Multiphysics modeling of the initiating capability of detonators

Part I: The underwater test

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Detonators are explosive devices used for the initiation of secondary explosives in commercial and military applications. They are characterized by their initiating capability which is a critical factor for their safe and effective use but challenging to assess accurately. In this two-part study, we employ numerical simulations to investigate the blast wave generated by detonators and examine their initiating capability. The first part, presented here, follows the European underwater test of initiating capability which evaluates detonators in isolation (direct method) and the second part considers detonators placed within a receiving explosive charge (indirect method). In the underwater test, the detonator is ignited inside a water tank and the initiating capability is assessed through pressure measurements in the far field.

We employ a multiphysics methodology that allows the use of distinct mathematical models for each component such as two-phase reactive materials, elastic-plastic solids, and inert fluids. The computational implementation is validated against underwater experiments and is employed for the simulation of the blast wave generated by different types of detonators. The initial focus is on the general characteristics of the blast wave and subsequently on the differences between detonators of different shell material and thickness. Results show that the blast wave in the near field is asymmetric and varies significantly between detonators, but these features do not persist in the far field. The underwater test considers only the far field and is thus unable to capture the near field differences which have a significant impact on the initiation of secondary explosives.

Keywords: detonator initiating capability, booster devices, shock desensitization, numerical simulation, condensed-phase explosives, elastic-plastic solids

I. INTRODUCTION

Detonators (or blasting caps in mining terminology) are devices used to ignite insensitive explosive charges. They contain small quantities of sensitive high explosives and are designed to generate a shock wave that grows into a detonation in the secondary explosive. One of the first versions of a detonator was invented in 1864 by Alfred Nobel when he observed that a small quantity of a powerful explosive in a metal cup provided a more reliable and effective method for detonating nitroglycerin than simply using a flame¹.

In modern applications of explosives, safety concerns have led to the use of increasingly more insensitive explosives. To ensure their reliable ignition without requiring large quantities of sensitive explosives, a procedure called *explosive initiation train* is employed. This makes use of multiple explosives of decreasing sensitivity in increasing quantities. The sensitive explosives are used in small amounts, just enough to ignite a larger charge of a less sensitive explosive, and thus minimize the impact of an accidental ignition when not in use. Modern initiating trains can be either two-step, involving a detonator and the bulk explosive or three-step that also includes a booster between the detonator and bulk explosive. Three-step trains are commonly used in mining to initiate blastholes filled with a mixture of Ammonium Nitrate and Fuel Oil (ANFO) which has very low sensitivity and cannot be ignited by a detonator alone.

A standard detonator has a cylindrical metal shell which is commonly made out of aluminum, copper, steel or an alloy. The shell contains two different explosives, a small sensitive primary charge called primer and a larger, less sensitive explosive called base charge. In commercial detonators, the most commonly used explosives are Lead Azide for the primary charge and Pentaerythritol Tetranitrate (PETN) for the base charge. The initiation of a detonator begins with a small, non-explosive impulse such as heat, impact or friction to ignite the primary explosive which then detonates the base charge. This generates a shock wave in the metal shell which is transmitted into the explosive outside and ignites it.

Detonators used in mining operations are broadly classified into three types. These are non-electric, electric and electronic detonators. The non-electric detonators use a hollow plastic tube coated with explosive (shock tube) to deliver a low energy impulse to the detonator which makes them invulnerable to stray electrical currents and radio frequencies. Electrical detonators apply current to ignite an electric fuse that initiates the primary charge whereas electronic detonators are similar but have integrated circuits to receive commands and control the initiation time. Electric and electronic detonators have timing precision in the order of milliseconds. Applications with higher accuracy requirements use exploding bridgewire detonators which apply a larger current to a thin wire that explodes to ignite the base charge directly and can have nanosecond precision. Lastly, one of the latest developments in detonator technology is the use of a laser pulse to initiate the base charge which provides enhanced safety and reliability as well as high precision.

The reliable and efficient initiation of explosives is a matter

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of critical importance for the safety of explosion sites. In mining operations, a failure in the initiation of a blasthole filled with explosives will pose a severe post-blast hazard whereas an inefficient initiation may lead to partial detonation with unpredictable outcomes. In addition, initiation failures cause significant financial cost and delays especially in operations that involve time-critical processes such as the sequential detonation of multiple blastholes designed to increase the efficiency of rock blasting.

There is continuous research and development on detonators driven by strict safety requirements, increasing environmental concerns, cost and efficiency. Over the years, detonators have become more elaborate devices and a large range of detonators are currently produced to suit different applications. Historically, the base charge has been considered the only factor related to the initiating capability which is why the industry usually classifies detonators based on the type and quantity of the included explosive. Evidently the detonation characteristics and energy output of the base charge play a major role in initiating the surrounding explosive, but aspects such as the primary explosive, the use of a confining cup, the material and design of the outer shell also influence the initiating power of a detonator^{2,3}. However, the impact of each of these aspects on its initiating capability and the mechanisms by which they influence it are not fully understood.

The expanding range of available detonator devices has increased the need for standardized test procedures to assess and compare the performance of detonators. This subject has been explored by the explosives community for more than a 100 years and several tests have been devised but there has not been a clear consensus on an effective and practical test that reliably correlates with the initiating capability of the detonator. This is because initiation efficiency depends on multiple aspects of detonator design as well as on the characteristics of the receiving explosive charge and it cannot be represented by a single measurable parameter⁴.

Hall and Howell¹ classified detonator tests into direct and indirect methods. Direct methods measure the mechanical effect of the detonator directly, without inserting it into the explosive that is meant to initiate. The detonator is usually placed in sand, water or next to a metal plate and its effect on the surrounding material is measured. Direct tests are simpler and cost-effective but have shown contradictory results and have no proven correlation with the initiating capability of detonators^{4,5}.

Indirect methods place the detonator within an explosive and the configuration is tested as a whole. The surrounding explosive is a mixture of adjustable sensitivity such as Trinitrotoluene (TNT) and iron oxide⁵ or liquid Nitromethane and 2-Nitropropane⁴. The test procedure aims to determine the least sensitive explosive mixture that the detonator can initiate based on a specified criterion for assessing whether the explosive has detonated. Since these tests involve the actual initiation of an explosive, they are considered superior to direct tests. Indirect tests should be preferred for the assessment of initiating capability and also be used to verify direct tests.¹

Despite lasting concerns about the suitability of direct tests

in assessing the initiating capability of detonators, one of the most widely used tests is the direct underwater test specified in the European standard EN 13763-15:2004⁶. This test places the detonator inside a water tank and uses a pressure gauge to capture the generated blast wave and determine the total energy output of a detonator. The energy is calculated as the sum of the energy of the shock wave and the energy of the gas bubble oscillations. These are calculated based on measurements of pressure over time at a distance of 400 mm from the detonator and use expressions originating from the classical work of Cole on underwater explosions⁷. The results are compared to reference detonators of given characteristics to determine the initiating capability of the detonator.

Orica, a leading manufacturer of mining products including detonators, underwent an effort to determine the energy output of its detonators according to the underwater test of the European standard⁸. They used the detonators of varying mass of PETN base charge and different shell material as well as the reference detonator 4⁶. Their results show that the total energy output increases monotonically with the mass of the explosive charge and that detonators made from different shell material have similar shock energy but different bubble energy. The shock energy of all considered detonators was equivalent to the reference detonator but the bubble energy was 5% lower for the copper/zinc detonator and 14% higher for the aluminum detonator compared to the reference detonator. It also reports that previous experimental studies, which assessed the initiating power of detonators using different tests, have shown that the initiating capability of copper detonators is less than that of the corresponding aluminum detonators. However, the reasons behind this discrepancy are not known and the significance of the bubble energy in determining the initiating capability has not been shown.

