Diameter-Effect Modelling in Unconfined Steady Non-Ideal Detonations

Paulo Couceiro, MAXAM

Abstract

Since explosives are the source of all energy used for rock blast fragmentation and heave, multi-dimensional effects in the detonation driving zone become essential to better describe the detonation process. In order to use the explosive as an energy source-information for more realist blasting performance simulations, a simple and effective modelling strategy is desirable. Facing this challenge, an engineering approach to two-dimensional unconfined non-ideal detonation is proposed. Based on the elliptical construction of the shock locus, the model combines the axial cylindrical stick Q1D solution with some additional limiting conditions to determine the sonic edge of the charge. For a given set of rate law parameters and velocity of detonation, a complete axial solution is firstly computed through the Q1D model. From this solution, a vital relationship between the axial shock curvature with the shock shape parameters can be stablished. Once this relationship is found, the problem simply reduces in finding the shock shape parameters subject to the sonic edge condition. As a result of this calculation, the corresponding charge diameter can be found. Consequently, the proposed model can map the diameter-effect curve by relating the unconfined velocity of detonation with its corresponding diameter. Finally, because of its low computation cost, the proposed engineering approach can be also used for characterizing the rate law parameters by fitting to data from unconfined detonation experiments.

Introduction

The complex energy release mechanisms involved in a detonation of heterogeneous non-ideal explosives, such as those ammonium nitrate-based explosives, has being the subject of intense investigations in the past years. In the blasting and mining field, the interest is mainly motivated by the need of providing a reliable source energy-term information for rock blasting simulations. The optimization of mining operations through the energy-chain optimization, which is strongly influenced by an efficient blasting process, is key for sustainable mine exploitation. Thus, the characterization of non-ideal detonation process become essential to understand the source of all blasting phenomenologies.

Non-Ideal detonation modelling

The rock blasting process is complex. The interaction of the explosive and inert confiner material during the detonation is still a matter of research and discussion, especially in cases where the sound speed of rock is higher than the velocity of detonation (Sharpe et al., 2009; Sharpe & Braithwaite, 2005; Braithwaite et al., 2010; Sellers, 2007; Braithwaite & Sharpe, 2013; Sellers, 2013; Esen, 2008; Sellers et al., 2012). Most of the non-ideal detonations approaches in condensed phase are based on the reactive Euler equations or conservation of mass, momentum and energy. From one side, there is the direct numerical simulation (DNS) method, which demand intensive computation time to solve the equations' problem, remaining as an academic approach or to provide invaluable data for use as benchmark against more approximate analysis (Braithwaite et al., 2010). On the other side, some classes of quasi-one dimensional analysis, such as slightly divergent flow analysis (Fickett & Davis, 1979; Kirby & Leiper, 1985) or Q1D models (Sharpe & Braithwaite, 2005), applied to axial solutions and extended approaches to two dimensional geometries like the Detonation Shock Dynamic (DSD) analysis (Stewart & Bdzil, 2007) or the Straight Streamline Approach (SSA), proposed by Watt et al. (2011), have been using with different degrees of success in non-ideal steady detonation modelling.

In multi-dimensional analysis, while DSD normally works well for weakly curved and strongly confined detonations, although some attempt to extend the theory for highly non-ideal explosive have been reported (Watt et al., 2011), SSA has supposed an important improvement toward the highly non-ideal steady detonation calculations, where the velocity of detonation can reach even 50% of the D_{CJ}. The SSA is a novel method where the reactive Euler equation are written in a streamline-based co-ordinate system. Given the streamline shapes, the two-dimensional problem reduces to an ordinary differential equation eigenvalue problem along each streamline (Watt et al., 2011). The structural description of the detonation driving zone (DDZ) arouses great interest for the bi-dimensional understanding of the detonation. A direct consequence of this knowledge is the possibility to develop the diameter effect curve. In this field, the SSA model has been an interesting alternative to the DNS due to its good prediction capability and cheap computational cost. However, the SSA tends to under predict the length of the detonation driving zone (DDZ) and shock locus shape (Watt et al., 2011; Cartwright, 2016; Croft, 2017), leading to a regular description of the DDZ when compared with the shock shapes from DNS.

