990) emulsion
ρ_0 (g/cm^3)	0.800	1.150	1.248
D_{CJ} (km/s)	4.845	6.218	6.382
q (MJ/kg)	3.833	2.976	2.609
γ_{CJ}	2.777	2.999	2.981
γ_R	1.339	1.338	1.336
MFL	0	0.65	1
ρ_S (g/cm^3)	1	1	1
ρ_L (g/cm^3)	1.00	1.39	1.39
C_0 (km/s)	0.92	1.85	2.036
s	1.40	1.40	1.923
d (mm)	152	152	152
ρ_r (g/cm^3)	2.264	2.264	2.264
v_p (km/s)	2.521	2.521	2.521

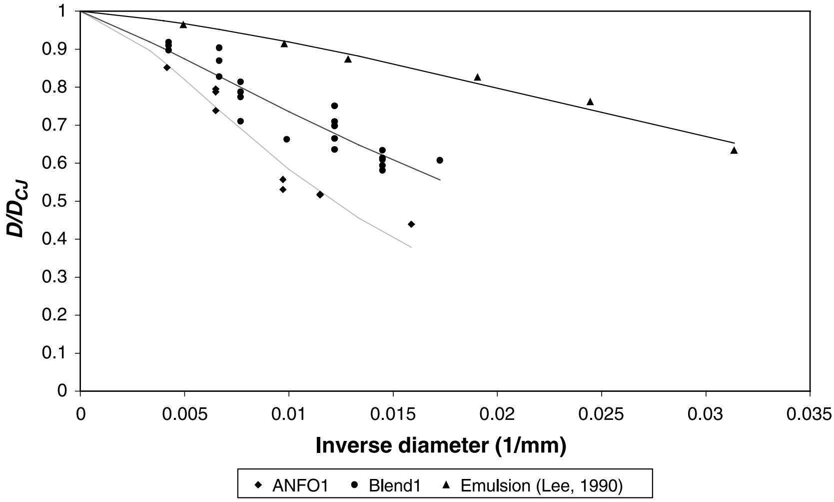

Fig. 5. D/D_{CJ} versus inverse diameter relations for the explosives included in the sensitivity analysis

of these. Simulated densities of these explosives were 0.80, 1.15 and 1.248 g/cm^3, respectively. Table 3 gives the input parameters for the simulated explosives. Simulations have been carried out for 152 mm charges confined in kimberlite (Table 2).

The code also requires the experimental unconfined size effect data as input in the form of an expression as shown in Eq. (32). Figure 5 illustrates the D/D_{CJ} versus inverse diameter relations for these explosives. The constants m and n in Eq. (32) for ANFO1, Blend1 and Lee's (1990) emulsion are 16.53, 5468.75; 21.47, 1441.69; and 4.93, 383.54, respectively.

6.1.2 Sensitivity Studies on the Parameters

The sensitivity analysis has been carried out by changing the selected input parameters at 3, 5 and 10%. The responses of each feature (VoD, pressure and extent of reaction at a given diameter of 152 mm) and the sensitivity, S_1, to changes in each input parameter are evaluated in detail.

Figures 6–8 illustrate the response of the sensitivity S_1 to changes in the detonation parameters (VoD, pressure and extent of reaction) at a 152 mm charge diameter for ANFO1, Blend1 and emulsion explosives, respectively. In this analysis, the sensitivities at the initial state are compared.

The following conclusions can be drawn from this sensitivity analysis:

- Liquid density and *MFL* have no effect on ANFO1's performance (Fig. 6). Similarly, solid density does not alter the performance of the emulsion (Fig. 8).
- The only parameters included in the sensitivity analysis that affect the VoD of the explosive are the confinement parameters (ρ_r and v_p).
- In general, the most sensitive parameters that affect the feature pressure and extent of reaction are ρ_s, s and C_0 for ANFO1 (Fig. 6); ρ_L, C_0 and *MFL* for Blend1 (Fig. 7); and v_p and *MFL* for the emulsion explosive (Fig. 8).

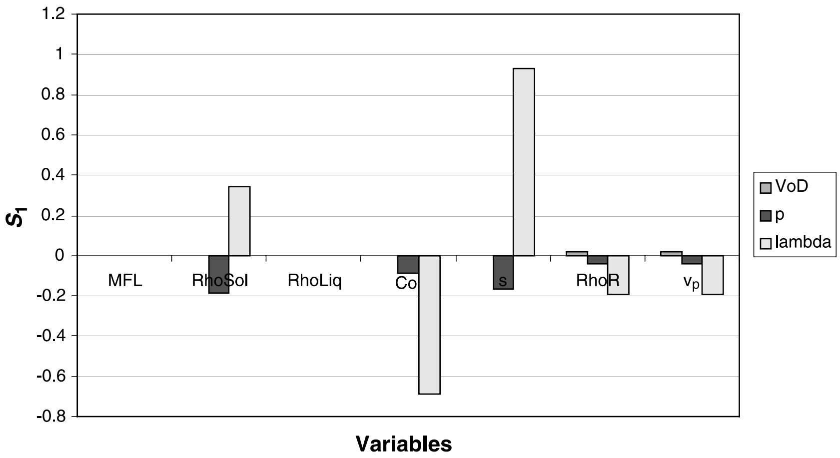

Fig. 6. Response of the sensitivity S_1 to changes in the detonation parameters for ANFO1. RhoSol: ρ_S; RhoLiq: ρ_L; RhoR: ρ_r