The widespread use of the European underwater test provides the necessary standardization for comparing detonators but its appropriateness for assessing the initiating capability of detonators has not been established. Fundamentally, the initiation of an explosive by a blast wave is a complex interplay of shock strength, duration and geometry⁹. Historically, the shock energy output of the detonator has been associated with criteria used to determine the initiation threshold of explosives¹⁰. However, this corresponds to the blast wave right next to the detonator where the explosive is placed (near field). The European standard test examines the blast wave at a distance of more than 100 times the radius the detonator (far field) where the near field characteristics of the blast wave have decayed. At large distances, the blast wave becomes spherical and eventually degenerates to a near acoustic wave independent of the nature of its source¹¹. In addition, the initiation of a heterogeneous explosive requires a blast wave strength above a certain shock threshold regardless of the shock energy⁹ which cannot be determined by examining the blast wave in the far field. Moreover, while the connection of the shock wave energy with the initiation threshold of an explosive is evident, there is no such connection for the bubble energy. This process has a much slower timescale than the initiation process and there are no empirical or theoretical arguments for its influence on the initiation of an explosive.

The accurate characterization of the initiating power of detonators requires consideration of the blast wave generated in the near field in its full extent, not only at a single point. This can be accomplished with optically-based tests that use high-speed imaging and are able to capture the blast wave in the near field³. However, the obtained data are of shock radius over time and additional quantities (such as shock pressure) are determined based on empirical expressions, whereas the flow state behind the shock cannot be determined.

Numerical simulations can provide the complete picture of the blast wave which includes all flow state parameters at any point from the detonator. The wealth of data provided by computer simulations is particularly useful in the assessment of the initiating capability of detonators since the complexity of the subject requires the consideration of several characteristics of the blast wave that are often not captured by experimental setups. The peak pressure, duration and decay rate of the blast wave in the near field are needed to determine if the generated impulse exceeds the initiation threshold of the explosive. Also important is to consider the directional variation which has been shown to cause differences in the initiating capability of detonators depending on their orientation⁴. Lastly, the availability of complete data on the formation and expansion of the blast wave enables the extraction of more characteristic quantities that can be potentially related to the initiating power of detonators. Indirect tests can be used to examine the applicability of such quantities which will provide a reliable and proven method for assessing the initiating capability through a direct test.

The work presented here is the first part of a two-part numerical study on the initiating capability of detonators and how it is influenced by the shell of the detonator. The first part considers the blast wave generated by detonators underwater following the test described in the European standard. Initially, we examine the nature of the blast wave generated by the underwater explosion of a detonator in the near and far field. Results show the asymmetry of the blast wave in the near field as well as how it decays and transforms into a spherical wave in the far field. Subsequently, the study considers the effect of shell material and thickness on the blast wave strength. It is shown that while the far field measurements are not considerably affected, the blast wave in the near field has significant differences between shells which are expected to impact the initiating capability of the detonator. The second part of this work¹² will examine the initiating capability of detonators when placed within an explosive charge. In particular, the detonator is placed inside a booster device which follows the typical configuration of a three-step initiation train. The aim is to examine the initiating capability of detonators through the setup of an indirect test which includes the explosive that the detonator is intended to initiate. This provides further insights into the effect of the shell on the initiating capability of detonators and allows to relate the variation of the generated blast wave with the actual ability to ignite the explosive of the booster.

The numerical simulations employ a multiphysics methodology which allows for the use of separate governing equations and accurate material models to represent the physical

system. The base charge of the detonator is PETN, commonly used in commercial detonators, and is modeled with a two-phase reactive formulation with distinct equation of state (EOS) for reactants and products. The PETN in the detonator is porous due to the manufacturing process which involves pressing the explosive into the detonator shell up to a specified compacting pressure. This influences the explosive properties of the base charge and thus, the reactants EOS has been extended with a porosity model along with a calibration of the products EOS to match the experimental values for the PETN porosity considered in this study. The metal shell of the detonator is modeled with the elastic-plastic formulation for solids and the surrounding water is modeled as an inviscid fluid with the stiffened gas EOS.

The mathematical formulation is presented in the following section and the numerical methods used for their solution along with the problem setup are presented in section III. Validation test cases are shown in section IV where the underwater detonator configuration is validated against the experimental study of Klapötke et al.¹³ that follows the European standard test. Results on the nature of the blast wave generated by the detonator and variations between the considered detonator types are presented in section V followed by the conclusions in section VI.

II. MATHEMATICAL FORMULATION

The physical system considered in this study involves several physical processes occurring in materials with different properties. The explosive inside the detonator undergoes chemical reactions that transform solid reactants to gaseous products. The shell of the detonator is metal and is subjected to elastic and plastic deformation, while the whole device is submerged in liquid water where a blast wave is generated. To accurately capture the physical behavior of these materials, we employ the multiphysics methodology by Michael and Nikiforakis¹⁴ which allows the use of distinct mathematical models for each material and provides appropriate coupling methods to model their interaction.

The mathematical models include a multiphase hydrodynamic formulation which is used to model the explosive as a two phase reactive material and the water as a single phase compressible material. The metal materials are represented with an elastic-plastic formulation which accounts for material strength. The multiphysics methodology involves the formulation of all systems of equations in an Eulerian framework which allows for their independent solution on the same fixed mesh. The rest of this section presents an overview of the mathematical models whereas the numerical methods used for their solution are presented in section III.

A. Multiphase hydrodynamic model

The mathematical model used to represent the explosive and water is the hydrodynamic, multiphase formulation by Michael and Nikiforakis (MiNi16)¹⁵. It is a hybrid diffuse

interface formulation, which can model one reactive and one inert hydrodynamic material but can be extended to include additional hydrodynamic materials. The reactive material is further divided into two phases which allows for modeling the explosive with two distinct equations of state, one for reactants and one for products. The formulation is reduced to a simpler set of equations if only one of the materials is present. These are the augmented Euler approach for two-phase explosives if only the reactive material is present and the inviscid Euler equations if only the inert material is present. The setup of the simulations performed in this study does not lead to contact between the explosive and water which are always separated by the metal components of the detonator. Thus, there is no region of diffused interface forming between them and the two materials are essentially represented by reduced versions of the multiphase model.

The hydrodynamic model is defined by the following system of equations

$$\begin{aligned}
 \frac{\partial z\rho_1}{\partial t} + \frac{\partial z\rho_1 u_k}{\partial x_k} &= 0, \\
 \frac{\partial (1-z)\rho_2}{\partial t} + \frac{\partial (1-z)\rho_2 u_k}{\partial x_k} &= 0, \\
 \frac{\partial \rho u_i}{\partial t} + \frac{\partial (\rho u_i u_k + p\delta_{ik})}{\partial x_k} &= 0, \\
 \frac{\partial \rho E}{\partial t} + \frac{\partial (\rho E + p)u_k}{\partial x_k} &= 0, \\
 \frac{\partial z}{\partial t} + u_k \frac{\partial z}{\partial x_k} &= 0, \\
 \frac{\partial z\rho_1 \lambda}{\partial t} + \frac{\partial z\rho_1 \lambda u_k}{\partial x_k} &= z\rho_1 \mathcal{R},
 \end{aligned} \tag{1}$$

where Einstein notation has been used. It features two continuity equations which represent the discrete conservation of mass for each material as well as conservation laws for the momentum and energy of the mixture. Quantities ρ_1 and ρ_2 correspond to the density of the explosive and the inert material respectively. Quantities ρ , $\mathbf{u}$, p and E are the mixture density, velocity, pressure and total specific energy defined as $E = e + \frac{\|\mathbf{u}\|^2}{2}$, where e is the specific internal energy of the mixture. The composition of the mixture is determined by the quantity $z \in [0, 1]$ which represents the volume fraction of the explosive and $\lambda \in [0, 1]$ which is the mass fraction of the reactants. The source term $\mathcal{R}$ is the reaction rate that governs the conversion from reactants to products.