Q1D Engineering Approach Model

A simple engineering approach to two-dimensional steady non-ideal unconfined detonation is proposed. It is based on the argument that there is a spatial coherence between the axial solution and the explosive/inert edge conditions. The model combines the axial steady non-ideal detonation solution from the Q1D model developed by Sharpe and Braithwaite (2005) with assumptions upon shock and locus shape functions. Once the sonic edge condition is defined by shock-polar analysis, an additional condition is needed in order to calculate the explosive radio (or diameter) for given set of rate burn parameters and velocity of detonation. This engineering model, coded as Q1D EA, has been used for a simple polytropic and pseudo-polytropic equation of state (EOS) with surprising level of success. Comparisons with DNS, DSD and SSA (Sharpe & Braithwaite, 2005; Watt et al., 2011; Cartwright, 2016) are performed to assess the Q1D EA capability. Finally, the last section of this paper exemplifies the Q1D EA capability to efficiently calibrate the burn rate parameters for a given set of unconfined detonation experiment data.

Model description

The proposed engineering approach is founded on the spatial construction of the DDZ based on the axial solution and additional geometrical conditions to determine the sonic edge of unconfined steady non-ideal detonations. Consequently, it is possible to determine the diameter effect curve for a specific set of unconfined experimental data by calibrating rate parameters.

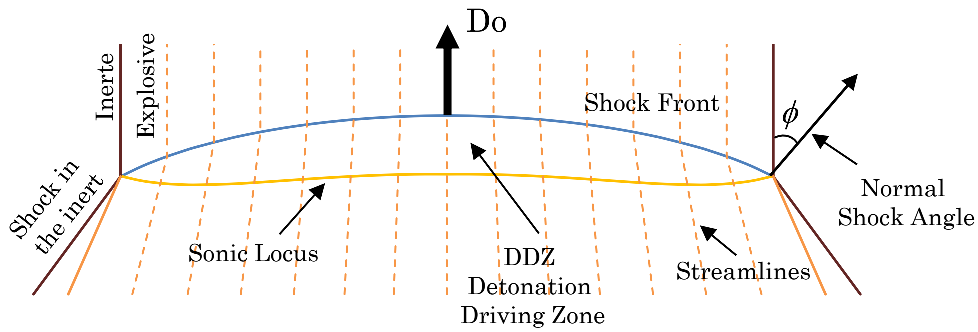

Figure 1. Idealized scheme of two-dimensional steady non-ideal detonation. The detonation is propagating upward with a constant velocity of Do.

In the case of non-ideal detonation, direct numerical simulations DNS indicates that shock shapes can be well fitted by an arc of ellipse (Sharpe & Braithwaite, 2005; Kennedy, 1998). Thus, an ellipse of the following form

$$\frac{{z_f}^2 + \alpha^2}{\alpha^2} + \frac{r^2}{\beta^2} = 1 \qquad \textbf{Equation 1}$$

can be assumed to well represent the shock shape. Where z and r are the axial and radial directions, respectively; and α e β are the ellipse or the shock shape parameters.

An assumed shock shape function allows one to calculate the slope angle ϕ and curvature κ at any point along of the shock z_f. Thus, the shock slope z_f' can be calculated by

$$z_f' = -\frac{\alpha r}{\beta^2}\left(1 - \frac{r^2}{\beta^2}\right)^{-1/2} \qquad \textbf{Equation 2}$$

In the case of unconfined detonation, the sonic condition, through shock polar analysis, applies at the charge edge, $r = R$, leading the Equation 2 be equal to the sonic edge angle

$$z_f'(R) = -\left(\frac{\gamma - 1}{\gamma + 1}\right)^{1/2} \qquad \textbf{Equation 3}$$

Thus, the normal shock angle makes with the direction of propagation z at the charge edge, ϕ_{edge}, can be calculated by

$$\phi(R) = \phi_{edge} = -\tan^{-1}\left(z_f'(R)\right) \qquad \textbf{Equation 4}$$

Axial solution

The axial solution for a steady-state non-ideal detonation is required to estimate both shock and sonic locus shapes. Although any model can be used to determine the axial solution, such as the slightly divergent flow theory, the quasi-one-dimensional (Q1D) analysis proposed by Sharpe and Braithwaite (2005) is preferred for their advantages. The Q1D model has demonstrated very good capabilities in predicting axial solutions for both confined or unconfined detonations.

