Multi-phase simulation of ammonium nitrate emulsion detonations

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Abstract

Ammonium-nitrate-based explosives used by the mining industry exhibit strong non-ideal detonation behaviour. Detonation velocities in rate-sticks with radii close to the failure radius, can be as low as one third of the ideal detonation velocity, which poses a significant challenge for their accurate predictive computational modelling. Given that these emulsions are highly heterogeneous, multi-phase formulations are well suited for their representation in numerical hydrocodes. To this end, a single-pressure, single-velocity multi-phase model is employed for the simulation of an explosive emulsion widely used by the mining industry. The model is modified to rectify a problem related to the calculation of a unique detonation state, and is evaluated using a high-resolution, shock-capturing Riemann problem-based scheme. In order to perform high-resolution numerical simulations at a reduced cost, a shock-following method is implemented and validated against the full-domain solutions. An improved iterative fitting procedure for steady-state detonation kinetics is also presented. Validation against experimental evidence shows that the model can reproduce confined VOD experimental data, solely by adjusting the reaction kinetics to match unconfined experimental VOD data. Furthermore, the model can match experimental front curvature measurement without further adjustments.

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1. Introduction

Ammonium-nitrate-based explosives are widely used by the mining industry due to their low manufacturing cost, ease of handling and low risk of accidental ignition. There is a strong interest within the industry to predict the performance of these explosives in confined environments in order to optimise the fracture and heaving process of rock.

The objective of this study is to identify, assess and implement a model appropriate for truly predictive simulations of detonation propagation and early-time response of the confinement material. To this end, the selected model should only rely on experimentally-determined values for the equation of state and reaction rate, without any use of additional user-adjusted parameters. In addition, the model should be able to accommodate a range of equations of state (e.g. Mie-Grüneisen, JWL [1], WMBG [2]) and arbitrary reaction rate equations, so that it can reproduce realistic material behaviour and non-ideal detonation behaviour. The model should also be able to deal with strong pressure and density gradients arising from confinement conditions. Multi-material capabilities are needed to deal with mixture cells across which appropriate interface conditions have to be fulfilled. It is also desirable that the reaction kinetics can be calibrated from simple unconfined detonation experiments.

Research and development in detonation modelling is dominated by military applications, thus yielding a plethora of specialised models for military explosives. The research and development requirements of the mining industry, despite being fundamentally related, have different emphasis. Military research aims to optimise maximum power generation in combination with a long shelf life. In contrast, the mining industry is mainly driven by cost factors (e.g. production and transport) and has an interest in “moderate” pressure detonations with a long pulse duration [3], i.e. energy is released over a longer period of time. Energy released over a short period of time would result in detonation pressures that would pulverise, instead of fracture and move, the rock around drill holes.

In the modelling framework these differences create two additional challenges in simulating mining explosives. Firstly, typical ammonium nitrate mining explosives have relatively high voidage, either for sensitising the explosive or lowering the explosive density. This voidage can be as low as 10% and can go as high as 60%. Also, the oxidiser and fuel are located on different molecules, leading to non-ideal detonation behaviour over a large range of charge radii. This means that in this range, the velocity of detonation (VOD) strongly depends on the confinement material as well as the charge radius and cannot be accurately predicted by simple detonation models, e.g. Chapman-Jouguet (CJ) theory.

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Despite the drawbacks of these simple models, there are some successful reduced models like Detonation Shock Dynamics (DSD) [4] and models based on the Wood–Kirkwood theory [5]. The DSD approach has proven itself as a useful model in military applications and is based on a unique detonation velocity–shock curvature law \( D_0 = a \). First-order DSD theory is known not to perform well for highly non-ideal detonations: Second-order extensions have been developed, but are restricted to simple reaction rate laws [6]. Nevertheless, first and second-order DSD theory is still based on the assumption that reaction zones are very thin in comparison to the radius of curvature. This assumption holds true for most military explosives but approaches the limits of its validity when dealing with highly non-ideal explosives. The Wood–Kirkwood based models, which are mainly used in mining industry, rely on a streamline approach. The underlying PDE system is transformed into the detonation frame and expressed in rotational symmetry. The resulting model reduces to an ODE along the centre streamline containing an unknown divergence term, which is usually supplied in some empirical form. Determination of the front dynamics is thus not enough to predict propulsion effects as a large amount of the energy is released out of the sonic surface during detonation products expansion. Furthermore, the relationship between front curvature and explosive diameter is not known and needs to be supplied from experiment. Taking into consideration the limitations of the current approaches outlined above, we assess in this work a multi-dimensional, unsteady, reactive, multi-phase approach for the purpose of investigating the post-initiation behaviour of mining explosives.

A popular class of multi-phase models are based on the formulation by Baer and Nunziato (BN) [7–9] and its reduced formulations, see for example [10]. To the best of our knowledge, no multi-phase model has yet been applied to mining explosives in combination with realistic equations of state (e.g. Mie-Grüneisen, JWL, WMGB).

For the class of explosives in which we are interested, a single-pressure and single-velocity multi-phase model is likely to be well-suited due to the fast mechanical relaxation between the explosive’s constituents. We propose to adopt a continuum hydrodynamic representation of each phase, where every material is represented by an independent set of state variables in order to allow temperature disequilibrium. A number of such formulations exist [11–13,10], and we chose the approach of Petitpas and Saurel [11,12], for reasons that will become apparent below.

In this work, the single-pressure and single-velocity multi-phase model described in [12] is modified to allow simulations of ammonium-nitrate-based emulsion explosives, as used in industrial applications. During the analysis of the model, a dependence of the detonation solution on the initial value of the product density was identified. This product density is not known at the very start of the detonation front. To rectify this problem, we suggest a physically-based approach to determine a unique product density at the shock front. In addition, the steady-state ODE system along the centre streamline for arbitrary materials with embedded front curvature effects is derived. An iterative process to fit the reaction kinetics for the purpose of steady-state calculations is presented. In order to allow high resolution simulations in multidimensions, rotational symmetry terms are derived and a simple method is developed which can significantly reduce the amount of computational cells. This approach is suitable for ratestick-based performance calculations (velocity of detonation (VOD), front curvature, detonation driving zone (DDZ), etc.).

The remaining section in this paper are organised as follows: In Section 2 we summarise the mathematical model as derived in the papers by Kapila et al. [10] and Saurel et al. [11]. The section is closed with the final formulation for the physical model, including the constitutive law and the reaction kinetics. Section 3 presents the algorithms used to solve the mathematical system, comprising the numerical method, the rotational symmetry source terms and the shock-following method. The steady-state ZND structure for a two-phase ideal detonation and for arbitrary materials with embedded front curvature effects, are derived in Section 4. The problem of the detonation dependency on the (yet unknown) initial product density is explained in Section 5, followed by a constant volume approximation to rectify the problem. The model is validated in Section 6 with a set of inert and reactive test cases, and the accuracy and efficiency of the shock-following method is demonstrated by comparisons against whole-domain simulations. The experiments of Dremin are outlined in Section 7, followed by a presentation of the reaction-rate fitting procedure and comparison of the numerical results to the experimental evidence. A discussion and concluding remarks are made in Section 8.

### 2. The mathematical and physical model

The emulsion explosive EM120D is used as the vehicle for this research; this is a mixture of ammonium nitrate (oxidiser), water, oil (fuel) and emulsifier. The ammonium nitrate is first dissolved in water forming an aqueous oxidiser solution, which is then emulsified into the fuel phase. The condensed emulsion may be sensitised by means of glass micro-balloons, which may also be used to control the explosive bulk density. The unreacted EM120D emulsion is represented in this study by a two-phase mixture of the liquid condensed emulsion and the gaseous void phase, the reaction products are represented by a single gaseous phase.

A starting point for a suitable formulation is the BN model [7,14], which provides a comprehensive description of the material behaviour at the continuum scale, but with significant overhead in terms of computational expense and algorithmic complexity, especially if three phases have to be considered. Even the two-phase version of the BN model is currently undergoing further mathematical and algorithmic development, and has not been extended to accommodate complex equations of state. Reduced versions of the BN model offer a good compromise, if the behaviour of the explosive warrants simplifications.