A diffuse interface formulation allows for the materials to mix which requires the definition of a set of mixture rules. These rules relate the thermodynamic variables of the mixture to those of the individual constituents and are given by

$$\begin{aligned}
 \rho &= z\rho_1 + (1-z)\rho_2, \\
 \rho e &= z\rho_1 e_1 + (1-z)\rho_2 e_2, \\
 \frac{1}{\rho_1} &= \lambda \frac{1}{\rho_a} + (1-\lambda) \frac{1}{\rho_b}, \\
 e_1 &= \lambda e_a + (1-\lambda) e_b,
 \end{aligned} \tag{2}$$

where quantities with subscript 1 and 2 correspond to the explosive and the inert material respectively and subscripts a and

b denote quantities of the reactants and the products that comprise the explosive. The formulation allows for each material to have a distinct equation of state (EOS), $e(\rho, p)$, but closure conditions are required for the thermodynamic state to be fully determined. These are selected to be pressure equilibrium between the explosive and inert material, for better stability at the interfaces¹⁶, and pressure and temperature equilibrium between the reactants and products as in similar studies^{17–20}.

B. Elastic-plastic model

The metal confining materials are described by an elastic-plastic model for solids based on the Godunov-Romenskii formulation²¹. In contrast to the traditional Lagrangian description of solid mechanics, this formulation presents the equations in an Eulerian frame and conservative form. This allows for their solution using Finite Volume Methods (FVM) as done for the hydrodynamic equations and the seamless incorporation of this formulation into the multiphysics methodology used in this study. The model is defined by the following system of equations

$$\begin{aligned}
 \frac{\partial \rho}{\partial t} + \frac{\partial (\rho u_k)}{\partial x_k} &= 0, \\
 \frac{\partial (\rho u_i)}{\partial t} + \frac{\partial (\rho u_i u_k - \sigma_{ik})}{\partial x_k} &= 0, \\
 \frac{\partial (\rho E)}{\partial t} + \frac{\partial (\rho u_k E - u_i \sigma_{ik})}{\partial x_k} &= 0, \\
 \frac{\partial \rho F_{ij}^e}{\partial t} + \frac{\partial (\rho u_k F_{ij}^e - \rho u_i F_{kj}^e)}{\partial x_k} &= -u_i \frac{\partial \rho F_{kj}^e}{\partial x_k} + \mathcal{P}_{ij},
 \end{aligned} \tag{3}$$

where

$$F_{ij} = \frac{\partial x_i}{\partial X_j} = F_{ik}^e F_{kj}^p,$$

and Einstein notation has been used.

The first three equations represent the conservation of mass, momentum and energy as in the hydrodynamic formulation (1) with the difference of replacing pressure by the Cauchy stress tensor $\boldsymbol{\sigma}$. In addition, because of using Eulerian coordinates, the deformation gradient $\mathbf{F}$ needs to be tracked. Following the example from Barton et al.²², the equations evolve only the elastic deformation gradient F_{ij}^e which is determined after performing a multiplicative decomposition of the deformation gradient into an elastic and a plastic component, $F_{ij} = F_{ik}^e F_{kj}^p$. Source terms are included to satisfy the compatibility constraints and the change in the elastic deformation due to plasticity, $\mathcal{P}_{ij}$. The plastic update follows the work of Miller and Colella²³.

The stress at each point in the domain is determined from the deformation of the material through the definition of a constitutive law in the form $e = e(\mathbf{F}^e, S)$ where e is specific internal energy and S is entropy. This expression represents a hyperelastic equation of state which defines the physical response of the solid. Stresses are obtained by direct differenti-

ation of the hyperelastic EOS

$$\sigma_{ij} = \rho F_{ik}^e \frac{\partial e}{\partial F_{jk}^e}.$$

C. Equations of state

An equation of state (EOS) must be defined for each material in order to close the system of equations for both the hydrodynamic and elastic-plastic formulation. The explosive in the detonators considered in this work is PETN and is modeled using two distinct Jones-Wilkins-Lee (JWL) EOS for the reactants and products. However, the explosive used in industrial detonators is often porous which influences its mechanical and reactive properties. Thus, a porosity model is incorporated into the JWL EOS of the reactants accompanied by an adjustment of the parameters of the products EOS to match the reactive characteristics of the porous version of the explosive. The modifications to the JWL EOS to accommodate the snow plow porosity model is described in section II C 1 and the parameter set is presented in section II C 2.

The water is modeled with the stiffened gas EOS with parameters from Shyne²⁴. These parameters were chosen because they yield a sound speed value of 1450 ms^{-1} which corresponds to water at 10°C ²⁵ as were the conditions in the experiment by Klapötke et al.¹³.

The elastic-plastic materials use a hyperelastic equation of state which is a function of the principal invariants of the Finger deformation tensor and entropy²⁶ and is described in the work of Barton and Drikakis²⁷ along with the parameters for the materials aluminum, copper and steel. For plastic flow we use the perfect plasticity model of constant yield stress²³.

1. The JWL EOS with the snow plow porosity model

The JWL equation of state²⁸ written in the Mie-Grüneisen form

$$e - e_{\text{ref}}(\rho) = \frac{p - p_{\text{ref}}(\rho)}{\rho \Gamma(\rho)}, \quad (4)$$

has a constant Grüneisen coefficient $\Gamma(\rho) = \Gamma_0$ and isentropic reference curves that have the following expressions

$$p_{\text{ref}}(\rho) = A \exp\left(-R_1 \frac{\rho_0}{\rho}\right) + B \exp\left(-R_2 \frac{\rho_0}{\rho}\right) + C \left(\frac{\rho_0}{\rho}\right)^{-(\Gamma+1)}, \quad (5)$$

$$e_{\text{ref}}(\rho) = \frac{A}{\rho_0 R_1} \exp\left(-R_1 \frac{\rho_0}{\rho}\right) + \frac{B}{\rho_0 R_2} \exp\left(-R_2 \frac{\rho_0}{\rho}\right) + \frac{C}{\rho_0 \Gamma} \left(\frac{\rho_0}{\rho}\right)^{-\Gamma}, \quad (6)$$

where A , B , C , R_1 and R_2 are parameters calibrated for the particular explosive.

The expressions of the reference curves are usually written without the third term because they cancel each other when replaced in equation (4). Without the third term, the $p_{\text{ref}}(\rho)$ and $e_{\text{ref}}(\rho)$ curves do not correspond to the isentropic values, but this does not affect calculations which require only an incomplete, mechanical EOS $p(e, \rho)$. However, the MiNi16 formulation has closure conditions that use material temperature which requires the definition of a thermal equation of state $T(p, \rho)$ for its calculation. An extension to a complete EOS is achieved with the use of a thermal EOS

$$T - T_{\text{ref}}(\rho) = \frac{p - p_{\text{ref}}(\rho)}{c_v \rho \Gamma(\rho)}, \quad (7)$$

which requires the definition of a temperature reference curve²⁹. The reference curve can be determined by considering that for JWL, the curve must be isentropic and thus satisfy the thermodynamic identity

$$\frac{\Gamma(V)}{V} = -\frac{1}{T} \left(\frac{\partial T}{\partial V} \right)_S. \quad (8)$$

In the case of JWL EOS, Γ is a constant and the integration yields

$$T_{\text{ref}}(\rho) = T_0 \left(\frac{\rho_0}{\rho} \right)^{-\Gamma}, \quad (9)$$

where T_0 is the initial temperature.

The temperature reference curve $T_{\text{ref}}(\rho)$ corresponds to actual values of temperature and if expression $p_{\text{ref}}(\rho)$ is written without the third term, it will not correspond to the actual isentropic pressure value and the temperature calculated using expression (7) will be invalid. Thus, all terms of the JWL reference curves must be used when employing the complete form of the JWL EOS. It is interesting to note that expression (9) has the same form as the third term of the energy reference curve of expression (6). This means that the two terms may cancel each other when replaced in a thermal EOS if the parameters for an explosive are such. This would allow the use of reference curves that omit the temperature curve and the third term of the pressure and energy reference curve without leading to the calculation of unphysical temperature values. However, the accuracy of the calculated values will depend on the particular parameters of the explosive and a general set of parameters may not produce physical temperatures without the use of appropriate reference curves.