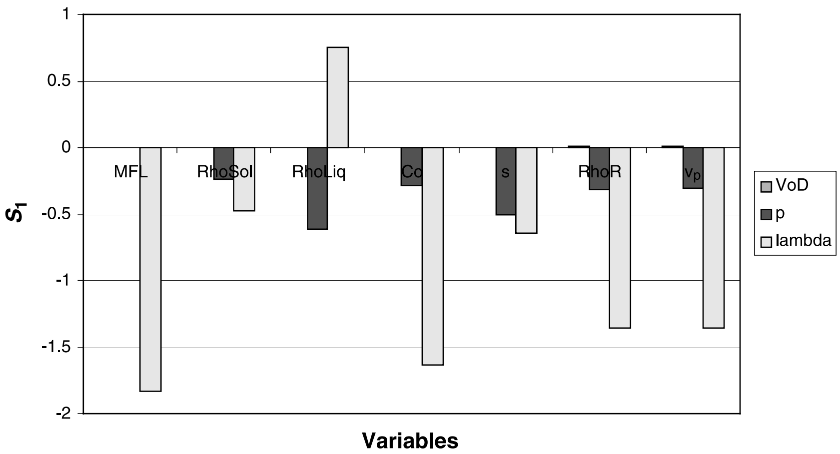

Fig. 7. Response of the sensitivity S_1 to changes in the detonation parameters for Blend1

6.1.3 Sensitivity of the Model to the Blasthole Diameter

Figure 9 plots the pressure and extent of reaction histories of ANFO at 152 and 250 mm diameter blastholes confined in Breccia confinement (Table 2) at the DDZ. It is shown that ANFO reacts 75 and 88% at 152 and 250 mm, respectively. In other words, the larger the diameter is, the more the explosive reacts at the sonic locus. Detonation pressure at the sonic locus is approximately 1.3 times more at larger diameter. Therefore, it can be concluded that the blasthole diameter affects the performance of the explosive significantly.

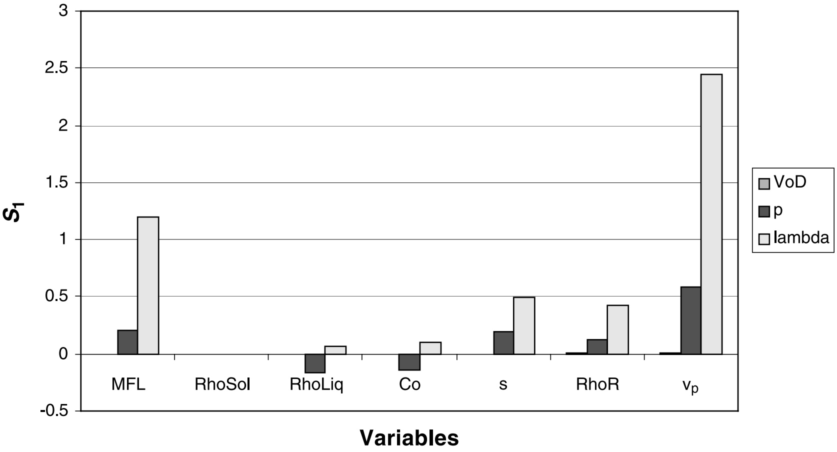

Fig. 8. Response of the sensitivity S_1 to changes in the detonation parameters for Lee's (1990) emulsion

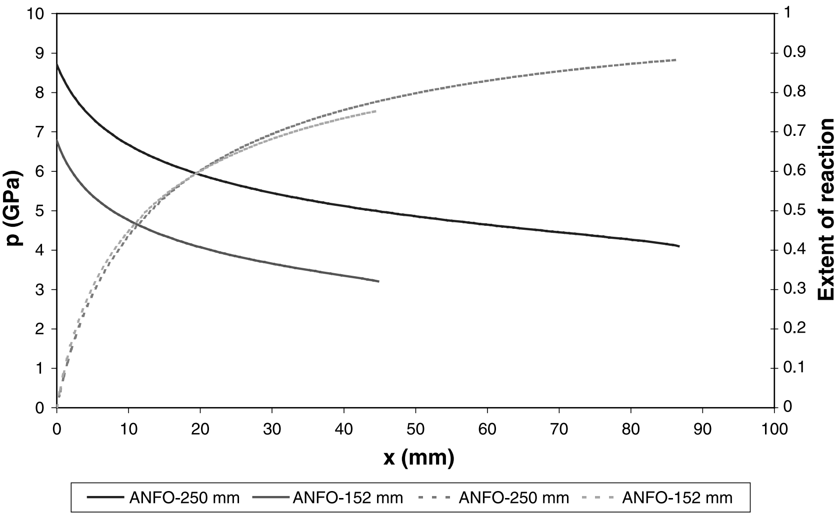

Fig. 9. Pressure and extent of reaction histories of ANFO at 152 and 250 mm in Breccia confinement