To make this assessment, we first need to consider a relaxation timescale estimate. Petitpas et al. [12] offer such an estimate for arbitrary explosives, based on the knowledge of the constituents densities, sound speeds, particle sizes and volume fractions. Following the procedure in [12], with representative values for the emulsion explosive EM120D, results in mechanical relaxation times\( \tau \propto 10^{-8} \text{s} \), justifying the use of a single-velocity and single-pressure model.

We note here that emulsion explosives exhibit relatively closer-to-ideal behaviour as compared to other explosives used in the mining industry. Mechanical relaxation times for ANFOs, depending on their prill size and detonation velocity, can range in between\( \tau \propto 10^{-6} – 10^{-7} \text{s} \). In comparison, the mechanical relaxation timescales for granular HMX under detonation conditions was shown to be of the order\( \tau \propto 10^{-8} \text{s} \) [10].

Due to the aforementioned timescales of pressure and velocity relaxation in the emulsion explosives, instantaneous relaxation may be reasonably assumed. Thus a reduced version of the Baer–Nunziato model is adopted in this study, obtained in the limit of stiff mechanical relaxation, which results to a single-pressure and single-velocity multi-phase model, as proposed by Kapila et al. [10].

The following sections outline the model and its adaptation for the explosives of interest. Section 2.1 summarises the previously derived single-pressure and single-velocity multi-phase model. Sections 2.2 and 2.3 complete the model description with the
equation of state and its reaction rate law for the emulsion of interest.

2.1. Single-pressure and single-velocity multi-phase model

The single-pressure and single-velocity multi-phase model with mass transfer can be stated as

\[
\frac{\partial \chi_k}{\partial t} + \nabla \cdot \mathbf{u} = -\chi_k \left( \frac{p c_k^2}{\rho_k c_k^2} - 1 \right) \nabla \cdot \mathbf{u} = \chi_k + \mathbf{H}_k.
\]

(1)

\[
\frac{\partial \rho_k}{\partial t} + \nabla \cdot \rho_k \mathbf{u} = \rho_Y k,
\]

(2)

\[
\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) + \nabla p = 0,
\]

(3)

\[
\frac{\partial \rho E}{\partial t} + \nabla \cdot ((\rho E + p) \mathbf{u}) = 0.
\]

(4)

The subscript \( \chi \) indicates the material to which the value applies, \( \chi_k \) the volume fraction, \( \rho_k \) the density and \( c_k \) the sound speed. The velocity vector is denoted by \( \mathbf{u} \) and the mixture quantities of total energy \( E \), total density \( \rho \) and the Wood sound speed \( c \) are given by

\[
E = e + \frac{\rho u^2}{2},
\]

(5)

\[
\rho = \sum_k \rho_k 
\]

(6)

\[
\frac{1}{\rho c^2} = \sum_k \frac{\chi_k}{\rho_k c_k^2}
\]

(7)

with the mass fraction \( Y_k = \frac{\rho_k}{\rho} \) and internal energy \( e = \sum Y_k e_k(\rho_k \rho_k) \). We neglect the heat transfer between the various constituents due to their small interfacial area and short resident time (i.e. \( H_0 = 0 \)). For big enough particles, the accuracy of this assumption has been demonstrated by Baudin et al. [15]. We note that the definition of specific alphanumeric material indices will be supplied in each section individually.

In order to complete the reactive mass transfer, \( \rho_Y k \), needs to be defined. Initially, this mass transfer will lead to a pressure disequilibrium between the different components, which is mechanically relaxed by means of emission of acoustic waves, thereby affecting the volume fractions of the mixture. The volume fraction source term, \( \chi_k \), based on this assumption was determined previously by Petitpas et al. [16] as

\[
\chi_k = \frac{\rho_Y k}{\rho_k c_k^2} - \frac{\chi_k}{\rho_k c_k^2} \rho c_k^2 \sum_j \frac{\rho_Y j}{\rho_j}.
\]

(8)

Note that the volume fraction source term in this form depends on all the constituents’ densities. The implication is that the model is ill-posed for zero \( \chi_k \) so it is necessary to assign a very small volume fraction \( \chi_k = 1 \times 10^{-8} \), even if a phase is not present. We note that the volume fraction source term was originally derived for phase transition problems, where densities for all constituents (i.e. the liquid and vapour phases) are known. In detonation problems this is not the case; the density of the product gas is not known at the very start of the detonation front, thus a method is suggested to determine a unique reaction product density. The problem and the suggested solution will be discussed in detail in Section 5.

Since the model is not in conservation form, appropriate shock conditions need to be prescribed in order to regularise it [10]. This study employs the shock conditions as derived by Saurel et al. [17] in the limit of weak shocks:

\[
\forall k, \quad Y_k = \frac{Y_k^0}{\gamma_k - 1}.
\]

(9)

\[\rho(u - D) = \rho_0 (u_0 - D) = m,
\]

(10)

\[p - p_0 + \gamma \rho (u - v_0) = 0,
\]

(11)

\[
\forall k, \quad e_k - \frac{\rho_0}{\rho_k} + \frac{\gamma_0}{2} (v_k - v_0^2) = 0,
\]

(12)

where D denotes the shock speed (or detonation speed), the superscript \( ^0 \) refers to the unshocked material. This algebraic model was compared and validated against strong shock data in the same reference.

When compared to the full Baer–Nunziato model [7,14], the set of reduced equations simplifies the wave structure of the Riemann problem and allows for faster numerical multi-phase calculations. Nevertheless, the reduced equations possess numerical challenges which need to be addressed. In particular, the non-conservative volume fraction equation causes difficulty in combination with the non-monotonic sound speed speed behaviour. The velocity divergence term can cause volume fractions to become negative within strong shocks or strong expansion waves and the non-monotonic sound behaviour in diffusive interfaces leads to inaccurate wave dynamics [11].

To overcome these problems, Saurel et al. [11] constructed a pressure non-equilibrium model in combination with a stiff relaxation method. The numerical treatment of the single-pressure and single-velocity multi-phase model will be summarised in Section 3.1.

2.2. Equation of state

For closure, the above system of equations requires an appropriate equation of state (EoS) for every constituent and a reaction rate equation to specify the conversion from reactants and products. This section describes the equation of state for reactants, products and the inert confiner material.

The reactants are described with a Shock-Mie-Grüneisen (SMG) [18] equation of state, the products are represented with a Willansborg (WMBG) equation of state [2] and the inert confiner material is represented by means of a SMG equation of state, or Ideal Gas (IG) in the unconfined case.

All the equations of state employed can be cast in Mie-Grüneisen form, which can be represented in mechanical and thermal form as

\[
e_k(p, v_k) = e_{k,ref}(v_k) + \frac{v_k}{\Gamma_k(v_k)} (p - p_{k,ref}(v_k)),
\]

(13)

\[
e_k(v_k, T) = c_k v T + e_{k,ref}(v_k),
\]

(14)

\[
p_k(v_k, T) = \Gamma_k(v_k) p_k + c_k v T + p_{k,ref}(v_k),
\]

(15)

where \( \Gamma_k(v_k) \) represents the Grüneisen coefficient and \( (p_{k,ref}, e_{k,ref}) \) is a reference curve for pressure and energy.

The simplest EoS, i.e. the IG EoS, is defined through the trivial reference curves:

\[
p_{k,ref}(v_k) = 0,
\]

(16)

\[
e_{k,ref}(v_k) = 0,
\]

(17)

\[
\Gamma_k(v_k) = \gamma_k - 1.
\]

(18)

In the case of the SMG EoS, the reference curves are determined in such a way that the given reference curves lie exactly along the linear shock expression relating particle speed, \( u_p \) and shock speed, \( u_s = c_0 + s u_p \):

\[
p_{k,ref}(v_k) = \begin{cases} 
\frac{c_k^2 (v_k - v^p_k)}{u_s - c_0} & v_k < v^p_k \\
\frac{c_k^2 - c_0^2}{u_s - c_0} & v_k > v^p_k,
\end{cases}
\]

(19)
The term in front of the brackets provides the regressiveness at the end of the reaction with the regression index \( \text{indx} \). The first term in the brackets represents the hot-spot reaction, with the critical pressure \( p_b \), below which reaction fails. The second term in the brackets represents the pressure dependent bulk burning term.