The porosity model chosen for this study is the snow plow model³⁰. The model assumes that the work required to compress a porous material of density ρ_0 up to its skeletal density ρ_{00} (density of the material without the pores) is negligibly small. This is based on the fact that during the compression of a porous material, the closing of voids happens first and requires little work compared to compression above the skeletal density. Evidently, this assumption is more accurate for strong shocks that compress the material to high densities and less appropriate for weak shocks where difference between the work for compressing up to the skeletal density and beyond that is not high. A detonation wave compresses the material to densities much higher than the skeletal density which

FIG. 1. Comparison of the regular and porous reactants Hugoniot along with the products Hugoniot and the Rayleigh line for the PETN parameters used in this study. The von Neumann point is determined by the intersection of the reactants Hugoniot and Rayleigh line and its pressure is reduced for the porous explosive. The Rayleigh line is tangent to the products Hugoniot at the CJ point.

justifies the use of the snow plow model. In addition, it is simple to implement and does not introduce additional parameters that would require calibration. In the case of an explosive, the skeletal density corresponds to the theoretical maximum density (TMD) that the explosive can be pressed into a charge.

The compression work is defined by the integral of pressure over volume. To minimize the work for compressing up to the skeletal density, the pressure reference curve is set to zero for densities lower than the TMD. To maintain continuity of the reference equations, pressure should be zero at the TMD value as well. However, the condition $p_{\text{ref}}(\rho_{00}) = 0$ is not generally satisfied by the form of the JWL reference curves and it is up to the parameters to satisfy this condition. In this work, the value of C is adjusted so that it satisfies the above condition.

The complete expressions for the reference curves with the snow plow porosity model are

$$p_{\text{ref}}^{\text{sp}}(\rho) = \begin{cases} 0 & \rho \leq \rho_{00} \\ p_{\text{ref}}(\rho) & \rho > \rho_{00} \end{cases}, \quad (10)$$

$$e_{\text{ref}}^{\text{sp}}(\rho) = \begin{cases} e_0 = e_{\text{ref}}(\rho_{00}) & \rho \leq \rho_{00} \\ e_{\text{ref}}(\rho) & \rho > \rho_{00} \end{cases}, \quad (11)$$

$$T_{\text{ref}}^{\text{sp}}(\rho) = \begin{cases} T_0 & \rho \leq \rho_{00} \\ T_{\text{ref}}(\rho) & \rho > \rho_{00} \end{cases}. \quad (12)$$

and the parameters for PETN are given in table I.

2. Parameter set for the explosive

The explosive used most widely in industrial-grade detonators is PETN. However, the manufacturing and packing pro-

cess varies significantly within the industry which results in explosives of different characteristics. During manufacturing, the PETN is machined or hand pressed in the detonator shell. In the case of the Orica i-kon II detonator, the density is 1.5 g cm^{-3} . Given that the density of PETN crystals is 1.778 g cm^{-3} , the void fraction is approximately 16%.

The porosity of the explosive has a great impact on the characteristics of the explosive. Critically, it sensitizes the explosive since the voids and grains that make up a porous explosive are locations where hotspots are formed. These hotspots eventually coalesce and lead to the formation of a detonation wave in the explosive. The sensitizing effect is valid up to a certain value of porosity. At larger values, it actually has the opposite effect and causes the desensitization of the explosive. The initial density of the explosive also influences the Chapman-Jouguet (CJ) and von Neumann states of the detonation wave. The pressure of both states reduces with increasing porosity as the reactants Hugoniot steepens and the energy density reduces. Thus, it is critical to use explosive EOS and parameters that produce the experimental detonation properties of the explosive in order to accurately simulate the underwater explosion of the detonator. For the explosive considered here, the difference between the regular and porous Hugoniot can be seen in figure 1 and results in a 11% difference in the pressure of the von Neumann spike.

The explosive characteristics of pure PETN crystals have been extensively studied and there exist well verified parameters for PETN at the theoretical maximum density (TMD) of $\rho_{\text{TMD}} = 1.778 \text{ g cm}^{-3}$. In the case of porous versions of PETN the data are not so extensive. The LLNL High Explosives Handbook³² provides JWL parameters for a range of porous versions of PETN. However, Green and Lee³³ reported flaws in the calculations of the study that the LLNL EOS parameters are based on and redid the experiments with significantly different results. They provide revised values for the velocity of detonation (VOD) and CJ density and pressure for a range of initial densities which are mostly lower than the original study. Thus appropriate calibration of the explosive parameters is required.

In the two-phase model, the CJ state and the VOD are controlled by the products equation of state. The initial parameter set is taken from the LLNL High Explosives Handbook³² but the coefficients A and B are adjusted to match the CJ state from the study of Green and Lee³³. Since the study has no data for the exact initial density of $\rho_0 = 1.5 \text{ g cm}^{-3}$, the values are interpolated from the two closest densities and are given in table I. The coefficient C is determined from the condition $p_{\text{ref}}(\rho_0) = 0$ for the porous reactants and $p_{\text{ref}}(\rho_{\text{CJ}}) = p_{\text{CJ}}$ for the products. The parameters for the reactants are taken from a study of Tarver et al.³¹ and correspond to PETN of density $\rho_0 = 1.778 \text{ g cm}^{-3}$ which is at the TMD. The snow plow model is used to model the porous PETN of density $\rho_0 = 1.5 \text{ g cm}^{-3}$. Lastly, the parameter set for the reaction rate is taken from the study of Lee and Tarver³⁴ which matched initiation experiments for porous explosive at density $\rho_0 = 1.6 \text{ g cm}^{-3}$.

Parameters	PETN	
	Reactants	Products
Γ_0	0.5675	0.28
A [10^{11} Pa]	202.80	6.51712
B [10^{11} Pa]	-0.03752	0.19187
C [10^9 Pa]	0.4596	1.308
R_1	10	6
R_2	1	2.6
Q [10^6 m ² s ⁻²]	0	5.975
c_V [m ² s ⁻² K ⁻¹]	1528.4	625
T_0 [K]	293	3811
ρ_0 [kg m ⁻³]	1500	1500
ρ_{00} [kg m ⁻³]	1778	-
D [m s ⁻¹]	7370	
ρ_{CJ} [kg m ⁻³]	2016.2	
p_{CJ} [10^9 Pa]	20.86	
ρ_{vN} [kg m ⁻³]	2752.4	
p_{vN} [10^9 Pa]	37.07	

TABLE I. JWL EOS parameters for PETN^{31–33}.

III. NUMERICAL SOLUTION

The simulations are performed on a fixed Eulerian mesh where the mathematical model corresponding to each material is solved independently using a dedicated numerical solver. The multiphysics methodology allows the use of any number of materials represented by different mathematical models and provides sharp interface resolution for tracking material interfaces while also handles the interaction between materials through appropriate material boundary conditions. The explosive and water are modeled with the multiphase hydrodynamic formulation but there is no diffused interface arising between them due to having material regions that are never in contact during the simulations. The metal components (detonator shell and cup) are modeled with two distinct instances of the elastic-plastic formulation.

The hydrodynamic and elastic-plastic formulations are both solved using FVM for the homogeneous part and the 4th order Runge-Kutta method for the source terms. The FVM used is the Monotonic Upwind Scheme for Conservation Laws (MUSCL)-Hancock with the van Leer limiter³⁵ with a different Riemann Solver (RS) for each model. The MiNi16 hydrodynamic model uses the Harten–Lax–van Leer contact wave (HLLC) RS and the Godunov advection method for the non-conservative equation of the volume fraction¹⁵. The elastic-plastic model is solved using the Harten-Lax-van Leer (HLL) RS³⁶. These methods constitute a high-resolution, shock capturing scheme where discontinuities are directly calculated as part of the solution and are well-suited for the study of deto-

nation and blast waves which are considered in this work.