6.1.4 Sensitivity of the Model to the Explosive Type

Figure 10 shows the confined (in kimberlite) and unconfined D/D_{CJ} versus diameter relations of ANFO, Blend1 and emulsion. The differences between unconfined and confined VoDs become more than 5% when the charge diameter is below 200, 100 and 30 mm for ANFO, Blend1 and emulsion respectively. These explosives approach to ideality ($D/D_{CJ} > 0.95$) at 360, 330 and 140 mm, respectively. Given that the most surface mines utilise drilling machines with a range from 89 to 351 mm and ANFO and blend type products, these explosives are non-ideal and their performance should be predicted using a non-ideal detonation code.

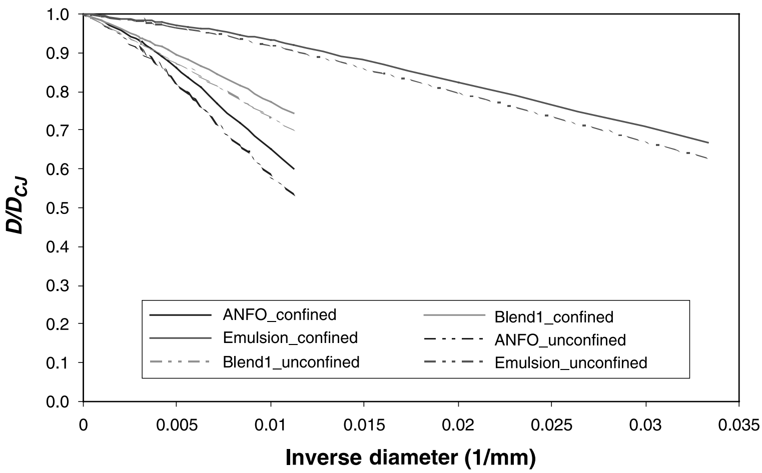

Fig. 10. Unconfined and confined (kimberlite) D/D_{CJ} versus diameter relations of ANFO, Blend1 and emulsion

Table 4. Performance of the explosives at 152 and 250 mm diameter blastholes confined in kimberlite

	250 mm			152 mm			Difference (%)		
	ANFO1	Blend1	Emulsion	ANFO1	Blend1	Emulsion	ANFO1	Blend1	Emulsion
D (km/s)	4.325	5.701	6.246	3.822	5.32	6.129	13.2	7.2	1.9
P (GPa)	3.944	9.234	12.098	3.025	7.797	11.438	30.4	18.4	5.8
v (cm^3/g)	0.958	0.673	0.606	0.993	0.687	0.613	3.5	2.0	1.1
λ	0.874	0.942	0.968	0.681	0.835	0.942	28.3	12.8	2.8

Table 4 shows the performance of the explosives at 250 and 152 mm diameter blastholes confined in kimberlite confinement. For a given blasthole diameter and rock type, the performances of ANFO, blend emulsion type explosives are different. In particular, ANFO1 has a lower pressure and reacts less at the sonic locus compared to the other explosive types. Furthermore, the degree of non-ideality is more pronounced in order as follows when the blasthole diameter is decreased from 250 to 152 mm: ANFO1, Blend1 and emulsion.

6.1.5 Sensitivity of the Model to the Rock Type

The sensitivity analyses have been further carried out to investigate the effect of rock type on the model responses. Three rock types kimberlite, monzonite and hematite whose properties are given in Table 2 have been included in the analysis to represent low, medium and high strength rock types. Intact rock classification is based on the Young's modulus (Lama and Vutukuri, 1978). Table 5 shows the predictions of the code for ANFO1 at 165 and 250 mm diameter blastholes confined in these rock types.

As shown in Table 5, the performance of ANFO1 varies with changes in rock properties at a given blasthole diameter. The results follow the expected trends: the stiffer the rock, the higher the VoD, pressure and extent of reaction and the lower the

Table 5. Comparison of the performance of ANFO1 at 165 and 250 mm diameter blastholes confined in kimberlite, monzonite and hematite

	165 mm			250 mm			Difference (%)		
	Kimberlite	Monzonite	Hematite	Kimberlite	Monzonite	Hematite	Kimberlite	Monzonite	Hematite
D (km/s)	3.927	4.005	4.071	4.325	4.374	4.416	9.2	8.4	7.8
P (GPa)	3.212	3.350	3.483	3.954	4.067	4.146	18.8	17.6	16.0
v (cm^3/g)	0.984	0.983	0.979	0.957	0.951	0.946	2.8	3.4	3.5
λ	0.720	0.766	0.802	0.873	0.887	0.889	17.5	13.6	9.8

Table 6. Comparison of the performance of Blend1 at 165 and 250 mm diameter blastholes confined in kimberlite, monzonite and hematite

	165 mm			250 mm			Difference (%)		
	Kimberlite	Monzonite	Hematite	Kimberlite	Monzonite	Hematite	Kimberlite	Monzonite	Hematite
D (km/s)	5.398	5.459	5.511	5.701	5.741	5.776	5.3	4.9	4.6
P (GPa)	8.090	8.357	8.483	9.193	9.399	9.470	12.0	11.1	10.4
v (cm^3/g)	0.686	0.682	0.679	0.672	0.668	0.665	2.1	2.1	2.1
λ	0.877	0.886	0.889	0.932	0.940	0.942	5.9	5.7	5.6

specific volume. When the performance of ANFO1 is compared at 165 and 250 mm diameters, the differences in the model predictions vary between 2.8 and 18.8%.