The function \( \alpha_h \) is a switching function. At ignition the hot-spot behaviour dominates \((a_h = 1)\) and then transfers to the bulk burning \((a_h = 0)\). The parameter \( \omega_h \) in \( \alpha_h \) defines the fraction of explosive that burns in the hot-spot process and the constant \( N_p \) prescribes how quickly this transition between both processes takes place. The burn time parameters, \( \tau_h \) and \( \tau_s \), are constants that determine the burn time of the hot-spot \((\times \tau_h)\) and bulk reaction \((\times \tau_s)\), respectively. To allow for different hot-spot burn behaviour, the pressure power dependence, \( N_p \), can be varied.

The method to determine the reaction parameters is presented in Section 7.2. The obtained parameters for the emulsion explosive \( EM120D \) are

\[
\begin{align*}
\tau_h &= 22.0 \text{ } \mu\text{s \ GPa}, & \tau_s &= 20.0 \text{ } \mu\text{s \ GPa}, & p_b &= 1.51 \text{ } \text{GPa}, \\
\text{indx} &= 0.667, & \omega_h &= 0.95, & N_p &= 9.0, \\
N_p &= 1.51.
\end{align*}
\]

### 3. The numerical discretisation procedure

The complete reactive multi-phase problem, given by the equations in Section 2, is solved using an operator splitting approach. The hyperbolic left-hand side part of the system is evaluated by means of a second order of accuracy MUSCL reconstruction scheme, used in combination with the HLLC [24] Riemann solver. The numerical procedure is outlined in Section 3.1.

Since our interest focuses on cylindrical explosive charges, the three-dimensional system is reduced to a rotational symmetric system. The corresponding rotational source terms are derived in Section 3.2. For problems which converge to steady-state (e.g. detonation propagation in rate-sticks), we propose, in Section 3.3, a method based on the detonation frame of reference.

Operator splitting is applied to advance the numerical solution in time. The problem is therefore separated into two hydrodynamic steps, one for each spatial direction and two source term steps. The source terms, reactive and geometrical, are solved with a fourth order Runge Kutta method (RK4) [25], restricted by a maximum time-step estimated by the first order explicit Euler method.

#### 3.1. The algorithm

The numerical solution of the system (1)–(4), together with the equations as listed in the previous section, poses significant numerical challenges which cannot be addressed with standard procedures [13]. The challenges stem from the non-conservative compaction term and the non-monotonic sound speed behaviour with respect to mass and volume fraction. Here we follow the procedure developed in [11] and [12], where the system is expressed as a pressure non-equilibrium model in combination with a stiff pressure relaxation step. The three main steps, necessary to solve the inert part of the pressure non-equilibrium model, are summarised below:

1. **Hyperbolic step:** In the hyperbolic step, the pressure non-equilibrium model is advanced in time.

\[
\frac{\partial \rho_h}{\partial t} + \mathbf{u} \cdot \nabla \rho_h = 0, \tag{27}
\]

\[
\frac{\partial \rho_h}{\partial t} + \nabla \cdot \rho_h \mathbf{u} = 0, \tag{28}
\]

2. **Source term step:** In the source term step, the pressure non-equilibrium model is advanced in time.
\[
\frac{\partial x_k \rho_k e_k}{\partial t} + \nabla \cdot (x_k \rho_k u_k) + x_k p_k \nabla \cdot u = 0, \quad (29)
\]
\[
\frac{\partial p}{\partial t} + \nabla \cdot ((p \rho u) + p) = 0, \quad (30)
\]
\[
\frac{\partial E}{\partial t} + \nabla \cdot ((pE + p) u) = 0. \quad (31)
\]

In comparison to the single-pressure and single-velocity multiphase model of Eqs. (1)–(4), additional partial energies are introduced. In combination with the subsequent stiff pressure relaxation step, it is possible to eliminate the numerically complicated velocity divergence term in the volume fraction Eq. (1).

2. Pressure relaxation step:

Subsequent to the hyperbolic step, the pressure of the different constituents can be in non-equilibrium, so relaxation to a single pressure is necessary. With the exception of shock regions, the pressure relaxation is determined with the following constraint:

\[
\forall k \left\{ E_k(p_k, \nu_k^0) - E_k(p_k^0, \nu_k^0) + p_k(\nu_k^0 - \nu_k) = 0 \right. \quad \text{ where the superscript } ^0 \text{ denotes the initial state and the superscript } ^* \text{ the relaxed state. The interface pressure is chosen to be } p_0 = p^* \text{ as suggested in } [11].
\]

If relaxation is necessary within the diffused shock region, the analytically derived shock conditions [17] are employed. Inside shock regions, the pressure relaxed state is determined by

\[
\forall k \left\{ E_k(p_k, \nu_k^0) - E_k(p_k^0, \nu_k^0) + \frac{p_k^0}{2}(\nu_k^0 - \nu_k^0) = 0 \right. \quad \text{ where the superscript } ^{\text{ref}} \text{ denotes the reference state and the superscript } ^{\text{rel}} \text{ denotes the relaxed state. In this formulation, knowledge of the unshocked state being needed, the system (27)–(31) is thus complemented by the following equations:
\]
\[
\frac{\partial \nu_k}{\partial t} + u \cdot \nabla \nu_k = 0, \quad (36)
\]
\[
\frac{\partial p_k}{\partial t} + u \cdot \nabla p_k = 0. \quad (37)
\]

allowing the Hugoniot poles transport inside the multi-phase shock [12]. Both relaxation systems (32)–(35) are solved with a Newton–Raphson method.

The relaxation constraints also determine the volume fractions \( x_k = (xk) \cdot \nu_k \). Since the partial energies cannot be expressed in conservative form, total energy conservation can be violated. Therefore the partial energies need to be re-initialised to ensure total energy conservation.

In order to distinguish between continuous flow and shock region, a shock indicator is necessary. The detection method employed in [12], based on time variations, is replaced with the shock detection algorithm developed by Toro [24, §14.6.4] as part of an adaptive primitive-conservative scheme and is based on the solution of the Riemann problem. The algorithm reduces the numbers of wrongly identified shocks cells, which in turn increases the stability of the relaxation root-finding procedure.

3. Re-initialisation step:

In the re-initialisation step, the relaxed pressure is recomputed based on the total mixture internal energy \( \rho e \). The volume fractions \( x_k \) and partial volumes \( \nu_k \) determined by the relaxation steps, are applied to the mixture equation of state together with \( \rho e \), determining the pressure of the relaxed state:

\[
\rho e = \sum_k (x_k p_k) \left( e_k^{\text{ref}}(\nu_k^0) - \frac{\nu_k^0}{\gamma_k} p_k^{\text{ref}}(\nu_k^0) \right) \sum_k \frac{\nu_k^0}{\gamma_k}.
\]

Subsequent to the re-calculation of the relaxed pressure, the volume fractions \( x_k \) and partial internal energies \( x_k p_k \nu_k \) are updated with the calculated relaxed state.

This sequence of three steps results in solving the homogeneous part of the pressure equilibrium system (1)–(4). Although the above system holds for an arbitrary number of materials, the case-studies we consider are composed of four material components: the liquid reactant, the gaseous reaction products, void gas and an inert confiner material.

3.2. Rotational symmetry

Since all the three-dimensional computations presented in this study are axisymmetric, the problem can be reduced to a two-dimensional formulation with additional geometric source terms. These source terms arise from the divergence terms in the model, which become apparent once the divergence operator is cast into cylindrical coordinates:

\[
\nabla \cdot A = \left( \frac{\partial}{\partial t} + \frac{1}{r} \right) A + \frac{1}{r} \frac{\partial}{\partial q} A + \frac{\partial}{\partial z} A: (39)
\]

The extra term \( \frac{1}{r} A \) is treated as a forcing (source) term to describe three-dimensional axisymmetric geometries. The source term for the pressure non-equilibrium model on the right hand side of Eqs. (27)–(31) can be written as

\[
s_k(U) = -\frac{1}{r} A = -\frac{u_y}{y} \begin{pmatrix} 0 \\ x_k p_k \\ x_k (p_k e_k + p_k) \end{pmatrix} \quad \text{ with } U = \begin{pmatrix} x_k \\ (x_k p_k) \\ \frac{(x_k p_k)}{\rho} \\ \frac{(x_k p_k)}{\rho E} \end{pmatrix}.
\]

3.3. Shock-following method

In order to perform simulations on a desktop computer that resolve the detonation driving zone (DDZ) with a resolution of the order of 100 grid cells, the calculation cost for cells distant to the DDZ needs to be reduced significantly. This resolution was determined to be necessary in order to predict the detonation velocity to within 10 m/s accuracy [26] (see Fig. 1).