The mathematical formulation of Q1D theory is discussed elsewhere (Sharpe & Braithwaite, 2005). It assumes that the axial solution depends only parametrically on the axial velocity of detonation or shock front curvature. Based on reactive Euler equations, it is written in the shock-attached coordinate systems, since it is suggested to be governed by simple $D_n - \kappa$ law (Sharpe & Braithwaite, 2005). For a pseudo-polytropic equation of state, the Q1D set of ordinary differential equations are:

$$\frac{du_n}{dn} = \frac{Q(\gamma-1)W + \kappa(1+n\kappa)^{-1}c^2(u_n + D_n)}{c^2 - u_n^2} \qquad \textbf{Equation 5}$$

$$\frac{d\rho}{dn} = \frac{-Q(\gamma-1)\rho\dfrac{W}{u_n} + \kappa(1+n\kappa)^{-1}\rho u_n(u_n + D_n)}{c^2 - u_n^2} \qquad \textbf{Equation 6}$$

$$\frac{d\lambda}{dn} = \frac{W}{u_n} \qquad \textbf{Equation 7}$$

where u_n is the normal particle velocity; ρ is the density; D_n is the normal velocity of detonation; c is the sound speed; Q is the head of reaction; γ is the adiabatic gamma; $\kappa^* = \kappa(1+n\kappa)^{-1}$; and $W$is the reaction rate, given by a pressure dependent equation

$$W = \frac{1}{\tau}(1-\lambda)^m\left(\frac{P}{P_{ref}}\right)^n \qquad \textbf{Equation 8}$$

where n, m and τ are fitting parameter; P_{ref} is a reference pressure, 1GPa (145038 psi).

This set of ordinary differential equations form an eigenvalue problem in κ or D_n. The most common solution method is the shooting method subject to the jump shock and generalized CJ conditions (Sharpe & Braithwaite, 2005; Sharpe, 2000; Stewart & Jin, 1998).

Charge edge approximation

At the charge edge, the first boundary condition is defined in terms of shock slope, where the post-shock flow must be exactly sonic in the case of unconfined detonation (Cartwright, 2016). However, for a given axial solution, many possible sonic solutions can be found at different charge radios by assuming an elliptical shock shape function. Thus, an addition assumption in terms of shock shape parameters must be introduced about the charge radio.

For a given set of shock shape parameters, it is expected to find a charge radio R smaller than the highest ellipse radio $R_{max} = \beta$. Thus, the following proportion relationship can be formulated

$$\frac{R}{R_{max}} = f_R \qquad \textbf{Equation 9}$$

where f_R is an expression related to the degree of non-ideality of the explosive, given by

$$f_R = 1 - f_c \sqrt{\left(1 - \lambda_{CJ}\right)^m \frac{D_o}{D_{CJ}}} \qquad \textbf{Equation 10}$$

and λ_{CJ} is the reaction progress at the axis ($\lambda = 0$, for unreacted product and $\lambda = 1$ for a complete reaction process); f_c is a function to be defined; D_o is the velocity of detonation; and D_{CJ} is the thermodynamic ideal velocity of detonation. Then, the charge radio R or the steady velocity of detonation D_o can be related to the shock shape parameters by combining Equation 9 and Equation 10

$$R = R_{max}\left(1 - f_c \sqrt{\left(1 - \lambda_{CJ}\right)^m \frac{D_o}{D_{CJ}}}\right) \qquad \textbf{Equation 11}$$

From Equation 11, one can see that R increases when the D_o and λ_{CJ} increases. This behaviour is in line with the statement of Sharpe and Braithwaite (2005) that when the detonation speed increases, the shock locus always become flatter at the axis.