Table 6 shows the predictions of the code for Blend1 at 165 and 250 mm diameter blastholes confined in the above rock types. Similar conclusions have been found; however, because Blend1 is a less non-ideal explosive than ANFO1, the differences in the model predictions vary less, between 2.1 and 12.0%. This may suggest that the effect of confinement is more pronounced in low VoD explosives such as ANFO1.

6.1.6 Sensitivity Analysis for the Taylor Wave Model

Figure 11 shows the results of the Taylor wave model for ANFO confined in low (kimberlite) and medium (breccia) strength rock types at 152 and 250 mm blasthole diameters. It is shown that when ANFO is confined in stiffer rock, the Taylor wave is higher; that is, the $p-v$ curve is higher. Similarly, for a given explosive (ANFO in this case) when the blasthole diameter is increased, the Taylor wave is higher. Therefore, when the blasthole diameter is decreased for a given explosive and/or the rock is less stiff, the Taylor wave is lower. The shape of the Taylor wave is governed by a combination of the isentrope for expansion of the detonation gases, the blasthole diameter and the degree of confinement.

Figure 12 plots the $p-v$ curve and the work done by the detonation products for ANFO1, Heavy ANFO1 and Blend2 in 210 mm blasthole in fresh volcanics (Table 2).

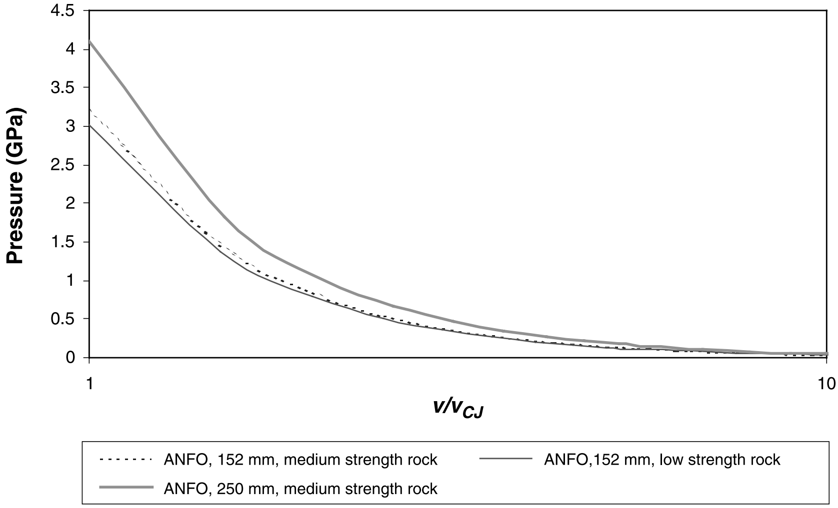

Fig. 11. The results of the Taylor wave model for ANFO confined in low (kimberlite) and medium (breccia) strength rocks at 152 and 250 mm diameter blastholes

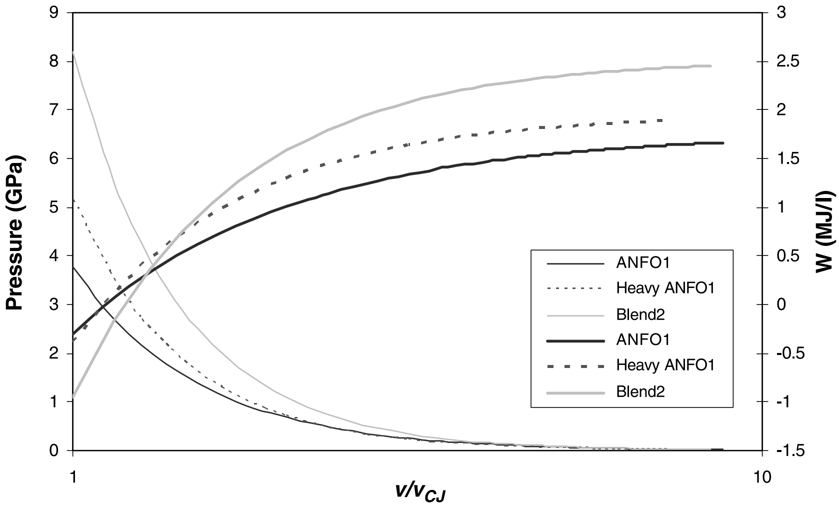

Fig. 12. p–v curve and the work done by the detonation products for ANFO1, Heavy ANFO1 and Blend2. Thin and thick lines represent the pressure and expansion work curves respectively for each explosive type

It appears that the p–v curve is higher for the Blend2 and more work is done by this product than Heavy ANFO1 and ANFO1.