In the case of steady-state detonations, which is the main interest in this study, it is sufficient to capture the flow to the extent of the sonic locus (including an additional buffer region as a precaution), which in turn will reduce calculation times. This could be achieved with traditional methods, like adaptive mesh refinement, but due to the fact that the flow is supersonic (i.e. disturbances cannot propagate ahead of the sonic line), we suggest an adaptive truncation of the computational domain.

The simplification, hereafter referred to as the shock-following method, is implemented in such a way that it automatically traces the detonation shock front in every time step. Based on the DDZ location, the simulation domain will be extended if the leading shock is closer to the domain head than a certain buffer region.
4. Steady-state ZND structure

In this section we derive the system of ODEs describing the structure of a steady-state ZND detonation wave. The motivation is twofold: firstly, the system can be used in order to validate the implemented unsteady hyperbolic model and moreover, the system is used to reduce the time overhead of the reaction rate fitting procedure of the rate law appearing in Eqs. (24), (25).

The system of Eqs. (1)–(4) can be transformed into the detonation frame of reference. The related coordinate transformation is given by $x = D \cdot t - x$ which yields the corresponding transformed differentials:

$$\frac{\partial}{\partial x} = -\frac{\partial}{\partial t}, \quad \frac{\partial}{\partial t} = \frac{D}{Dx} \frac{\partial}{\partial x}. \quad (41)$$

In Section 4.1 we describe the coordinate transformation for a two-phase system, unreacted explosive and reaction products. This system is of particular interest as it allows to validate the reactive part of the unsteady hyperbolic model for ideal detonations. In Section 4.2 we apply the same transformation, but for a steady-state ODE system that is generalised to arbitrary materials. Furthermore, we include front curvature effects, which is particularly useful for fitting reaction rates. The complete temperature non-equilibrium ZND system can be regarded as an extension of the quasi-one dimensional Wood–Kirkwood [5] front curvature model.

4.1. Two-phase ideal detonation

By applying the differentials (41) and (42) to the system of Eqs. (1)–(4) and considering one dimension and two materials, the steady-state ZND structure can be recovered. The system in the detonation frame for two materials may be written as

$$\frac{dY}{dx} = \frac{\dot{Y}}{u}, \quad (43)$$
$$\frac{dp}{dx} = -\rho \frac{du}{dx}, \quad (44)$$
$$\frac{dp}{dx} = -\rho u \frac{du}{dx}, \quad (45)$$
$$\frac{dz}{dx} = K \frac{du}{u} + \frac{pM}{u} \dot{Y}, \quad (46)$$
$$\frac{du}{dx} = \frac{\Gamma (h_2 - h_1) + \rho c^2 \left( \frac{h_1}{h_1 - 1} - \frac{h_2}{h_2 - 1} \right)}{c^2 - u^2} \frac{\dot{Y}}{u}. \quad (47)$$

with $K = \frac{\gamma_2 \gamma_1^{\gamma_1}}{\gamma_1 - 1}$ and $M = \frac{h_2 \gamma_1}{\gamma_1 - 1}$. The subscripts $1$ and $2$ indicate the material to which the value applies, the speed of sound is given by Eq. (7), the enthalpy by $h_k = e_k + p v_k$ and the mixed Grüneisen coefficient by $\gamma = \frac{1}{\gamma_1} + \frac{1}{\gamma_2}$.

The system of Eqs. (43)–(47) is solved between the Von Neumann spike, determined by the System (9)–(12), and the CJ point (defined by $u = c$ and $\dot{Y} = 0$). Values for the Von Neumann spike and the CJ point are obtained through the intersection of Rayleigh line with the Curvass Curve and the Hugoniot of the reactants. The full steady-state ZND solution is then recovered by integrating the system (43)–(47) along the Rayleigh line with a standard ODE solver. This ODE system is identical to the system derived in [12].

4.2. Arbitrary materials with embedded front curvature effects

In order to obtain the ODE system for arbitrary materials with embedded front curvature effects, the system of Eqs. (1)–(4) has to be transformed into cylindrical coordinates. The rotational symmetry allows the elimination of all derivatives in the angular direction, leading to the transformation for velocity times gradient and velocity divergence terms:

$$\mathbf{u} \cdot \nabla = u \frac{\partial}{\partial x} + \omega \frac{\partial}{\partial r}, \quad (48)$$
$$\nabla \cdot \mathbf{u} = \frac{\partial u}{\partial x} + \frac{\partial \omega}{\partial r} + \frac{\omega}{r}, \quad (49)$$

with $x$ being the axis of symmetry and $\mathbf{u} = (u, v, \omega)$ the velocity vector in cylindrical coordinates $(x, \phi, r)$. Subsequently the system is reduced to the centre streamline:

$$\lim_{r \to 0} \omega(r) = 0, \quad (50)$$
$$\lim_{r \to 0} \omega(r) = \frac{\partial \omega}{\partial r} = 0. \quad (51)$$

Finally, the differentials from Eqs. (41), (42) are applied to transform the system into the detonation frame.

The final system for arbitrary materials and embedded front curvature effects along the centre streamline is given by

$$\frac{dY_k}{dx} = \frac{\dot{Y}_k}{u}, \quad (52)$$
$$\frac{dp}{dx} = -\rho \left( \frac{du}{dx} + 2\omega \right), \quad (53)$$
\[ \frac{dp}{dx} = -\rho \frac{di}{dx}, \]  
\[ \frac{dz_k}{dx} = \frac{1}{\bar{u}} \left( K_k \left( \frac{di}{dx} + 2\omega_k \right) + H_k + M_k(\bar{Y}) \right). \]  
\[ \frac{du}{dx} = \frac{2\omega_k c^2 + \Gamma \sum \frac{h \bar{Y}}{\rho} - \rho c^2 \sum \frac{\rho Y_j}{\rho_j}}{\bar{u}^2 - c^2}, \]  
with the corresponding multi-phase term \( K_k \), heat exchange term \( H_k \) and mass transfer term \( M_k(\bar{Y}) \) defined by
\[ K_k = \frac{c g}{\rho_k c_k} \left( \frac{c^2}{\rho_k} - 1 \right). \]
\[ H_k = \left( \frac{Q_k}{\rho_k c_k} - \frac{c g}{\rho_k c_k} \right) \sum \frac{Q_k Y_j}{\rho_j}. \]
\[ M_k(\bar{Y}) = \frac{\bar{u} Y_k}{\rho_k c_k} - \frac{c g}{\rho_k c_k} \sum \frac{\rho_j Y_j}{\rho_j}. \]

Note that the heat transfer terms in the system (52)–(56) are only included for completeness and are not considered in this work.

This extended steady-state ODE system can be used to adjust reaction rates to match the corresponding VOD to inverse charge radius graphs. It is solved between the Von Neumann spike and the generalised CJ point (defined by \( \bar{u} = c \) and \( 2\omega_k c^2 + \Gamma \sum \frac{h \bar{Y}}{\rho} - \rho c^2 \sum \frac{\rho Y_j}{\rho_j} = 0 \) in the absence of heat exchanges), but since the detonation velocity is now front-curvature-dependent, a shooting method is necessary to obtain the ODE solution.

The above steady-state ODE model is not complete. One additional term needs to be supplied to make the solution unique and an extra relationship is necessary for fitting reaction rates. The term necessary to complete the model is the unknown divergence term \( \omega_k \). The term can be derived exactly at the detonation front by geometrical means but its flow dependency behind the shock is undetermined.

Analytical solutions for \( \omega_k \) only exist for very specific input parameters (see e.g. Bdzil [27]). However, various approximate estimates for \( \omega_k \) are available. The two most commonly used approximate estimates, which are also used in this study for the reaction rate fitting, are presented in Appendix A.