Further relationship between shock shape parameters α and β can be addressed to keep all equations as a function only of β. Since the axial solution is known, and its curvature κ_{axis} at the axis, the shock shape function z_f can be derivate twice to give

$$z_f'' = -\frac{\alpha}{\beta^2}\left(1 - \frac{r^2}{\beta^2}\right)^{-3/2} \qquad \textbf{Equation 12}$$

and by setting $r = 0$

$$z_f''(r = 0) = -\frac{\alpha}{\beta^2} \qquad \textbf{Equation 13}$$

This equation can be related to the axisymmetric cylinder shock front curvature by the following expression

$$\beta = \left(\frac{2\alpha}{\kappa_{axis}}\right)^{1/2} \qquad \textbf{Equation 14}$$

Therefore, given an axial solution for an unconfined steady detonation, the proposed approach requires to find the shock shape parameter α (since β can be written in function of α and R in function of β) in which the shock slope at the charge edge R become exactly sonic, as defined in Equation 3.

Model Validation

A simple polytropic equation of state with $\gamma = 3$ is examined for non-dimensional unconfined detonations. The calculations where performed for $m = 0.5$ and various n and compared with the results published by Watt et al. (2011). As can be seen in Figure 2(a) and (b), diameter curves predictions for $n = 0$ and $n = 1$ are in a very good agreement with DNS calculations. This is a good sign since the severest non-ideal detonation cases are very low state dependents (Watt et al., 2011). In comparison with SSA model, the Q1D EA seems to improve the diameter effect curve for larger radii whereas it is almost equivalent for smaller ones for $n = 0$ and slightly higher for $n = 1$.

