Multiphysics modeling of the initiating capability of detonators

Part II: Booster initiation

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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 follows the European underwater test which evaluates detonators in isolation (direct method). The second part, presented here, investigates detonators placed within a receiving explosive charge (indirect method). Specifically, the detonator is placed inside a booster device which contains secondary explosive and together form an initiating system used to ignite mining blastholes.

The physical system is modeled using a multiphysics methodology to accurately capture the response of the materials present in the configuration (explosives, metals and fluids). The reactive model is extended to account for shock desensitization where explosives become more difficult to initiate after the passage of weak shock waves. The variability of the blast wave generated by detonators, observed in the first part of the study, can lead to partial desensitization resulting in pockets of unreacted explosive which inhibit booster initiation and performance. The computational implementation is extensively validated and calibrated against experiment before employed for the study of booster initiation by a range of detonators. Results show that the booster is susceptible to shock desensitization which occurs in varying degrees for different types of detonators and can significantly impact the performance of the initiating system.

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

I. INTRODUCTION

Rock blasting is the practice of using explosives for rock fragmentation that is extensively used in the mining industry and other civil engineering applications. It typically involves drilling holes in rock, filling them with explosive and igniting them in a specific pattern designed to increase the efficiency of the process. The explosive that is most commonly used in mining is ANFO (Ammonium Nitrate mixed with Fuel Oil). It is a very insensitive explosive that has beneficial safety and usability characteristics in addition to low cost. However, its detonation is highly non-ideal with low detonation velocity and poor performance in small diameters^{1–3}. Furthermore, it requires strong stimulus for initiation and cannot be reliably ignited by standard detonators. The recommended practice is to use a three-step explosive initiation train which includes a detonator and a booster⁴.

A booster is an explosive device that is part of a blasthole initiating system. It provides an additional layer of explosive between the detonator and the tertiary explosive to ensure reliable initiation of non-detonator-sensitive explosives. It contains a secondary explosive that must be sensitive enough to be ignited by a detonator and powerful enough to provide sufficient impulse for the ignition of insensitive tertiary explosives such as ANFO. Similar to detonators, these devices exist in several designs which have different type and quantity of explosive as well as shell shape and material. Their design must

satisfy a long list of industry standards and specifications related to safety, cost and ease of use which inevitably leads to compromises in performance.

The performance of an explosive initiating system depends on the successful ignition of each explosive component. The detonator and booster must be appropriately designed and paired to ensure that the initiation sequence progresses reliably from the detonator to the booster and finally to the explosive in the blasthole. These configurations have a complex structure with multiple layers of materials and involve several physical processes associated with reactive and inert shock waves such as reflection, transmission, interference and diffraction (corner turning). The intricate ignition process and dependence on several characteristics of the design complicates the determination of the ability of the detonator to initiate the booster explosive.

The initiation process also depends on the reactive properties of the explosives. The base charge of the detonator is typically a sensitive explosive that promptly forms a steady detonation propagating in a straight charge. However, the explosive of the booster is usually a heterogeneous explosive that has more extensive run-to-detonation distance and can also exhibit *shock desensitization*. This is a phenomenon where the explosive becomes more insensitive or completely unable to ignite after the passage of a shock wave of lower strength than the initiation threshold of the explosive. When the shock wave transmitted into the booster is not strong enough to ignite the explosive, it may desensitize it and lead to the formation of non-reacting pockets of explosive called dead zones. Extensive dead-zones will obstruct the propagation of detonation and can be detrimental to the performance of the booster.

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Shock desensitization of solid explosives was first mentioned in a study by Campbell et al.⁵ which focused on shock initiation while more recent investigations have distinguished between different manifestations of shock desensitization^{6,7}. In the context of shock initiation, desensitization is observed as a delay in the transition to detonation for the case of double (or reflected) shock compared to the single shock case. In the regime of detonation propagation, shock desensitization manifests as the quenching of detonation in parts of the explosive that have been previously shocked. Drimmer and Liddiard⁸ performed one of the first experiments showcasing detonation failure in pre-shocked HMX-based explosives and Campbell and Travis⁹ observed similar behavior in RDX-based explosives.