The Wood–Kirkwood approach unfortunately does not provide an estimate for the relation between charge radius and front curvature. This relationship is necessary to allow reaction rate fitting to VOD versus inverse charge radius data, as done in this study. This connection can either be supplied through previous experimental results or be determined through a numerical simulation. The reaction rate fitting procedure is discussed in detail in Section 7.2.

5. Volume fraction source term

Considering two materials, namely reactants with subscript \( s \) and products with subscript \( g \), the volume fraction source term, as derived by Petitpas et al. [16] (see Eq. (8)) and later employed in an explosives study [12], depends among, other variables, on the gaseous product density. The reaction term \( \dot{x}_s \) depends on the density of the products even in the limit of \( \dot{x}_s \to 1 \) (i.e. in the absence of products):
\[ \lim_{x_s \to 1} \dot{x}_s = \lim_{x_s \to 1} \frac{\rho \dot{Y}_s}{\rho_s} - \frac{\dot{x}_s}{\rho c_k} \rho c^2 \sum \frac{\rho Y_j}{\rho_j}. \]  
\[ = \dot{Y}_s - \sum \frac{\rho \dot{Y}_s}{\rho_j} = \frac{\rho \dot{Y}_s}{\rho} \dot{Y}_s. \]

Due to this dependency in the limit of \( \dot{x}_s \to 1 \), the product density needs to be uniquely specified at the detonation shock front. There are two obvious choices for the density of the initially non-existent product gases.

One choice is to specify the product density in the ambient explosive such that thermal equilibrium holds amongst all components. This is how we calculate the densities of existing inert materials. The product density at the shock front is then automatically determined through the mixture shock conditions (9)–(12).

This approach is limited in most reactive cases because the thermal behaviour of the detonation product gases is mostly unknown at ambient conditions, as most real gas EoS have limited domains of validity. Another choice is to determine the product density at the shock front based on a constant volume explosion. This approach is generally applicable in practice and is therefore the method of choice in this work.

The volume fraction dependency on the initially chosen product density, \( \rho_k \), in the limit of \( \dot{x}_s \to 1 \) is confirmed by numerically-obtained ZND structures (not displayed here). Although the Von Neumann spike and the CJ point stay the same for ideal simulations, the behaviour within the reaction zone will be different, even in one-dimensional ideal simulations.

5.1. Constant volume approximation

The model needs to be supplied with a physically meaningful and unique way of determining the product density. The assumption made to derive the product density for the reaction rate is based on a constant volume explosion (an instantaneous explosion) of a very small amount of reactants to products with a subsequent pressure relaxation process.

The assumptions expressed in mathematical form for a two-phase system can be summarised as
\[ e_x := e_s, \quad v_x := v_t, \quad p_x := p_t(e_x, v_x), \]
which is applied at the numerical Von Neumann spike. The multi-phase system with condition (62) is in general not in pressure equilibrium. The mechanically relaxed state is found with the relaxation method given in (32), (33) with the conditions (62) determining the initial state.

This constant volume explosion–pressure relaxation procedure is just a “discrete” analogue of the source terms related to mass transfer present in system (1)–(4). It closes this system in the limit \( \dot{x}_s \to 1 \).

Note that, for a heterogeneous explosive with explicit phase representation of the voidage (two-phase reactant consisting of a condensed phase and a voidage phase) the numerical Von Neumann spike is determined by the two-phase shock relations. As this explosive–air mixture represents the reactant phase a constant volume explosion is assumed from the post-shocked mixture to gaseous products. This implies that the energy \( e_x \) and specific volume \( v_x \) in Eq. (62) are given by the energy and specific volume of the two-phase reactant.

6. Test problems and validations

In this section we validate the above model for inert and reactive case-studies. In order to demonstrate convergence of the model at the inert limit, the most commonly studied and published inert multi-phase test cases have been summarised in Table 2 and compared to the results obtained with the current code in Section 6.1. The reactive part of the model is validated in one dimension by comparing the solution of the unsteady hyperbolic model to the solution of the steady-state ODE model in Section 6.2. This is first done for a test case previously studied by Petitpas et al.
[12] and later repeated for the emulsion explosive of interest. The one-dimensional grid convergence study for EM120D is then extended to an unconfined three-dimensional axisymmetric rate stick problem in Section 6.3. The validation section is closed with a comparison between the full domain solution and the developed shock-following method in Section 6.4.

6.1. 1D inert test cases

The numerical solver employed for the system of Eqs. (27)–(38) is first validated using a set of inert multi-phase test case-studies compiled from [12,11] and [13].

The first test is a simple air–water interface advection problem, chosen because it demonstrates that the numerical method does not cause spurious oscillations around material interfaces. These oscillations are also observed in augmented Euler formulations widely used to study detonations, and they have to be rectified by means of an additional procedure [28]. The second and third test cases are air–water shock tubes with different (moderate and extreme) pressure differences. These two tests show that, although the current formulation was developed as a mixture model, it is also capable to deal with material interfaces separating two pure materials even in combination with strong pressure gradients.

The following test cases all involve multi-phase mixtures. The fourth and fifth tests are air–water mixture problems and demonstrate the model’s ability to deal with high density and pressure gradients for mixtures. Case six and seven are mixture test cases involving the materials epoxy and spinel. These are known to be challenging mixture tests, especially for capturing the correct compression (volume fraction) within the shocked region [11].

All the test cases are summarised in Table 2 and the results are presented in Figs. 2–4. An exact Riemann solver is implemented as part of this work, based on the derivation of Petitpas et al. [29]. Comparisons between the exact solution and the numerical solution with 1000 cells are provided in Figs. 2–4 demonstrating a good agreement between numerical and exact solution. In addition it can be observed that the test cases with strong pressure and density gradients as well as material interfaces do not cause computational difficulties.

6.2. Reactive test case – quasi-1D comparison

The reactive part of the numerical solver is validated against the solution of the steady-state ODE model (see Eqs. (43)–(47)) for two detonation test cases.

The first reactive test case is a two-phase stiffened gas detonation problem, as presented in [12]. The second test involves the ammonium-nitrate-based mining explosive EM120D. In both tests, the reference ODE solution is compared to the results of the hyperbolic unsteady model.

The first two-phase reactive test is specified through the stiffened gas parameters for the solid reactant $\gamma_s=4$, $p_{\text{r,s}}=1 \times 10^9$ Pa and the ideal gas parameter $\gamma_g=3$ for the product gases. The corresponding energy release is given as $Q = 3.68$ MJ/kg. The reaction law for the first test only depends on the mass fraction of the reactants, $Y_s = k v Y_t$, with the reaction constant $k = 2 \times 10^6$ s$^{-1}$.

The solution of the steady-state ODE model is illustrated, in both cases, with a blue line, the numerical results at different computational mesh resolutions with: green triangles (fine), red squares (medium) or black dots (coarse). The results for the first reactive test case can be seen in Fig. 5, showing a very good agree-

![Fig. 2](image-url)

Fig. 2. Plots of (from left to right) $\rho$, $u$, $p$ and $s_t$. The top row shows an air–water advection problem (Test Case 1), the bottom row an air–water shock tube with moderate pressure ratio (Test Case 2). The numerical solution is given by red points; the exact solution is displayed as the green line. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)
We estimate that this resolution is sufficient to represent the solution of the steady-state ODE model once the resolution exceeds 1000 cells (i.e. \( \approx 30 \) cells in the ZND reaction zone).

In the second reactive test case, the mining explosive EM120D is considered, with the EoS parameters as in Table 1. Similar to the first reactive two-phase case, a good agreement between steady-state ODE model and full hydrodynamic solution can be observed once the resolution exceeds 15,000 cells (i.e. \( \approx 60 \) cells in ZND zone) (see Fig. 6).