6.1.7 The Effect of the Variation in the Unconfined VoD on the Confined Detonation Parameters

As the variations observed in unconfined VoD data may have a direct impact on non-ideal detonation modelling results, a series of non-ideal simulations have been carried

Table 7. The impact of the variation in the unconfined VoD on the confined (in fresh volcanics) non-ideal detonation parameters

Explosive	d (mm)	Unconfined VoD (km/s)	Confined detonation state parameters				Difference (%)			
			VoD (km/s)	p_{CJ} (GPa)	λ_{CJ}	v_{CJ} (cm^3/g)	VoD	p_{CJ}	λ_{CJ}	v_{CJ}
ANFO1	154	Max = 3.854	4.096	3.527	0.786	0.971	2.1	4.6	3.4	−0.8
		Mean = 3.749	4.012	3.371	0.760	0.979				
		Min = 3.577	3.873	3.115	0.705	0.990	−3.5	−7.6	−7.2	1.1
Heavy ANFO1	154	Max = 3.856	4.218	4.441	0.596	0.790	6.7	17.1	21.9	−1.5
		Mean = 3.555	3.952	3.794	0.489	0.802				
		Min = 3.302	3.723	3.204	0.440	0.833	−5.8	−15.6	−10.0	3.9
Blend1	130	Max = 5.061	5.288	7.784	0.840	0.527	4.4	10.9	11.7	−24.0
		Mean = 4.797	5.067	7.016	0.752	0.693				
		Min = 4.417	4.743	5.958	0.627	0.703	−6.4	−15.1	−16.6	1.4

out using the DeNE. Simulations have been conducted for three different explosive types, namely ANFO1, Heavy ANFO1 and Blend1. As discussed in Section 5, the variations in the unconfined VoDs depend on a number of factors including the explosive type and may vary by as much as 0.305 km/s. In order to investigate the possible impacts on the non-ideal detonation simulation results, this sensitivity analysis is conducted. Modelling results are summarised in Table 7. The comparison is made relative to the mean properties (VoD, pressure, degree of chemical reaction and specific volume). % differences in these properties due to the discrepancies in the unconfined VoDs (0.105, 0.172 km/s for ANFO1; 0.301, 0.253 km/s for Heavy ANFO1; 0.264, 0.380 for Blend1) are given.

As shown in Table 7, the variations in unconfined VoD data appear to have significant effects on the simulated non-ideal detonation parameters. It is shown that these variations are particularly more pronounced for the Heavy ANFO1 and Blend1. The simulation results suggest that the variations in the detonation pressure range from 4.6 to 17.1%. However, the impact of this on the overall blast results is still unknown and should be explored further.

6.2 Validation of the DeNE

The validation for the code DeNE has been carried out in three parts: (a) comparison of the results of DeNE and detonation shock dynamics (DSD) simulations conducted by Lee (1990) and Sharpe (2003); (b) comparison of the results of DeNE and Braithwaite et al.'s (1989) code; and (c) in-hole VoD data collected from mine sites.

6.2.1 Comparison of the DeNE and Hydrocode Simulations

Sharpe (2003) has carried out a number of hydrocode (COBRA) simulations of time-dependent 2-D reactive Euler equations to test the assumptions and approximations

Table 8. Comparison of the Sharpe's (2003) hydrocode and the proposed model for the unconfined ANFO charges

Modelling method	d (mm)	VoD (km/s)	R_s (mm)	p_s (GPa)	p_{CJ} (GPa)	x_{CJ} (mm)	λ_{CJ}
Sharpe's (2003) hydrocode	100	3.13	127.3	4.32	2.01	14.9	0.73
DeNE			117.8	3.95	1.90	13.6	0.47
Sharpe's (2003) hydrocode	150	3.73	207.2	6.12	2.89	16.2	0.86
DeNE			229.5	5.99	2.85	15.4	0.68
Sharpe's (2003) hydrocode	200	4.02	309.2	7.09	3.37	17.3	0.91
DeNE			344.3	7.12	3.40	17.9	0.80

used in the slightly divergent flow theory. Sharpe (2003) has presented the hydrocode results for the unconfined ANFO charges with density of $0.8\,\mathrm{g/cm^3}$.

A comparison of the detonation properties at the charge axis determined by the hydrocode (Sharpe, 2003) and the proposed model is given in Table 8. It is shown that the results at the detonation and shock states are comparable. The discrepancies are believed to be due to the use of different models with different flow theory. Furthermore, the above discrepancies may also be attributed to the poor approximation of the shock shapes in unconfined detonation used in the slightly divergent flow theory. However, the approximations used in the theory is valid for the confined detonations (2003). This suggests that the use of DeNE in confined blasting is reliable.

Lee (1990) has developed a hydrocode which uses the DSD theory. He has used the Mie-Gruneisen EoS and β EoS for the unreacted and reacted (product) phases. He has employed a reaction-rate equation (as a function of p and λ) that was calibrated for an emulsion explosive with a density of $1.248\,\mathrm{g/cm^3}$. The DeNE is run for the unconfined explosive with diameters of 32 and 72 mm.