The multiphysics methodology is a combination of Level-Set (LS) methods for interface tracking and a Ghost-Fluid method for capturing the interaction between materials. The interface of the material is represented by the zero LS of a signed-distance function which is updated based on the state of the cells at the interface. The state of these cells is calculated using the Riemann Ghost fluid (GF) method³⁷. For every interface cell, the Riemann GF method identifies two points, one point in each material, which are equidistant from the interface. The states at these two points, which correspond to different materials, present a *mixed* Riemann Problem and its solution is the new state at the interface cell. The solution of a Riemann Problem between states of different mathematical models is provided by mixed RS which have to be specified for every combination of mathematical models used in the simulation. The mixed RS used to solve between the hydrodynamic and the elastic-plastic model are described in the work of Michael and Nikiforakis¹⁴. The computed states at the interface provide the velocity that is used to advect the LS of each material and are also extrapolated to fill the ghost cells at the boundary of each material using a fast-marching method. With the boundary states determined, the solution of each material is advanced with its own numerical solver.

The numerical methods mentioned above are implemented within a general Computational Fluid Dynamics code developed at the Laboratory for Scientific Computing (LSC) of the University of Cambridge. This framework incorporates hierarchical, block-structured Adaptive Mesh Refinement (AMR)³⁸ for increased resolution in areas of interest and is fully parallelized which allows the distribution of the computational workload on multiple processors.

A. Problem setup and Convergence

The problem setup follows the underwater detonator test described in the European standard EN 13763-15:2004⁶. The basic components are a detonator and a pressure gauge placed in a water tank and separated by a distance of 400 mm. The computational setup is axisymmetric around the axis of the detonator and the equations are solved in cylindrical coordinates in a two-dimensional domain.

The design of the detonators is based on actual devices produced by Orica and is also similar to the design of the reference detonator provided by the European standard. It includes an explosive column of radius $R = 3.3$ mm and length that is determined from the mass and density of the explosive for each simulation. The charge is confined by a thin metal shell of thickness $T = 0.5$ mm which is representative of most industrial detonators. A metal cup of thickness $C = 6.2$ mm is placed above the explosive charge to emulate the actual cup and additional components placed on top of the charge in detonators. The length of the simulated detonator shell is shorter than in industrial detonators and covers only the explosive charge and cup, as shown in figure 2. A longer detonator shell does not change the solution since the blast wave depends only on the section that contains the explosive charge.

FIG. 2. (a) A close-up of the detonator configuration which involves an explosive charge of radius R and length L placed in a metal shell of thickness T and enclosed by a cap of thickness C . (b) The detonator is placed in water in a domain of dimensions 500 mm by 400 mm along with gauges at several points in the axial and normal direction (represented by the dots). The refinement criterion is reduced for areas of the domain that are further from the detonator to ensure proper refinement of the expanding blast wave.

Actual detonators have longer shells for practical reasons such as for housing the circuitry required for their operation and for the insulation and protection of its components.

The rest of the domain is filled with water. The domain size is 500 mm by 400 mm. The boundary conditions are reflective along the axis of the detonator and transmissive at the rest. The transmissive condition is not perfect in multi-dimensional problems and partial reflections occur which can influence the flow inside the domain. Thus, we ensured that the domain boundaries are sufficiently far as to not influence the blast wave in areas of interest.

The charge in the detonator is initiated by a hemispherical high pressure region of radius $0.3R$ and pressure 20 GPa. This ensures a prompt formation of a detonation in the base charge of the detonator without influencing the generated blast wave. The detonation propagates in the explosive and induces a shock wave in the confining metal which is subsequently transmitted in the water.

The domain is considerably extensive compared to the length-scale of the detonator. The distance of 400 mm at which the pressure is measured is more than 100 times the radius of the detonator and four orders of magnitude larger than the resolution required to adequately resolve the reaction zone of the explosive. Such simulations are made possible with the use of adaptive mesh refinement (AMR). The grid is refined according to refinement criteria shown in table II which increase the resolution around the detonation and shock waves in the metal and water in addition to continuous refinement

FIG. 3. Convergence study for the numerical solution of the pressure pulse measured at 400 mm for the configuration of 0.5 mm thick aluminum shell detonator.

at material interfaces. In the case of water, the refinement criterion is lowered for regions further from the detonator, as shown in figure 2b, to keep the blast wave refined as it expands.

The convergence of the numerical solution is assessed by

Material	Variable	Threshold
Explosive	λ	10^6
Metal	$\log(\rho/\rho_0)$	10^6
Water	ρ	$10^3 - 10$

TABLE II. The refinement criterion uses a different variable for each material. The area is refined if the normalized gradient $(\nabla v/v)^2$, of the corresponding variable v , exceeds the prescribed threshold.

examining the blast wave in water for a series of simulations of increasing resolution. The detonator has an aluminum shell and the comparison is on pressure over time at a distance of 400 mm which will also be used for validating the solution against experimental data. The initial resolution is set to $\Delta x = 200 \mu\text{m}$ and is halved for every subsequent simulation.

Figure 3 shows pressure over time in water for increasing resolution. The solution convergences in an expected rate and the difference between resolution $\Delta x = 50 \mu\text{m}$ and $\Delta x = 25 \mu\text{m}$ is very small in the context of this study. Thus the selected resolution is $\Delta x = 50 \mu\text{m}$ which is adequate for comparing the experimental results and for assessing the differences in the blast wave strength between different detonators.

IV. VALIDATION

A. One dimensional steady detonation

The structure of the steady one-dimensional detonation wave is described by the Zel'dovich–von Neumann–Döring (ZND) detonation model³⁹ and characteristic quantities, such as the states at the von Neumann and CJ points are calculated analytically and used to verify the implementation of the model.

The setup considered in this section is one-dimensional and contains solely the explosive. The initial conditions consist of a small region of high pressure, equivalent to a booster, placed at the left end of the domain and the rest of the explosive is at ambient conditions. The pressure in the booster region is set to 20 GPa which is close to the CJ pressure of the explosive. This causes the rapid expansion of the explosive in this region, which compresses and ignites the explosive ahead, leading to the quick formation of a steady detonation wave.

The numerical solution of the one-dimensional detonation wave is shown in figure 4 for a resolution of $\Delta x = 25 \mu\text{m}$. The solution is presented in a series of pressure plots, for times after the detonation has settled to steady state and the density, pressure and mass fraction profile of a single instance of the wave. The solution demonstrates the almost ideal detonation of PETN with a very thin reaction zone of approximately $150 \mu\text{m}$ or 20 ns. The von Neumann and CJ points of the numerical solution match the values calculated analytically.

(a)

(b)

FIG. 4. Plots of the numerical solution of the one-dimensional steady detonation wave in PETN along with the von Neumann and CJ values determined analytically. (a) The propagating detonation wave. (b) Steady detonation wave with scaled values of density, pressure and reactant mass fraction.

B. Underwater initiating capability test

The blast wave generated by the underwater detonator is validated against the experimental work of Klapötke et al.¹³. The experiments follow the methodology of the underwater initiating capability test described in the European standard⁶. The detonators have an aluminum shell and are filled with different amounts of PETN charge. The European standard specifies the pressure that the charge is pressed into the shell. The density for the detonators with explosive mass of 500 mg and 700 mg was measured at $\rho_0 = 1.5 \text{ g cm}^{-3}$ which is the density that corresponds to the explosive parameters presented in section II C 2.

FIG. 5. Comparison between experiment and numerical solution for the blast wave pressure measured at 400 mm for detonators containing different amounts of explosive. The experimental measurements are overlaid over the numerical results. The time is simulation time and does not correspond to experimental time from initiation.

Figure 5 shows the pressure trace measured experimentally against the results of the simulation. The numerical solution shows stronger blast waves than reported experimentally for both amounts of explosive. The differences can be seen quantitatively in table III. The numerical peak pressure differs by approximately 10% and the equivalent energy by almost 30%. A higher energy output is expected from the numerical simulation because some of the energy released by the explosive is spent in fracturing the metal shell which is not modeled in this study. However, this cannot account for the whole difference since the amount of energy lost in fragmenting the shell is not more than 7% of the shock wave energy, even with the most favorable metrics³.