The reason that a higher amount of cells is necessary for EM120D is related to the two-stage reaction behaviour. The initial, faster hot-spot burn is followed by a slow bulk burning process of the ammonium nitrate. Although the slow burning elongates the reaction zone, the steep part of the reaction still needs to be resolved accurately. The resolution of 15,000 cells within a domain length of 1.5 m corresponds to a physical resolution of \( \Delta x_{DP} = 0.1 \) mm. We estimate that this resolution is sufficient to

Fig. 3. Plots of (from left to right) \( \rho, u, p \) and \( \phi \). The top row shows an air–water shock tube with extreme pressure ratio (Test Case 3), the bottom row an air–water mixture problem (Test Case 4). The numerical solution is given by red points; the exact solution is displayed as the green line. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Fig. 4. Plots of (from left to right) \( \rho, u, p \) and \( \phi \). The top row shows an air–water shock mixture problem (Test Case 5), the middle and bottom row show an epoxy-spinel mixture problem (Test Case 6 and Test Case 7). The numerical solution is given by red points; the exact solution is displayed as the green line. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)
achieve convergence in the multi-dimensional simulations but we will provide an additional quantitative comparison in the next section.

6.3. Reactive test case – convergence study

This section provides a qualitative and quantitative comparison between the two spatial resolutions $\Delta x = 0.2$ mm and $\Delta x = 0.1$ mm. The test case under consideration is a cylindrical slab of explosive $D = 20$ mm) surrounded by air. The emulsion is initiated by a high-pressure booster at the end of the charge; the detonation is then allowed to travel twenty times its charge radius to transition to steady state.

The numerical results for total density and reactant volume fraction are shown in Fig. 7. The top half in every contour plot represents the numerical result obtained with the coarser resolution and the bottom half the finer resolution. The two simulations exhibit very similar physical features. Both resolve an ejected, partially burned explosive layer, visible in the density as well as in the volume fraction contour plots. A closer look in the volume fraction plot reveals a thin layer of compressed unburned explosive ahead of the detonation wave (darker red contour), which is also resolved in both simulations. In addition, the contours across the DDZ are virtually identical for both simulations. Nevertheless, some minor differences can be detected; the most pronounced difference being the lag of the less resolved simulation (see Fig. 7). Therefore, a quantitative comparison between the measured detonation velocity (which is a quantity of interest in this study) is done for both numerical resolutions and compared to the results obtained using the shock following method (see Table 3).

The detonation velocity is determined by averaging over the last 500 time steps once the detonation has reached steady state. The error in determining the numerical detonation velocity in Table 3 arises from the uncertainty in peak pressure location to within the width of one computational cell.

The time-dependent VOD, compared to the steady-state VOD, is shown in Fig. 8. The figure demonstrates the numerically observed transition to steady state. In the strong booster ignition case (high-pressure region with unreacted emulsion explosive at an initial pressure of $p = 3$GPa) it can be seen that shortly after ignition, the detonation wave initially runs behind (ignition state), then a little ahead (overdriven state) and then settles quickly to steady state. For the selected rate stick dimension, the steady-state detonation is achieved about 20$\mu$s after initiation, which corresponds to a physical distance of roughly 100 mm, a quarter of the chosen domain length.

Based on the results shown in Fig. 8, the chosen domain length, of twenty times the charge radius, is considered sufficient to transition to steady state before reaching the end of the domain.

The relative experimental errors in VOD are stated by Dremin [30] to be between $\Delta_{\text{rel}}$VOD = 1.0–3.0% depending on the charge radius, which translates in absolute values of the order $\Delta_{\text{abs}}$VOD > 50 m/s. Thus the resolution of $\Delta x = 0.1$ mm can be regarded as sufficient to approximate the explosive within its experimental errors and is chosen from now on for all multi-dimensional simulations in this study.
6.4. Shock-following method

As well as the quantitative comparison of detonation velocities between the full domain simulation and the shock-following method (see Table 3), a comparison for density, pressure and reactant volume fraction contours is provided in Fig. 9. The top half displays magnified results of the full domain simulation, already exhibited in Fig.7 at the last output stage $t = 80 \mu s$ (steady state), which can be compared to the results obtained with the shock-following method in the bottom half.

It can be seen that the domain in the shock-following method is limited to double the DDZ length. Nevertheless, the DDZ region (black dashed line) completely matches the one within the full domain simulation. The same matching behaviour can be found for the interface position of the air confiner (white dashed line). Figure 9, together with the detonation velocity results in Table 3, demonstrates the equivalence of both methods for steady-state detonation waves.

7. Comparison to experiment

The goal of this study is to demonstrate the usability of the presented model, with its modifications, for mining applications.

First, input parameters are fitted to existing experimental data. The emulsion investigated, EM120D, is a typical explosive used in the mining industry and was previously investigated experimentally by Dremin [30] and later numerically by Chan [19].

Shock data is supplied as parameter input for the equation of state of the condensed explosive. The porous unreacted explosive behaviour is predicted by mixing the condensed phase together with air to decrease the mixture density to $q_{EM120D} = 1200$ kg/m$^3$.

The product equation of state is fitted to an ideal detonation code (IDeX) and the kinetics parameters are adjusted to match unconfined velocity of detonation measurements.

Subsequent to the fitting of the input parameters, predictions are made for two different confinement types: concrete and steel.
In addition, a comparison to existing front curvature measurements is done to complete the validation.

7.1. Summary of the Dremin experiments

The experimental results of Dremin [30] were obtained by contract with ICI Explosives Canada. The task was to replicate a research emulsion of ICI explosives and complete various detonation tests.

The research emulsion EM120D, a mixture of ammonium nitrate, water, fuel and emulsifier, had a condensed phase density of \( \rho_c = 1400 \text{ kg/m}^3 \). It was later sensitised with glass micro-bal- loons (hollow glass spheres), which yielded an average mixture density of \( \rho = 1200 \pm 10 \text{ kg/m}^3 \). The ideal detonation velocity, determined with IDex, is \( D_{id} = 6385.35 \text{ m/s} \).

Detonation velocities were obtained for unconfined (paper confinement), concrete confined and steel confined charges. The unconfined tests were accomplished for nine different diameters, ranging from 17–120 mm. The paper casing was produced by gluing layers of paper together with silicate glue, with paper wall thickness in the range of 1.1 ± 0.1 mm. The average unconfined detonation velocity results are summarised in Table 4.

The steel confinement tubes for the small diameter (7–10 mm) were machined from cylindrical steel rods with a stated ultimate strength of \( \sigma_{UTS} = 0.48 \text{ GPa} \). Larger diameter experiments (14–75 mm) were done with weld free steel tubes with a stated ultimate strength of \( \sigma_{UTS} = 0.56 \text{ GPa} \). The thickness of the steel walls were measured to be \( 4.0 \pm 0.3 \text{ mm} \). The corresponding detonation velocities for steel confinement are summarised in Table 5.

Concrete confinement tubes were produced by pouring the cement (27%), sand (54%) and water (19%) mixture in steel moulds. The mixture was allowed to harden over the course of 18 days. The concrete reached its maximum compressive strength (\( \sigma_c = 27 \text{ MPa} \)) after two weeks and did not change after longer hardening periods. The inner diameter for the concrete confinement ranged from 14–120 mm; all concrete tubes had a wall thickness of \( 30 \pm 0.5 \text{ mm} \). The recorded detonation velocities are summarised in Table 6.

Fig. 8. Time dependent VOD \( D(t) \) (blue circles) compared to the determined steady- state VOD of \( D = 4931 \text{ m/s} \) (black line) for charge radius \( r = 20 \text{ mm} \). Transition to steady state is achieved after 20 \( \mu \text{s} \). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Table 4

<table>
<thead>
<tr>
<th>( r ) (mm)</th>
<th>13.5</th>
<th>15.0</th>
<th>18.0</th>
<th>20.0</th>
<th>30.0</th>
<th>40.0</th>
<th>60.0</th>
</tr>
</thead>
<tbody>
<tr>
<td>( D ) (m/s)</td>
<td>4000</td>
<td>4207</td>
<td>4780</td>
<td>4920</td>
<td>5470</td>
<td>5690</td>
<td>5900</td>
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</table>

Table 5

<table>
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<tr>
<th>( r ) (mm)</th>
<th>7.0</th>
<th>10.0</th>
<th>15.0</th>
<th>21.0</th>
<th>27.0</th>
<th>37.5</th>
</tr>
</thead>
<tbody>
<tr>
<td>( D ) (m/s)</td>
<td>4900</td>
<td>5400</td>
<td>5800</td>
<td>5900</td>
<td>6000</td>
<td>6000</td>
</tr>
</tbody>
</table>

Fig. 9. Comparison between full domain simulation (upper half) and shock-following method (lower half). The DDZ was marked in all contour plots with a black dotted line. The pressure plot contains an additional white dotted line which represents the explosive–confiner interface.
Table 6
Velocity of detonation, \( D \), for radii, \( r \), for concrete confined EM120D.