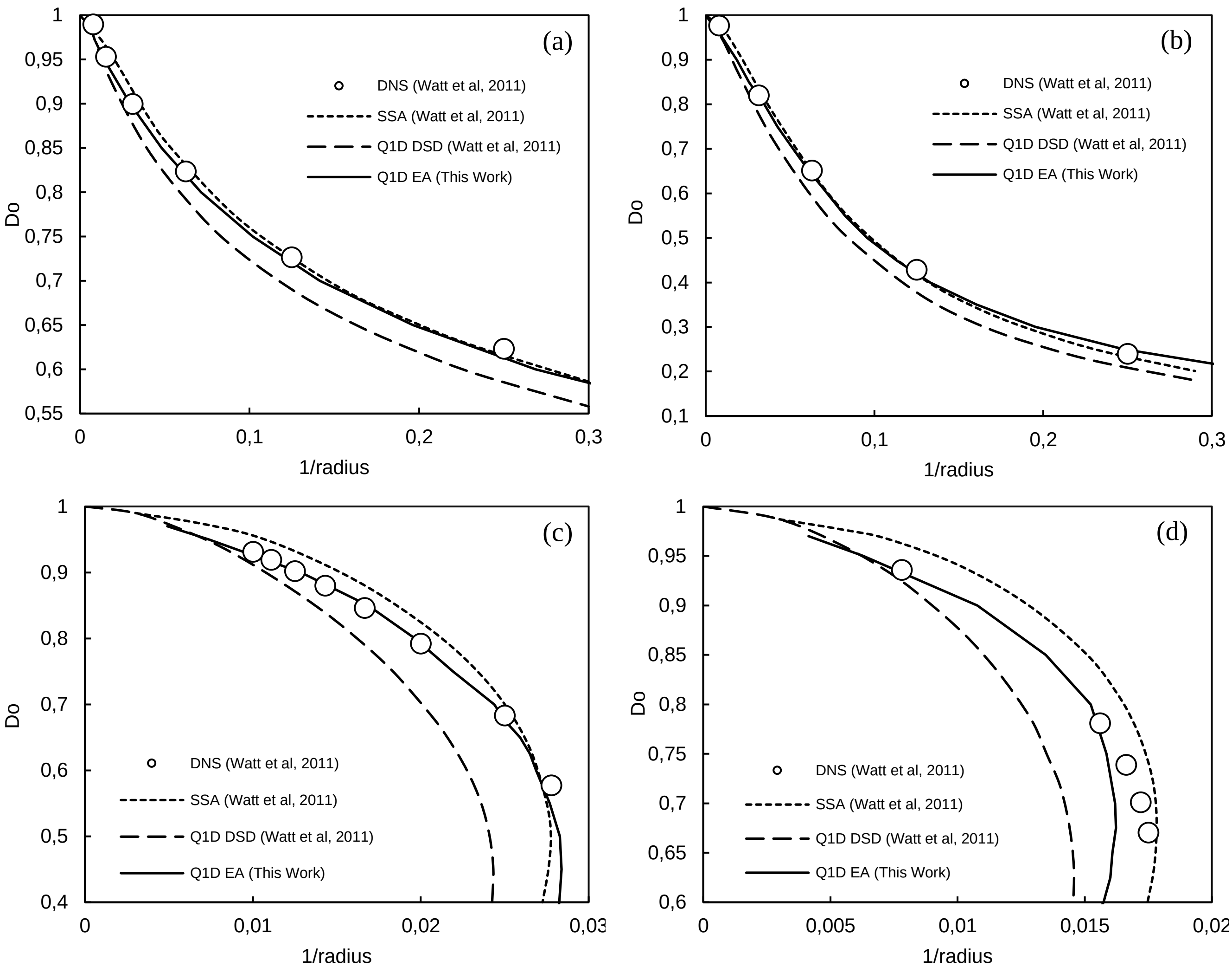

Figure 2. Diameter effect curve for cylindrical geometry. Solid line (Q1D EA), dotted lines (SSA), dashed lines (Q1D DSD) and Circles (DNS).

Moving to higher values of n, Q1D EA has presented notable improvements over Q1D DSD and SSA models, especially for $n = 1.7$, as can be seem in Figure 2(c). Very good predictions could be achieved for all large and small radii. In this case, the critical diameter predicted by the Q1D EA is slightly smaller than the predicted by Watt et al. (2011) SSA model, although the DNS curve seems to predict even smaller critical diameter.

Nevertheless, for $n = 2$, the Q1D EA well predicts medium-larger radii while over-estimates the critical diameter when compared to the DNS (Watt et al., 2011). In this case, the SSA model better predicts the critical or failure diameter in comparison with the Q1D EA. On the other hand, the most interesting diameter sizes are the medium-larger ones because of its practical application in mining and blasting operations. Surprisingly, the Q1D EA has achieved interesting results diameter predictions for this zone of the diameter effect curve, not only for $n = 2$, but in all other scenarios.

Fitting to experimental data

The proposed approach model (Q1D EA) has been verified in predicting diameter effect curves for unconfined non-ideal explosives. As the model is coupled with the Q1D for the axial solution (Sharpe & Braithwaite, 2005), it is possible to calibrate burn rate parameters from a set of experimental unconfined detonation data. As the Q1D EA just need to solve a system of ordinary differential equations once for a given set of rate parameters, the computation time required to perform the fitting process is attractive.

Once the experimental results are available, the fitting process can be performed. The strategy is simple: minimize the square of the diameters residues for a given set of initial rate law parameters, an initial diameter effect curve can be generated. Consequently, the residues formed between the calculated and experimental diameters can be determined. Then, the sum of all these residues is minimized by varying the rate law parameters.