Advances in experimental diagnostics have enabled the detailed study of dead zone formation which has been shown to occur for all polymer bonded explosives⁷. The explosive setup in such studies involves an abrupt change in geometry such as an increase in charge radius which forms a corner. As the detonation moves into the wider explosive region, it is diffracted and propagates in the radial direction which is referred to as “turning the corner”. The detonation in the radial direction is established at some distance from the corner which results in some parts of the explosive remaining unreacted. Cox and Campbell¹⁰ performed one of the earliest experiments involving detonation diffraction and reported dead zone formation in a Triaminotrinitrobenzene (TATB)-based explosive. Similar experiments performed by Held¹¹ showed dead zone formation in an RDX-based explosive as well.

The effects of shock desensitization on mining operations have been considered in several studies by the mining industry. The investigations mostly focused on the effect of shock waves from neighboring blasts in situations where multiple blastholes are initiated sequentially^{12–14}. The generated shock waves travel through rock at high velocities and can reach adjacent blastholes ahead of their initiation. Depending on the strength of the shock, this can cause an untimely initiation of the blasthole or desensitization of the explosive and loss of performance of the blast. In addition, it has been observed that the shock wave can also interfere with initiating devices such as the detonator¹⁵ and render them unable to initiate the blasthole.

The impact of shock desensitization during the initiation of boosters used in mining has not been extensively investigated. Orica performed internal experimental studies which placed the detonator and booster configuration in aquariums and used ultra-high-speed photography to capture the initiation of a commercial booster placed underwater. They made observations of the detonation front on the surface of the booster which demonstrated the complex initiation process as well as indicated that certain regions of the explosive were desensitized, leading to the formation of dead-zones. This is also recognized in accompanying numerical investigations¹⁶ which noted that several regions of the explosive of the booster were not promptly ignited when shocked, because of low shock strength, and would have been desensitized. However, no desensitization was included in the mathematical model to allow for the study of its effect.

The heterogeneous nature of the explosive and the geometry of the booster indicate that its initiation can be affected by shock desensitization. This is further supported by the results of the first part of this study¹⁷ where the blast wave obtained by the detonator was observed to have variable strength along its front. This can lead to the partial initiation of the explosive while some regions become desensitized by the weaker parts of the blast wave. To this date, experimental studies investigating the effect of shock desensitization on the initiation of a booster device do not exist in the literature. Such experiments can utilize x-ray or proton radiography to analyze the extent of reactions within the initiating system and provide valuable insight into the influence of shock desensitization on the initiation of booster devices.

In this study, we perform numerical simulations to investigate the ability of detonators to initiate a booster explosive device in a configuration used for blasthole initiation in mining. This constitutes an indirect test of initiating capability and is an extension of the first part of this study¹⁷ which considered a direct test. The use of indirect tests is the only conclusive method for assessing the initiating capability of detonators since direct tests have no proven correlation with initiation efficiency^{18–21}. Further, the study considers the influence of shock desensitization on the initiation process of the booster explosive and by extension on the performance of the initiating system. The configuration examined in this study is based on actual designs of devices used in initiating systems by the mining industry. The detonator is made out of a thin metal shell and contains Pentaerythritol Tetranitrate (PETN) as base charge whereas the booster has a plastic shell and contains 400 g of composition B.

The mathematical modeling of the physical system follows the multiphysics methodology presented in the first part of the study¹⁷ and more extensively in the work of Michael and Nikiforakis²². This allows for the independent use of different governing equations for each component of the configuration and enables the use of suitable material models that properly capture the response of each material such as explosives, metals and fluids. Further to the first part of the study, the reactive model is complemented with a desensitization model to account for the process of shock desensitization. This is required for pressure-based reactive models because they have been shown to be unable to capture the effects of shock desensitization in both shock initiation²³ and dead zone formation²⁴.