<table>
<thead>
<tr>
<th>Concrete confinement</th>
<th>5</th>
<th>7.5</th>
<th>10</th>
<th>15</th>
<th>20</th>
<th>25</th>
<th>30</th>
<th>35</th>
<th>40</th>
<th>50</th>
<th>60</th>
</tr>
</thead>
<tbody>
<tr>
<td>( r ) (mm)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>( D ) (m/s)</td>
<td>13.5</td>
<td>15.0</td>
<td>20.0</td>
<td>29.0</td>
<td>39.0</td>
<td>4800</td>
<td>5000</td>
<td>5300</td>
<td>5800</td>
<td>6000</td>
<td></td>
</tr>
</tbody>
</table>

The errors in the measured detonation velocity are stated in the report to be between 1% and 1.5% for charges with large diameter and 2–3% for charges near failure. The error in manufacturing the inner tube radius for unconfined and steel confined charges are given as \( \Delta r < 0.05 \text{ mm} \); for concrete confined charges, \( \Delta r < 0.1 \text{ mm} \).

The equation of state parameters used for steel and concrete in this study were chosen in accordance with the previous ICI study by Chan [19], which also analysed the same experimental data. The EoS parameters are summarised in Table 1.

In addition to velocity of detonation measurements, front curvature measurements were taken for the unconfined, as well as for the concrete confined, charges. The front shapes were obtained with a high speed streak photograph. The test charges length for front curvature measurements were equal to 5–6 times their diameters; the resolution time of the camera was stated by Dremin [30] to be 0.015 \( \mu \text{s} \). The streak pictures of the breakout are fairly rough (see Fig. 16), thus Dremin supplied smoothed outlines in order to analyse the data. This roughness is claimed to be due to the intrinsic heterogeneity of the explosive. The smoothed data, as stated in Dremin’s report [30], is supplied for the unconfined explosive in Table 7 and in the concrete confined case in Table 8. Since the detonation front in steel confinement is fairly flat, no detailed front curvature information was provided in the report.

7.2. Reaction rate fitting procedure

The commonly-used procedure for determining the reaction rate parameters in the rate law Eq. (26) for steady-state detonations, is to fit the parameters to experimental VOD and front curvature data. The parameters are determined by reverse engineering of the VOD data with a Wood–Kirkwood type model [31]. There are two drawbacks in this approach:

1. the front curvature data is not available for the majority of mining explosives;
2. an estimate of the velocity divergence term, \( \omega_s \), is necessary, and this is not known \textit{a priori}.

To rectify these drawbacks we adopt in the present work a different fitting procedure that only makes use of the unconfined VOD data for EM120D from Dremin [30]. The front curvature vs charge radius data can be recovered from the unsteady numerical code, which provides the numerical solution to the System (1)–(4). The final parameters were obtained by running this unsteady numerical code with a set of initial parameters and by reverse engineering the reaction rate as described below. Since the fitting was done manually, the parameters \( \text{indx} = 0.667 \) and \( N_p = 9.0 \) were used in the fitting procedure. The remaining parameters, \( \tau_s, \tau_p, p_s \), and \( N_p \) were then adjusted to match the experimental data points within their error limits.

The recursive fitting process described here takes advantage of the speed of the steady-state code, which provides the solution to the system (52)–(56); the complete procedure can be summarised as follows:

1. \textit{Adjust reaction rate parameters:} In the first iteration, a guess is made of the initial reaction rate parameters. Subsequent iterations take the parameter estimates from the steady-state code.
2. \textit{Run the unsteady numerical code:} In this step, the unsteady model is evaluated with the latest parameter set and the results compared to the experimental data. When the numerical results qualitatively fit the experimental data, the recursive procedure can be stopped and the final parameters found. If the current iteration is not accurate enough, we extract the front curvature vs charge radius relationship from the numerical results to supply to the steady-state code.
3. \textit{Supply front curvature vs charge radius relationship:} The relationship between front curvature and charge radius, a necessary input to the steady-state ODE model, can be updated with the latest prediction from the unsteady numerical code. Without this relationship the steady-

Table 7
Front curvature data extracted from [30] for unconfined detonation. The first column identifies the experiment with different charge radii, the following columns give detonation front arrival times (\( \mu \text{s} \)) at certain distances (mm) away from the charge axis.

<table>
<thead>
<tr>
<th>( r ) (mm)</th>
<th>Distance from charge axis (mm)</th>
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<tbody>
<tr>
<td></td>
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</tr>
<tr>
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</tr>
<tr>
<td>20</td>
<td>0.04</td>
</tr>
<tr>
<td>30</td>
<td>0</td>
</tr>
<tr>
<td>40</td>
<td>&lt;0.01</td>
</tr>
<tr>
<td>60</td>
<td>&lt;0.01</td>
</tr>
</tbody>
</table>

Table 8
Front curvature data extracted from [30] for detonation in concrete confinement. The first column identifies the experiment with different charge radii, the following columns give detonation front arrival times (\( \mu \text{s} \)) at certain distances (mm) away from the charge axis.

<table>
<thead>
<tr>
<th>( r ) (mm)</th>
<th>Distance from charge axis (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
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<td>&lt;0.01</td>
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<td>60</td>
<td>&lt;0.01</td>
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</tbody>
</table>
state code could only predict the detonation velocity vs front curvature relationship. The front curvature vs charge radius relationship for the final kinetic parameters is shown in Fig. 10.

4. **Run the steady-state code:** The objective of this step is to bound the reaction parameters by using the lower and upper limit estimates for $\omega_r$ (see Appendix A) in the steady-state numerical code. This means that the parameters are adjusted and the steady-state code is run until the area between the upper and lower estimated VOD graphs contain the experimental data points. The overall fitting procedure is accelerated, since the steady-state code can be run within seconds on a desktop computer. The estimated parameters are then supplied to the unsteady numerical code (step 1). The numerical VOD results obtained with the final fitting parameters, together with the lower and upper steady-state approximations are shown in Fig. 11.

![Fig. 10. Front curvature vs charge radius graph including fit of analytical function (green) to numerical results (red points). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)](image1)

![Fig. 11. Reaction rate fitter graph (blue line) together with experimentally measured VOD (blue bars). The upper limit steady-state solution (flexible $\alpha_r$, red dotted line) together with the lower limit steady-state solution (constant $\alpha_r$, orange dotted line) are added to demonstrate the fitting recursion process. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)](image2)

By following this iterative process, a final set of reaction parameters can be found after 3–5 iterations, depending on the experience of the user, thus saving many computations with the expensive, but more accurate, unsteady numerical code.

7.3. **Concrete and steel confinement**

One of the objectives for this model is to be able to simulate mining type explosives; that is, it should be able to predict the VOD graph of confined explosives within, or close to, the experimental error after the kinetic decomposition rate parameters have been adjusted in the model. Ultimately, it is desirable to be able to reproduce most of the available experimental evidence as accurately as possible.

All of the numerical experiments presented hereafter are accomplished at a spatial resolution of $\Delta x = 0.1$ mm (see Section 6.3). The length of the rate-sticks are chosen to be $l = 20r$, with $r$ being the explosive charge radius. The emulsion explosive is initiated by introducing a booster region at the left edge of the stick, modelled as an unreacted emulsion explosive at an initial pressure of $p = 3$ GPa. This setup was efficient in reaching a quick transition to steady state, as the detonation is initially overdriven and decays swiftly to its natural detonation state as described in Section 6.3. The steady-state detonation is usually reached after $t_{steady} \approx 5 \tau$ (see Fig. 8). In addition, it is checked that the detonation velocity is constant over the last 500 time steps.

In order to determine the numerical detonation velocity, line-outs from the centre streamline are provided and the average velocity of the pressure peak is calculated. The experiments are repeated at the exact same radii as chosen by Dremin, but with additional radii to allow plotting of smooth continuous curves in the VOD graph. The VOD curves in Fig. 12 are based on approximately 10 different radii runs.