Furthermore, the blast wave from the experiments appears significantly diffused. Experimental studies of blast waves in water estimate the shock front thickness between 10^{-8} m – 10^{-7} m and a rise time of less than 1 ns^{7,40} even for a weak wave traveling close to the speed of sound. The numerical solution shows a sharp discontinuity that is expected as a weak solution of the Euler equations which do not include viscous or heat conduction terms. The choice for omitting these terms is justified for this application as the Reynolds number is of the order of 10^6 and the inclusion of diffusion terms has negligible impact.

However, the experimental data show a more extensive front with a rise time of around 5 μ s which is not physically justified. The appeared diffusion is due to limitations of the pressure gauge. Even though the European standard specifies the use of gauges with response time of less than 2 μ s this usually corresponds to static load and the transient response characteristics are worse due to the finite size of the sensor. The distortion of the blast wave because of their finite size is a fundamental problem of piezoelectric sensors⁷. This dis-

tortion manifests as increased rise times and lower peak pressures because the shock wave requires time to cover the entire piezoelectric crystal. The increased rise time is of the order of the time required for the shock wave to cover the entire sensor and the reduced pressure measurement is caused by the fact that the electric signal generated is proportional to the total compression of the piezoelectric crystal.

The pressure sensor used in the experimental study is the PCB Piezotronics Inc, model 138A5. It uses a cylindrical tourmaline crystal of 3.2 mm in diameter and 1 mm in length. It has a rise time of less than 1.5 μ s and a bandwidth of 2.5 Hz – 10^6 Hz. A study by Zhou et al.⁴¹ analyzed the performance of two commercial piezoelectric pressure sensors (one of which was the sensor used in the experiment) in capturing blast waves in water generated by electric wire explosions. Results showed that the PCB sensor severely distorted the wave forms resulting in a more extensive front and a lower and rounder peak compared to the sensor of smaller size and lower response time.

The limitations of the pressure gauge is thus the main cause of the discrepancy between the experimental and numerical results of table III. Cole⁷ reported that measurements of the blast wave produced by a 25 g explosive charge had an error of 17% for the peak pressure and Zhou et al.⁴¹ reported lower peak pressures for the PCB sensor ranging from 9% up to 27%. Several studies considered reconstruction techniques for obtaining the correct blast wave from the gauge data but these have been application specific and are validated by actual measurements using sensors of higher specifications. A study of the blast wave using sensors of nanosecond response time and large frequency bandwidth is required to reveal the true characteristics of the blast wave produced by detonators.

V. RESULTS

We perform numerical simulations of the underwater explosion of a detonator and examine the blast wave generated in water. We initially focus on the characteristics of the blast wave and analyze the pressure trace over time obtained from a series of gauges aligned in two directions. The directions are along and normal to the axis of symmetry of the detonator, as shown in figure 2b. The positions of the gauges cover the near field and the far field, starting at distances of a few mm from the detonator and reaching the distance of 400 mm which is specified in the European standard for determining the initiating capability of detonators.

Subsequently, we compare the blast wave generated by detonators of different metal shells. The shells differ in terms of material and thickness. The analysis is concerned with the effect of the shell on the characteristics of the generated blast wave along the two aforementioned directions and how the differences evolve during the expansion of the blast wave. The materials considered are aluminum, copper and steel. They have different densities with aluminum being the lighter (2710 kg m^{-3}) whereas copper (8930 kg m^{-3}) and steel (8030 kg m^{-3}) have approximately three times larger density. Similar differences exist in terms of specific acoustic

	Mass	Experiment	Simulation	Difference
peak P [MPa]	700 mg	8.06 (0.04)	9.02	11.9%
	500 mg	7.12 (0.12)	7.73	8.6 %
equiv E_S [10^6 Pa ² s]	700 mg	463 (5)	598	29.2%
	500 mg	339 (5)	430	26.8%

TABLE III. Comparison of the numerical and experimental values for maximum pressure and equivalent shock wave energy.

impedance which determines the ratio of transmitted and reflected waves at material interfaces. Water has much lower impedance than metals and among the considered materials, aluminum has the lowest value whereas copper and steel have similar impedance which is approximately three times larger than aluminum. Lastly, the materials also differ in terms of yield strength. Copper has the lowest yield point at 140 MPa and will exhibit more plastic deformation, followed by aluminum (298 MPa) and steel (1370 MPa) which has the highest value.

A. The nature of the blast wave

We examine the blast wave produced by a detonator which has an aluminum shell of 0.5 mm in thickness and a base charge of 700 mg of PETN which is sealed with a copper cup placed on top of it. Figure 6 shows selected times in the formation and expansion of the blast wave. Initially, the blast wave is ellipsoidal due to the geometry of the charge. The major axis of the ellipse is in the direction of the axis of symmetry of the detonator and the blast wave is stronger and faster in this direction. As the blast wave expands, the magnitude of the shock decays at different rates in each direction and eventually, the difference between the axial and normal direction is minimized leading to a spherical blast wave.

The initial stages of the blast wave are characterized by a complex wave structure which varies along the front of the blast wave. As can be seen in figure 6b, certain sections of the blast wave show additional wave fronts behind the primary blast wave which have higher pressures than the leading blast wave. These secondary waves are produced by the internal reflections inside the base charge and shell of the detonator. Hence, the generated blast is formed by the coalescence of several blast waves of different strength and radii. As these expand, they combine and form a regular blast wave with a single shock discontinuity followed by falling flow parameters.

Along with the formation of the blast wave, the shell and cup of the detonator are compressed and deformed by the detonation wave and the expanding gaseous products. Initially, the detonation propagating in the base charge pushes the surfaces of the shell in the normal and axial direction, causing the formation of an inverse corner. Then, the isotropic expansion of the products takes over and causes extreme elongation of the metal shell while leading to a more rounded shape that persists until the late stages. The metal cup is also compressed but

is significantly less deformed compared to the shell of the detonator. Since the mathematical formulation does not include a fracture model, the metal flows without breaking which would be expected in these conditions.

The pressure traces from the gauges positioned along the normal direction are shown in figure 7. The explosion of the detonator produces a pulse in the water with peak pressure of almost 6 GPa at a distance of 1 mm from the side of the detonator. As the wave propagates to larger distances, the peak pressure falls and the pulse width increases. In the first few mm (near field), the blast wave shows two peaks resulting from reflections of the shock wave within the metal shell. The first peak has larger magnitude and travels faster than the following peak. As they propagate, the peaks move away from each other and are eventually incorporated into a single peak blast wave at a distance of approximately 10 mm.

The pressure pulse in the axial direction is significantly stronger and has peak pressure of more than twice the values in the normal direction as can be seen in figure 8. This means that the blast wave is also faster in this direction which leads to the ellipsoidal shape of the blast wave with the major axis in the axial direction. The difference between the strength of the blast wave in the two directions persists until approximately 10 mm where the magnitude of the blast wave is approximately 1 GPa in both directions, but the blast wave has not attained a spherical front yet. Further, the blast wave in the axial direction also exhibits a secondary peak of lower magnitude. Similar to the normal direction, the two peaks move away from each other as they expand and eventually form a regular blast wave, but are seen to persist longer in this direction.

The decay of the peak pressure of the blast wave with distance is plotted in figure 9. The plot compares the two directions considered and illustrates the persistence of higher peak pressure in the axial direction up to the distance of 10 mm where the peak pressure in both directions becomes similar. At larger distances, the blast wave in the normal direction exhibits slightly higher values, suggesting a slower rate of decay compared to the axial blast wave. Overall, the decay behavior exhibits a similar trend in both directions. It starts with a slow decay rate which increases as the blast wave expands and reaches an approximately constant power law decay at the larger distances.