Table 9 tabulates and compares the results obtained from the Lee's (1990) DSD model and DeNE. In general, it is shown that the results compare well and the discrepancies are believed to be a result of the different modelling approaches employed and the limitation of the use of the slightly divergent flow theory in unconfined detonation cases as discussed in Sharpe's (2003) study.

6.2.2 Comparison of the DeNE and Braithwaite et al. (1989) Code

The code developed by Braithwaite et al. (1989) has been made available in this study. It is based on the Kirby and Leiper's (1985) slightly divergent flow analysis and uses the same EoS used in this study; however, it employs different rate law, shock and isobar curvature expressions, numerical technique, shock calculation method and ideal

Table 9. Detonation state parameters obtained from the DeNE and Lee's (1990) DSD model

Model	d (mm)	VoD (km/s)	p_s (GPa)	p_{CJ} (GPa)	x_{CJ} (mm)	λ_{CJ}
DeNE	32	4.00	5.098	2.814	6.098	0.279
Lee's (1990) DSD model			5.020	3.400	8.970	0.317
DeNE	72	5.50	12.364	7.998	4.005	0.647
Lee's (1990) DSD model			12.300	7.870	9.150	0.639

Table 10. Detonation state parameters obtained from the MPEX and DeNE

Model	d (mm)	VoD (km/s)	p_{CJ} (GPa)	v_{CJ} (cm^3/g)	E_{CJ} (MJ/kg)	u_{CJ} (km/s)	λ_{CJ}	x_{CJ} (mm)
DeNE	50	5.097	6.592	0.679	0.208	4.075	0.633	6.721
MPEX		4.960	6.372	0.689	0.095	3.953	0.714	2.203
DeNE	100	5.868	10.024	0.628	0.774	4.505	0.846	5.276
MPEX		5.500	8.536	0.651	0.447	4.271	0.846	2.486

detonation code. The code is named MPEX in this study. One explosive type (emulsion) has been compared.

The results of the DeNE and MPEX at the detonation state are compared in Table 10 at 50 and 100 mm charge diameters. In general, the results agree well except for the model responses E_{CJ} and x_{CJ}. The discrepancies are believed to be owing to the following: shock state calculation method, the fitting process, rate law (simple versus complex), different shock curvature expressions, divergent flow approximation and numerical technique (initial value versus boundary value).

6.2.3 Validation of the Confined VoD Expression Using the In-Hole VoD Data

As discussed in Section 5, numerous in-hole VoD data is collected as part of the study to prove the necessary data for the validation of the DeNE. The measured and predicted confined VoDs are tabulated in Table 11. It is shown that the average error in predicting the confined VoD is 3.6% and the error range is between 0.8 and 6.3%. This is considered sufficiently accurate for practical applications in rock blasting. Furthermore, the error is within the experimental error described as the standard deviation divided by the measured VoD. The average experimental error is computed as 3.5% with a range from 2.2 to 7.2%.

The comparison of the published and predicted in-hole VoDs is given in Table 12. The average error in predicting the confined VoD is 4.1% that is similar to the error observed in the comparison of the measured VoD data. Hence, it is believed that the predictive capability of the confined VoD expression is adequate for practical rock blasting applications.

Table 11. Comparison of the measured and predicted in-hole VoDs

Explosive	d (mm)	Rock	Measured VoD (km/s)	Predicted VoD (km/s)	Error (%)
Blend1	165	Kimberlite	5.079 ± 0.132	5.210	2.6
Blend2	210	Monzonite (Cadia Extension)	5.728	5.774	0.8
Blend2	210	Fresh Volcanics (North Wall)	5.479 ± 0.134	5.765	5.2
Blend2	222	Monzonite (610 m Level)	5.460 ± 0.121	5.805	6.3
Blend2	222	Monzonite (625 m Level)	5.613 ± 0.176	5.805	3.4
Blend3	311	East Porphyry	5.864	5.993	2.2
ANFO2	311	Metasediments	4.344	4.586	5.6
Blend1	165	Kimberlite (TKB)	5.159 ± 0.370	5.297	2.7

Table 12. Comparison of the published and predicted in-hole VoDs

Explosive	ρ_o (g/cm^3)	d (mm)	Rock	Published VoD (km/s)	Predicted VoD (km/s)	Error (%)
ANFO (Sarma, 1998)	0.80	169	Breccia	4.235	4.058	−4.2
ANFO (Sarma, 1998)	0.80	269	Sandstone	4.220	4.408	4.5
ANFO (Sarma, 1998)	0.84	310	Overburden	4.510	4.741	5.1
ANFO (Sarma, 1998)	0.80	311	Overburden	4.375	4.453	1.8
ANFO (Gill, 1995)	0.80	165	Copper ore	4.380	4.024	−8.1
ANFO (Vanbrabant, 2002)	0.75	140	Andesite	4.052	4.010	−1.0

7. Conclusions

A non-ideal detonation model for commercial explosives incorporating a statistical approach to an established theoretical model has been developed. The proposed hybrid model combines the slightly divergent flow analysis, polytropic equation of state, simple pressure dependent rate law and statistical expressions of the unconfined and confined velocity of detonation (VoD) and shock curvature. The effect of confinement on the detonation is taken into account by creating the statistical expressions of VoD and radii of shock curvature of the shock front.