Modelling the experimental setup in its full complexity is generally not possible but it is in our interest to eliminate possible side effects on the final results. We ensure that the fitting quality of the kinetic parameters is unaffected by the paper confinement chosen for the experiment. It is known that cardboard beyond a certain strength or thickness can affect the velocity of detonation measurements [32], thereby affecting the adjustment of the kinetic parameters. The paper confiner is represented by an inert material.
layer with density $\rho_{\text{paper}} = 500 \text{ kg/m}^3$ and thickness of $T_{\text{paper}} = 1.1 \pm 0.1 \text{ mm}$. The qualitative difference for the $r = 15 \text{ mm}$ charge can be seen by comparing the contour plots of air confinement (see Fig. 13a) and cardboard confinement (see Fig. 13b). The difference in the velocity of detonation measurements can be seen in Fig. 12 (air confinement (red), paper layer (dashed pink)). Based on the results observed in Fig. 12, the effects of the paper layer on the kinetic parameters are considered negligible in this instance.

The confined charges are run with infinite confiner thickness and the material parameters for the confiner are the same as those used by Chan [19]. The confined experiments were repeated but with a finite confinement with the same thickness as stated in the original report [30]. As can be seen in Fig. 12, the inclusion of finite confinement effects does not affect the velocity of detonation in this particular setup. Comparing both scenarios for steel in Fig. 13 shows that the reflected wave from the exterior wall does not interact with the DDZ inside, that intrinsically drives the detonation. This agrees with the lack of an observed effect on the VOD results in Fig. 12. As can be seen in Fig. 12, the numerical prediction for concrete confinement is very good. The steel confinement is also predicted very well, except for the two very small radii.

We believe that the VOD discrepancy is caused by the two different steel types having slightly different ultimate strengths. Evidence to support this assumption is that the numerically predicted VOD is higher than the experimentally observed VOD, which is consistent with this notion, since the numerical confiner represents a "stronger" material than it actually is. Another possibility is that the fluid model for the confiner material is too simplistic, and no longer applicable at small charge radii.

In addition to the VOD measurements, the qualitative difference between different confiner types is summarised in Fig. 13. As expected, the biggest expansion can be seen in the unconfined case, thus leading to the smallest detonation velocity. In the cardboard confinement, the shock transmitted in the confiner material can be seen, but the effects on the detonation driving zone are negligible, as mentioned above. The concrete confinement, in comparison, not only has a smaller interface deflection angle, but the effect on the detonation front, of a smaller curvature, is clearly visible. This effect is even more pronounced in the case of steel confinement. The confiner effect on the DDZ is also clearly visible, ranging from a convex lens type shape (unconfined) to a semi-convex shape (concrete) to an almost flat shape (steel). The confinement in steel and concrete, which results in high pressure within the explosive (even at a charge radius of $r = 15 \text{ mm}$), leads to an almost complete burn process at the end of the domain (double DDZ length). In contrast, air confinement at the same charge radius leaves behind around 10% unburned emulsion by weight at the same distance behind the front, which continues burning slowly since pressures are reduced down to approximately $p = 1 \text{ GPa}$.

In addition to the VOD data, Dremin also reported on front curvature measurements for the unconfined and the concrete confined emulsion explosive. Front curvature data can be obtained from the numerical results by extracting the highest pressure region along the front, shortly before the detonation reaches the
end of the domain. A comparison with the unconfined front curvature measurements of Dremin is shown in Fig. 14. The x-axis is perpendicular to the centre streamline, thereby representing the distance from the centre. The y-axis is along the centre streamline and provides the time difference between first breakout in the centre (t = 0) to breakout at the distance x from the centre. It is worthwhile mentioning that these results were obtained by simply adjusting the kinematic parameters to represent the correct VOD versus inverse radius relationship for the unconfined detonation.

The front curvature comparison with the unconfined data shows very good agreement, especially at smaller diameters; the larger diameter numerical experiments have a stronger lag, as compared to experiment. The concrete confined case exhibits a smaller detonation front curvature, as expected from a stronger confinement material. For small radius charges, experimentally observed lags can be half the timing compared to the unconfined case. The numerical prediction again matches the experimental data points well. The experimentally observed fluctuation in timing locations (e.g. r = 15 mm (exp)) seems to be greater than the difference between experimental data points and numerical simulation.

Furthermore, not much information is known about the smoothing algorithm applied by Dremin [30] or about the exact experimental procedure used in taking the front curvature streak pictures, thus the overall agreement is considered reasonable. A direct comparison between the experimentally recorded front curvature shape and the numerically obtained arrival times is shown in Fig. 16. The numerical prediction in the bottom half was coloured grey to allow easier identification. The rough structure of the front, as mentioned by Dremin, can be attributed to the heterogeneity of the explosive. The edge between explosive and confiner can be clearly seen in the numerical and experimental picture, despite the roughness. Both front structures are in good agreement, as already seen in Figs. 14 and 15. Obviously the numerical results will not exhibit the roughness shown in the experiment since it does not model the heterogeneities explicitly. Note that this case corresponds to the red coloured data set in Fig. 15 except that experimental data is scanned and smoothed for analysis and the numerical contour does not contain the shock in the confiner.

8. Conclusions

A single-pressure, single-velocity multi-phase model is employed for the numerical simulation of an explosive emulsion used in the mining industry. Analysis of the model revealed a dependency on the initial product density, unknown at the very start of the detonation front. To rectify this problem, we implemented an extension of the model, based on a constant volume explosion approximation, which allows an instantaneous conversion of a small amount of explosive to product gases, thus determining a unique density at the shock front. In addition, we presented a shock-following method to reduce the computational costs for steady-state calculations within an unsteady numerical code.

The model and the associated numerical method can accommodate complex equations of state, and can cope with strong density and pressure gradients, which are an essential requirement for this class of problems. Numerical results (validated against experimental data) from the modified model show that it can reproduce confined VOD experimental data (for concrete and steel) solely by adjusting the reaction kinetics to unconfined VOD experimental data (with no adjustment of any free parameters for the model or the numerical method), thus being truly predictive. Furthermore, the model can match experimental front curvature measurements without any further adjustments, which is also useful for improving reduced (ODE-based) formulations.

An improved iterative fitting procedure for steady-state detonations kinetics was also presented. The steady-state code is used to provide new parameter estimates while the unsteady code is used
to ensure accuracy of those parameters. The combination of both approximations can thus reduce the costly unsteady code iterations to a minimum, while keeping the accuracy of the parameter fit.

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Appendix A. Divergence term $\omega_r$ estimates

The divergence term $\omega_r(z)$ can be obtained exactly on the detonation front [33] through geometrical arguments:

$$\omega_r(0) = \frac{D - u(0)}{R} = \frac{\bar{u}(0)}{R}. \quad (A.1)$$

Determining the divergence term exactly behind the detonation front is only possible for special cases and has not been solved for the arbitrary case. If one wants to keep the simplicity of an ODE system further approximations need to be made concerning the divergence term. One assumption commonly made is to keep the divergence term constant along the centre streamline:

$$\omega_r(z) = \omega_r(0) = \frac{D - u(0)}{R} = \frac{\bar{u}(0)}{R}. \quad (A.2)$$

This corresponds to the assumption that the divergence term on the centre streamline some distance $z$ behind the front is equivalent to the divergence term at the same distance $z$ behind the front but off-axis enough to be on the curved shock front [33]. This assumption can be regarded as an upper limit of losses in the unconfined case, since usually the highest losses occur at the shock front and decrease with distance away from the shock front.

A different approximation can be obtained by comparing the detonation in slab geometry with a spherical detonation. Neglecting the unsteady terms of the spherical detonation in the limit of large radii leads to a $z$-dependent expression for $\omega_r(z)$ [33]:

$$\omega_r(z) = \frac{D - u(z)}{R} = \frac{\bar{u}(z)}{R}. \quad (A.3)$$

This approximation is quite similar to the constant approximation with a particle velocity dependency. The expression will always be smaller than the constant approximation and can be used as a lower loss limit in the unconfined case.

Both approximations have been used in this study for adjusting the reaction rate as they give a good approximation for the lower and upper detonation velocities expected with a certain reaction rate.

References