There is a clear distinction in the decay behavior between the near and far field. The initial decay of pressure is not linear in the log-log plot and therefore cannot be described by a single power law. In addition, it is slower than the in-

FIG. 6. Plots of pressure from the numerical solution of the blast wave generated by the detonator with 0.5 mm aluminum shell at times (a) 2 μ s, (b) 10 μ s and (c) 32 μ s. The blast wave is asymmetric in the near field and becomes progressively more spherically symmetric as it expands.

verse first power law (r^{-1}). This behavior has been observed in experiments and is a result of the finite time required for the energy transfer from the explosive to the surrounding material^{42,43}. The extent of this formation process depends on the ratio of energy release over the initial mass of the explosive. Brode⁴⁴ suggests that for a conventional explosive (e.g. TNT), the blast wave has fully formed when its radius engulfs a mass of the surrounding material that is roughly ten times the mass of the explosive. In the case of 700 mg PETN and water, which are considered in this study, this distance is at approximately 12 mm. This is the distance at which the change in the decay rate is observed in figure 9.

In the far field, the decay rate is increased and resembles a power law. A fit of the obtained peak pressures in the normal direction yields a power value of $-1.321(7)$ which also describes the axial values well. A value of higher than the inverse power law is expected for strong shock waves⁷. The rate of decay in this regime depends on the amplitude of the wave. The dissipation of energy at the shock front increases

with shock pressure, therefore there is smaller loss of energy as the blast wave expands and its peak pressure is reduced. This explains the lower decay rate of the blast wave in the normal direction which has lower pressures in the near field and thus dissipates less energy as it expands. At even longer distances, the blast wave becomes an acoustic wave and the decay is expected to reduce further and converge to the inverse first power law which is the asymptotic solution for spherical acoustic waves.

It should be noted that the classic Sedov-von Neumann-Taylor similarity solution for a point source explosion predicts a decay rate of r^{-3} . However, as mentioned in the original work of Taylor⁴², the range at which this solution can be compared to actual high explosives is limited. Firstly, the solution concerns point sources instead of an extensive explosive charge. This assumption sets a lower limit for the distance from the explosive charge that the solution applies, which is at the point where the involved mass of the surrounding material is several times the explosive mass. Secondly, an upper limit

FIG. 7. Pressure plots of the blast wave measured at several points along the direction normal to the axis of symmetry of the detonator in the (a) near field and (b) far field.

is also introduced from the assumption of strong shock waves. Taylor⁴² suggests that the solution is valid for shock pressures above 1 MPa in air. This corresponds to shock waves traveling with speed above Mach 3 or shock pressure of above 4.2 GPa in water. Shock waves of such strength are not observed after the blast wave has expanded beyond the lower limit and therefore, there is no range in which the similarity solution is applicable for the blast wave produced by the underwater detonator.

The characteristics of the blast wave in the near should be considered in the assessment of initiating capability since the placement of the detonator is within the receiving explosive charge. Most experimental tests, such as the widely used test specified by the European standard, consider only a single point in the far field. However, the asymmetric blast wave strength and low decay rate, that characterize the blast in the near field, do not persist in the far field. In addition, the overall decay rate is different between the two directions considered. The axial blast wave has higher pressure in the near field but decays faster and exhibits comparable and even slightly lower values of shock pressure than the normal direction in distances beyond 10 mm. The difference in blast wave strength between the two directions is a possible explanation for the observed variation in detonator strength depending on its orientation⁴. Given that the initiation of the neighboring explosive is heavily dependent on the shock pressure in the near field, tests that consider the blast wave only in the far field are not able to accurately capture the initiating capability of the detonator.

B. The effect of shell material

The material of the detonator shell is an important aspect of detonator design. The most commonly used metals are aluminum and copper, but manufacturers have been introducing new metal alloys in an effort to balance the requirements for low cost, efficiency and reliability. Experimental studies have shown that the initiating capability of the detonator is influenced by the type of shell^{2,8}, but the extent of its effect has not been established. The significance of the material of the shell is also evident when considering the physical processes involved in the generation of the blast wave. The detonation wave initiated in the base charge, induces a shock wave in the metal shell and subsequently in water through a series of transmissions and reflections at the material interfaces which depend on material properties. This section compares the blast waves generated from detonators made out of aluminum, copper and steel shell in order to identify the nature and extent of the influence of the detonator shell.

The flow field after the initiation of the copper detonator is shown in figure 10. The generated blast wave is initially ellipsoidal and progressively transforms into a spherical wave, as in the case of the aluminum shell presented in section V A. However, the initial wave transmitted in water (figure 10a) is seen to have multiple secondary peaks of similar strength. This is caused by strong reflections at the interfaces of the shell and leads to typical reverberations or 'ringing' in the metal⁴⁵. Once the reactions in the explosive have completed, the resulting blast wave has a complex structure and variable strength along its front which was observed in all materials. The deformation of the cup and shell is similar to the aluminum case for times up to 10 μs. In later times, the copper shell continues to feature the inverse corner and has more

FIG. 8. Plots of pressure obtained by gauges positions at several distances in the axial direction.

FIG. 9. Logarithmic plot of the decay of peak pressures of the blast wave with distance in the two directions considered.

anisotropic expansion compared to aluminum due to lower yield strength leading to more extensive plastic flow.

The comparison of the pressure pulses obtained at selected points in the near and far field of the detonators is shown in figure 11 for the three shell materials examined. The materials show little variation in the generated blast wave when observed in the far field but have stark differences in the near field. The peak pressure for the copper and steel detonators at the distance of 1 mm is a little over 2.5 GPa which is half the value of the aluminum detonator. Similar behavior is observed in the axial direction. The pulse of the aluminum detonator has almost double the pressure peak of the copper and steel detonators.

Furthermore, the copper and steel detonators also feature multiple peaks which are a result of stronger reflections of the shock wave within the copper/steel shell. This is caused by the higher impedance difference between copper/steel and water which causes strong reflection of the shock wave at the interface of metal and water and only a small portion is transmitted. The shock wave is also reflected at the inner interface between metal and explosive products where the impedance mismatch is also large. This results in more pressure peaks of lower amplitude compared to the case of aluminum case.

As the blast wave expands to larger distances, the stronger pressure peaks merge with the slower ones ahead while the weaker ones behind decrease further and are incorporated into the tail of the blast wave. After this equilibration process, only a single peak remains. At the distance of 400 mm the blast wave has peak pressure of around 9 MPa for both aluminum and copper and slightly lower for steel.

Figure 12 shows the decay of shock pressure with distance in the normal direction for all materials considered. The higher peak pressures observed in aluminum extend to a distance of 10 mm while copper and steel exhibit similar peak pressures and decay. At larger distances, the blast wave from all configurations shows nearly identical values of pressure

and the decay rate specified by the power law $r^{-1.321(7)}$ describes all materials within error. Similar results are observed for the blast wave in the axial direction.

Overall, the blast wave of the aluminum detonator differs significantly from the other configurations in the near field. As the wave expands, the blast waves converge and they are practically the same at the distance of 400 mm, especially in the case of aluminum and copper. Thus, shock energies measured at this point would be similar and the detonators would have equivalent initiating capability according to the European standard test. However, the strength of the shock is the leading factor in the initiation of heterogeneous solid explosives^{46,47}. The initial pressure pulse must be above a threshold to ensure the reliable initiation of the explosive and thus, the reduced peak pressure of the copper and steel detonator indicates lower capability in the initiation of secondary explosives. In addition, the weak blast wave can also lead to effects of shock desensitization which is common in heterogeneous secondary explosives. The important differences in the near field are not accounted for by tests that focus on the far field performance which suggests limited suitability for assessing initiating capability.

C. The effect of the shell thickness

We examine the effect of shell thickness on the blast wave generated by detonators. The mass of the shell, determined by its thickness, is expected to affect the equivalent energy yield of the device because the explosive charge and the shell have comparable masses¹¹. We consider detonators of 1 mm in shell thickness which is double the value of the configurations in section V B and made out of the same three materials.