The model developed in this study is named the DeNE (Detonics of Non-ideal Explosives). Data required for the DeNE are the explosive properties (ideal detonation parameters, unreacted explosive properties, unconfined VoD versus charge diameter data), blasthole diameter and intact rock data (density and P-wave velocity). It predicts the detonation state and subsequent rarefaction (Taylor) wave to provide the pressure history for different explosive, rock type and blasthole diameter combinations. It enables the prediction and comparison of the performance of the commercial explosives in different blasting environments (i.e. explosive and rock type, blasthole diameter).

Six commercial explosives including ANFO, Heavy ANFO and blend type explosives were tested to obtain a wide range of unconfined VoD versus charge diameter data. The variations in the unconfined VoDs were found to be between 7 and 305 m/s depending on the explosive type. The major factors affecting the variations in unconfined VoD are: a) variability in product mix for the small masses loaded directly from the bulk explosive vehicle; b) variability in the in-pipe density; and c) possible unstable behaviour of the bulk explosive in smaller diameter charges as they could be approaching the critical diameter.

A detailed sensitivity analysis was conducted to evaluate the model. The model was found to be most sensitive to the solid density and Hugoniot parameters for ANFO; liquid density, Hugoniot parameters and mass fraction of liquid for Blends; and mass fraction of liquid and P-wave velocity of rock for emulsions.

It is shown that the larger the blasthole diameter, the more the explosive reacts at the sonic locus and thus blasthole diameter affects the performance of the explosive. The analysis shows that for a given blasthole diameter and rock type, ANFO, blend and emulsion type explosives exhibit different behaviour. In particular, ANFO1 has a lower pressure and reacts less at the sonic locus compared to the other explosive types.

The performance of ANFO1 varies with changes in the rock properties at a given blasthole diameter. The stiffer the rock, the higher the VoD, pressure and extent of reaction and the lower the specific volume. It is shown that the effect of confinement is greater at smaller diameters and/or with the use of the low VoD explosives.

It is shown that when ANFO is confined in stiffer rock, the Taylor wave is higher; that is, the $p-v$ curve is higher. Similarly, for a given explosive when the blasthole diameter is increased, the Taylor wave is higher. Therefore, when the blasthole diameter is decreased for a given explosive and/or rock is less stiff, the Taylor wave is lower. The shape of the Taylor wave is governed by a combination of the isentrope for expansion of the detonation gases, the blasthole diameter and the degree of confinement.

When the performances of ANFO1, Heavy ANFO1 and Blend2 at the sonic locus in a 210 mm blasthole in fresh volcanics are compared, the $p-v$ curve is higher for the Blend2 and more work is done by this product than by Heavy ANFO1 and ANFO1.

It is shown that the variations in unconfined VoD data appear to have significant effects on the simulated non-ideal detonation parameters. However, the impact of this factor on the overall blast results is still unknown and should be explored further.

The DeNE has been validated using the results of the hydrocodes and the non-ideal detonation model developed by Braithwaite et al. (1989) as well as measured and published in-hole VoD data. It is shown that the results of the DeNE compares well with the hydrocodes and Braithwaite et al.'s (1989) code. The DeNE is further validated using in-hole VoD data which suggests that the average error in predicting the confined VoD is 3.6 and 4.1% for the measured and published VoD data, respectively. This is found to be within the experimental error range of 2.2–7.2%. Hence, it is believed that the predictive capability of the confined VoD expression is adequate for practical rock blasting applications.

This paper has aimed to present the current state-of-the art technology in non-ideal detonation modelling and a model of this type, which is shown to be potentially useable as a practical tool in rock blasting modelling. The blasting engineer can use the predictions of the DeNE in the determination of the realistic performances of the current and potential explosive products manufactured by the explosive companies for a given rock type and blasthole diameter. The comparison of the DDZ results, Taylor wave and the work done by the detonation products is a good starting point as an initial analysis. The explosive performance parameters determined by the DeNE can be integrated into any blasting model including empirical, kinematic, mechanistic and numerical models.

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Appendix A. Shock Jump Equations

The change in particle velocity, pressure, specific internal energy, density and specific volume across the shock front must be determined in order to determine the initial conditions at the shock front ($t = 0$). The usual way of treating shocks is to idealize

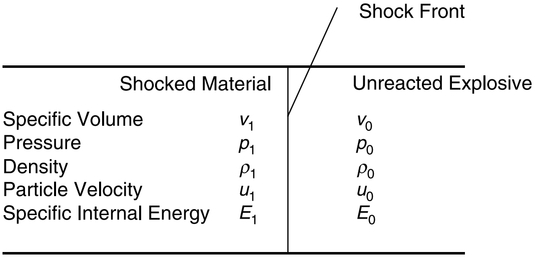

Fig. A.1. Shock parameters in front of and behind a shock wave front (Cooper, 1996)

them to jump discontinuities. They do not change gradually along some gradient or path but discontinuously jump from unshocked to shocked values (Fig. A.1). We use a system of shock coordinates, where we view the system as if we were sitting on the crest of the shock wave. We have five variables to deal with; so we will need five relationships to solve for all those variables (Cooper, 1996).