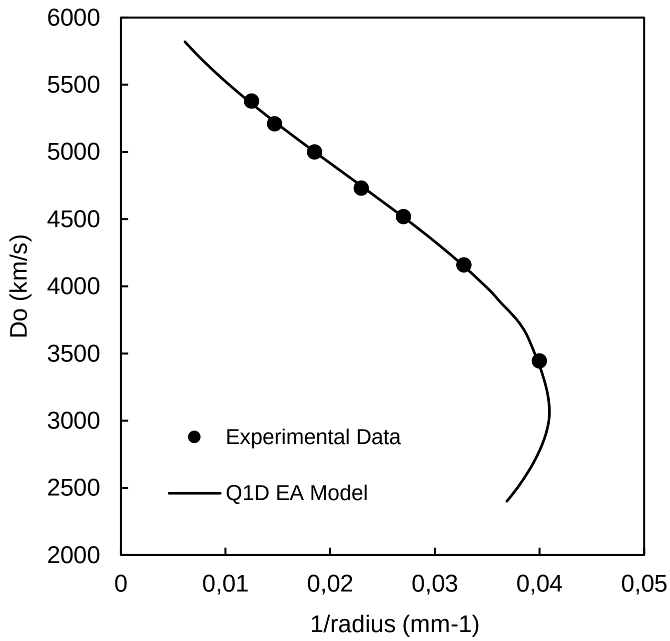

Figure 3. Fitted diameter effect curve for experimental data for a gassed Emulsion. The CJ detonation speed is D_{CJ} = 6000 m/s (19685 ft/s). Solid line (Q1D EA) and Circles (Experimental data).

The fitting capability of Q1D EA model is illustrated in Figure 3 by fitting the rate law parameters n, m and τ of Equation 8, combined with the pseudo-polytropic EOS with quadradic gamma, for a set of unconfined gassed Emulsion experimental data. A set of unconfined (cardboard) velocity of detonation were measured in order to characterize the critical diameter of this Emulsion explosive. These shots were carried out in diameters of 30mm (1.18in) and 50mm (1.97in), in a large range of densities. The results presented in this paper considers those results of an initial density of 1200 kg/m^3 (75 lb/ft^3).

Table 1. **Fitted Burn Rate Parameters from Q1D EA.**

Explosive	Gassed Emulsion
Initial Density	1200 kg/m^3 (75 lb/ft^3)
Ideal VOD	6000 m/s (19685 ft/s)
m	4.52
n	2.48
τ	5.69(-05)

The best fit values for n, m and τ are presented in Table 1. It was noted that a less weak state dependence of the rate law was required to fit the data, since $n = 2.48$ was obtained. Cowperthwaite (1994) first pointed out that when $n = 1.5$ there is always a turning point (Watt et al., 2011; Cartwright, 2016). Figure 3 shows the fitted diameter effect curve generated from Q1D EA model together with the experimental data. The presence of a turning point is evident, giving the critical or failure diameter of 49mm (1.93in), which is consistent with experimental critical diameter of 50mm (1.97in). The model well predicts the diameter effect curve for the full range of diameters of interest in the mining industry.

Conclusion

An engineering approach to two-dimensional steady non-ideal unconfined detonation, based on the spatial construction of the detonation driving zone, was presented. The model combines the cylindrical stick Q1D axial solution (Sharpe & Braithwaite, 2005) with some structural conditions to determine the unconfined explosive radio. It was found that the proposed functions related to the degree of non-ideality of the explosive, coupled with the Q1D axial solutions, provides exceptionally good predictions about both velocities of detonation and diameter effect curves, including good failure diameter predictions. Because of this remarkable predictive capacity and attractive computation cost, the Q1D EA model can be used to efficiently fit burning rate parameters to a set of unconfined experimental data.

The Q1D EA model was developed for unconfined detonations. It was shown that both polytropic and pseudo-polytropic with quadratic gamma equations of state worked well. There is no reason to believe that more sophisticated EOS would significant affect the structural conditions used to determine the unconfined explosive radio, since different EOS would only affect the Q1D axial solution. At this point, it is important to note that the proposed engineering approach works with other axial steady state non-ideal detonation solutions. However, the Q1D (Sharpe & Braithwaite, 2005) was chosen for its formidable capacity to find precise axial axisymmetric cylindrical stick solutions. Finally, an additional work is under way to extend this engineering approach to confined detonations cases, which will be reported in the future.

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