The plots of figure 13 compare the pressure pulse calculated for the thick detonators at selected points. Interestingly,

FIG. 10. Plots of pressure from the numerical solution of the blast wave generated by the detonator with 0.5 mm copper shell at times (a) $2\ \mu\text{s}$, (b) $10\ \mu\text{s}$ and (c) $43\ \mu\text{s}$. The blast wave is asymmetric in the near field similar to the aluminum case, but the internal reflections lead to multiple peaks of approximately half the strength of the blast wave generated in the case of aluminum.

the blast wave in the far field (400 mm) is not considerably different from the case of the thinner detonators. In particular, the pressure pulse of the aluminum shell is largely similar and for copper and steel the reduction in peak pressure is approximately 5%. The increased effect for the case of copper and steel detonators is caused by the fact that the increase in mass is much larger for these denser materials compared to aluminum.

In the near field, the relative differences between materials are also similar to the thin detonators. The aluminum detonator generates pulses of approximately double in pressure than copper and steel which have similar values. The existence of multiple peaks in the case of detonators made out of high impedance materials (copper/steel) is also observed, but the period of the oscillations is now larger due to the increased thickness and hence the larger time between reflections within the shell.

The increased shell thickness does cause a significant reduction in the strength of the pressure pulses observed in

the near field. All materials show decreased pressure pulses with the most extreme cases being the reduction of the pulse strength in the normal direction. The pressure peaks for this case have reduced to almost half. However, the reduction in the axial direction is less severe, with the aluminum reducing by 20% and the copper and steel by 35%.

An additional distinction to the case of thin detonators is the difference between the pressure pulses in the axial and normal direction which is larger for the thick detonators. In the 0.5 mm thick shells, the pulse in the axial direction had approximately twice the peak pressure in the normal direction, but for the shells of 1 mm this increases to three times larger pressure peaks.

A comparison of the decay of peak pressure of the blast wave between the thin and thick detonator is shown in figure 14 for the case of the aluminum shell. The plot shows that they deviate only in the near field where the doubling of the thickness leads to approximately halving of the pressure peak. However, at distances beyond 10 mm the shock pres-

(a)

(b)

(c)

FIG. 11. Comparison of the pressure pulse generated underwater for 0.5 mm thick detonators of different shell materials. (a) 400 mm in the normal direction, (b) 1 mm in the normal direction and (c) 1 mm in the axial direction.

FIG. 12. Logarithmic plot of the decay of peak pressure of the blast wave with distance in the direction normal to the detonator and for the three materials considered.

sure is similar for detonators of both thicknesses. This indicates that the mass of the shell mostly affects the formation regime of the blast wave. Once the energy of the explosive has been transferred to the surrounding material, the generated blast wave is similar for both sizes of detonator shell.

Overall, the results indicate that the increased thickness of the shell leads to a significant reduction in the near field pressure values. This suggests that the detonator will have lower capability in igniting an explosive. However, the impact of the shell thickness does not persist into the far field which follows the theme that is observed in sections V A and V B. Thus, direct initiating capability tests that consider the blast wave only at the far field are not able to fully capture the effect of the shell thickness and will demonstrate little difference in performance between the thin and thick detonators.

VI. CONCLUSIONS

The estimation of the initiating capability of detonators is a challenging topic due to the complex mechanisms involved in explosive initiation and the dependence on several aspects of the design of the detonator. In this work, we use numerical simulations to examine the blast wave generated by detonators underwater. It is the first of a two-part study in which the detonator is examined in isolation following the underwater test of initiating capability described in the European standard⁶. This is a direct test of initiation which has not been shown to correlate with the actual initiating capability of the detonators. However, it is widely used for assessing detonators and there are available experimental data of detonator initiation for this configuration. The focus of the study is on determining the general characteristics of the blast wave generated by detonators as well as the variations between detonators of different shell material and thickness.

(a)

(b)

(c)

FIG. 13. Comparison of the pressure pulse generated underwater for 1 mm thick detonators of different shell materials. (a) 400 mm in the normal direction, (b) 1 mm in the normal direction and (c) 1 mm in the axial direction.

FIG. 14. Logarithmic plot of the decay of peak pressure of the blast wave with distance in the normal direction for aluminum detonators of different shell thickness.

The simulations were performed following a multiphysics methodology that allows distinct mathematical models for each material that are appropriately selected for each component of the detonator. The explosive is modeled as a two-phase material with the Ignition & Growth reactive model. This was extended with the snow plow porosity model since the explosive used in detonators is highly porous due to the manufacturing process. The metal of the detonator shell and cup are modeled with an elastic-plastic formulation while the water is governed by the inviscid Euler equations for fluids.

The numerical solution is validated against the experiments of Klapötke et al.¹³ which used detonators of 500 mg and 700 mg of PETN of the same density (1.5 g cm^{-3}) as the Orica i-kon II detonator considered here. The numerical results show higher pressure peaks and larger shock energy than measured experimentally. This is attributed to imperfections of the experimental pressure measurement equipment. An experimental study by Zhou et al.⁴¹ examined the same piezoelectric sensor used in the experiments of Klapötke et al. and showed that the size of the sensor leads to increased rise times and reduced pressure values which explains the observed differences between the numerical and experimental results.

The study of the underwater explosion of the detonator examines the generated blast wave in the directions along and normal to the axis of the detonator and at several distances from the detonator ranging 1 mm – 400 mm. Results show that the blast wave exhibits distinct features in the near and far field of the detonator. In the near field, the blast wave has an ellipsoidal shape and is twice as strong in the axial direction than in the normal direction. As the blast wave propagates into the far field, the asymmetry is minimized and attains a spherical shape. Further, the blast wave in the near field goes through its formation regime which is characterized by a slow rate of decay and once the blast wave is established, it exhibits a faster rate of decay which follows a power law.

The blast waves produced by detonators of different shell types were analyzed to determine the effect of the shell material and thickness. This has revealed that certain types of detonators produce blast waves with significant differences in the near field, but these differences are minimized after the expansion of the wave into the far field. In particular, the pressure pulse in the far field is similar for aluminum and copper shells of 0.5 mm in thickness but in the near field, the blast wave is critically different for the case of aluminum which produces a pressure pulse with double the peak pressure of the denser metals, copper and steel. This is caused by the larger impedance difference between the water and copper/steel which leads to stronger reflections within the metal shell and results in blast waves with multiple peaks. The impact of the thickness of the shell also follows the same theme. In the far field, the aluminum detonators show very similar pressure pulses for both shell thicknesses and in the thicker copper and steel detonators, the reduction in peak pressure is approximately 5%. Contrary to that, the near field peak pressure of the pulse is reduced to half in the normal direction and by 20%–35% in the axial direction for all thicker shells.

The distinct features of the blast wave in the near field play an important role in the initiating capability of detonators because the initiation of heterogeneous explosives is believed to depend primarily on the strength of the blast wave. In addition, the experimental observations of lower effectiveness for copper detonators compared to aluminum as well as the change in initiating capability depending on the orientation of the detonator can be explained by considering the differences in the strength of the pressure pulse in the near field. However, this variation in the generated blast wave does not persist in the far field and thus cannot be captured by tests that examine the blast wave only in the far field. These tests, such as the standard underwater test, would show similar performance for most detonators which suggests that they are not able to fully assess the initiating capability of a detonator.

The outcomes of this work highlight the need for experimental studies that consider the full extent of the blast wave. These require advanced experimental techniques that are able to capture the short timescales and multi-dimensional character of the blast wave in the near field. Recent studies have proposed the use of high-speed imaging and optical techniques which are able to measure the near field blast wave strength and its variation with direction. A detailed description of the blast wave obtained from accurate experimental data will provide invaluable insight into the properties of the blast waves generated by detonators and can be used to validate the results of numerical studies. Lastly, the utilization of leading experimental techniques will also pave the way for the development of improved tests that will provide a more comprehensive evaluation of detonator performance.

The second part of this study extends the numerical investigation into detonator performance by considering detonators within a booster explosive charge. This configuration constitutes an initiating system that is used to ignite mining blast-holes and can be viewed as an indirect test of initiating capability. The aim is to compare the initiating capability of detonators in an actual configuration that they are designed

to operate in and relate it with the blast wave characteristics observed in this study.

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DATA AVAILABILITY

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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