The first three relationships can be derived from the fact that mass, momentum and energy must be conserved as material passes from one side of the shock front to the other. We call these three conservation relationships the "Rankine-Hugoniot jump equations". Let subscripts 0 and 1 refer to the states just in front of and just behind the shock front respectively.

The well known Rankine-Hugoniot jump conditions can be written (Cooper, 1996)

$$\text{mass equation: } \frac{\rho_1}{\rho_0} = \frac{D}{D - u_1} = \frac{v_0}{v_1} \tag{A.1}$$

$$\text{momentum equation: } p_1 - p_0 = \rho_0 u_1 D \tag{A.2}$$

$$\text{energy equation: } E_1 - E_0 = \frac{1}{2}(p_1 + p_0)(v_0 - v_1) \tag{A.3}$$

The strong shock conditions are employed by setting p_0 and E_0 equal to zero, which provides a common simplification used in condensed explosive modelling. In order to solve for these variables, we need the Hugoniot equation and also a relationship involving any two of the mass, momentum and energy.

The following equation is chosen in this study as the Hugoniot in the p–v plane (Cooper, 1996)

$$p = \frac{C_0^2(v_0 - v_1)}{[v_0 - s(v_0 - v_1)]^2} \tag{A.4}$$

where C_0 and s are shock Hugoniot parameters. C_0 is called the bulk sound speed with unit in km/s. s is dimensionless. C_0 and s values for a typical emulsion explosive are 2.04 and 1.91, respectively (Lee et al., 1989). These values for AN (Ammonium nitrate) with densities of 0.86 and 1.73 g/cm^3 are 0.84 and 1.42; and 2.20 and 1.96, respectively (Cooper, 1996).

It is often true that the Hugoniot curve can be represented over a reasonably wide range of pressures as a simple curve in U–u (shock velocity–particle velocity), ($U = C_0 + su$) which suggests that shock velocity is linearly related to the particle

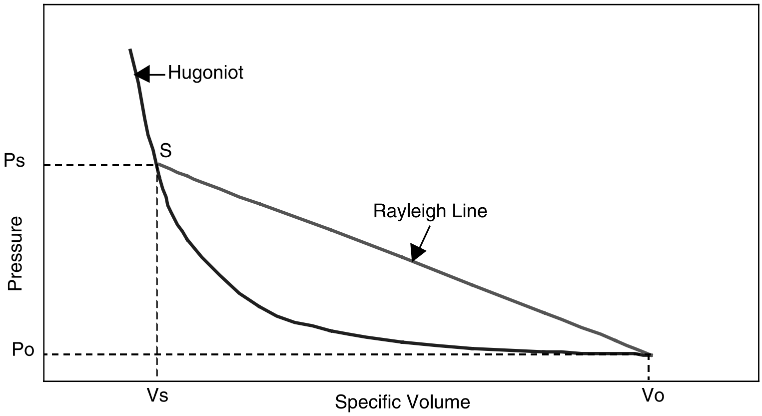

Fig. A.2. Typical $p-v$ Hugoniot for an unreacted explosive (Cooper, 1996)

velocity, for most solid materials. Solids can support many kinds of waves because they have strength. However, for many purposes, it is an adequate approximation to treat solids as fluids as long as the pressures are several times the yield strengths (Davis, 1998).

Figure A.2 plots a typical $p-v$ Hugoniot for an unreacted explosive. Hugoniot is not the path along which a material is stressed, but is the locus of all the possible equilibrium states in which a particular material can exist. Since the Hugoniot represents the locus of all possible states behind the shock front, then a line joining the initial and final states on the $p-v$ Hugoniot represents the jump condition. This line is called the "Rayleigh line" and is shown in Fig. A.2. Point S is the point in which the solution is sought.

If we eliminate the particle velocity term u by manipulating the mass and momentum jump equations, we get

$$p_1 - p_0 = \frac{D^2}{v_0} - \frac{D^2}{v_0^2} v_1 \tag{A.5}$$

Rankine–Hugoniot, Hugoniot and Rayleigh line relations are solved simultaneously to determine the shock parameters at the shock front (point S in Fig. A.2). For the $p-v$ Hugoniot given above, the solution is obtained analytically and is simply

$$v_s = v_0 \left[1 - \frac{(1 - C_0/D)}{s} \right], \tag{A.6}$$

and u_s, p_s and E_s, evaluated at the shock are obtained by substitution into Equations A.1, A.4 and A.3, respectively.

Author's address: Sedat Esen, Metso Minerals Process Technology (Asia-Pacific), Unit 1, 8–10 Chapman Place, Eagle Farm, Qld 4009, Australia; e-mail: sedat.esen@metso.com