Several extensions to pressure-based reactive models have been proposed for the purpose of capturing shock desensitization effects. Initial efforts introduced a switch to deactivate reactions if a critical range of shock compression is generated in the explosive²⁵. However, this method cannot replicate the time dependence observed in detonation quenching experiments. A more sophisticated approach was proposed by DeOliveira et al.²⁶ which suggested the addition of a desensitization parameter that is advected in the flow and is coupled with a desensitization rate which functions similar to a reaction rate. This modification has managed to match experimental results on detonation quenching²⁷ and corner turning²⁸ in TATB-based explosives. The concept of such desensitization

models follows the classical view on the cause of shock desensitization^{9,29} which argues that weak shock waves partially close the pores in the explosive and thus hinder the formation of hotspots by subsequent shocks that could potentially initiate the explosive.

Contrary to the above, reaction rates that depend on entropy or temperature are able to account for desensitization naturally⁷. In particular, the entropy-based reaction model CREST has been shown to agree with experimental corner turning data at different initial temperatures³⁰. This has given rise to an alternative view of desensitization proposed by James and Lambourn³¹ that is based on thermodynamic and hydrodynamic arguments. In this view, desensitization arises naturally when assuming that the reaction rate depends on a thermodynamic quantity that is greatly reduced behind multiple shocks compared to a single shock, such as temperature or entropy. The observed time dependence of the desensitization is then explained as hydrodynamic effects resulting from the reduced reaction rate which are different for each manifestation of desensitization, e.g. delay in run to detonation or detonation quenching. The debate between the two views is currently ongoing and the explosives community is showing increasing interest on the subject. A range of new experiments which utilize better diagnostic techniques are expected to provide more insights into the physical processes of shock desensitization as well as advance the computational models⁷.

The modeling approach in this study follows the classical view and uses the Ignition & Growth (I&G) reaction rate³² along with the desensitization model by DeOliveira et al.²⁶. This choice is facilitated by the availability of established I&G parameter sets for the explosives considered in this study in addition to the existence of experimental data that enable the determination of parameters for the desensitization model of composition B. The mathematical model is presented and discussed in section II followed by extensive validation in section III. Section IV presents the booster configuration and results from the examined configurations. The investigation considers the initiation process of the booster with and without the desensitization model, for different types of detonators, and for a configuration with different positioning of the detonator. The results indicate that the initiation of the booster explosive is significantly influenced by shock desensitization which leads to the formation of dead-zones of varying size depending on the detonator shell type.

II. MATHEMATICAL MODEL

The performance of the explosive initiating system consisting of a detonator and a booster depends on the interaction of several materials and physical processes. The numerical simulations follow the multiphysics methodology by Michael and Nikiforakis²² which enables the use of distinct mathematical models for each material. The mechanical response of each material and the corresponding physical processes are described by different sets of equations and parameters. The explosives are described by a two-phase hydrodynamic model that is a reduced version of the MiNi16³³ diffuse inter-

face method in which only the explosive material is present. The metal materials are described by an elastic-plastic formulation which models both normal and shear stresses in the material as well as the effect of strength and plastic deformation. Lastly, the plastic of the booster and the water which surrounds the setup are modeled using the inert Euler equations for compressible fluids. The employed multiphysics methodology provides sharp interface treatment between the materials and handles their interaction. The two-phase model for the explosives defines a diffused interface between the reactants and products phases within each explosive but they have sharp interfaces with the inert, confining materials.

The aforementioned models have been briefly described in the first part of this study¹⁷ and more extensively in the work of Michael and Nikiforakis²². Here, we restrict the discussion to the extension of the reactive model to account for shock desensitization in explosives. The Ignition & Growth (I&G) reactive model³² is used for both explosives, PETN and composition B. It features two Jones-Wilkins-Lee (JWL) equations of state that correspond to the reactants and products while the conversion from one phase to the other is governed by a multi-stage, pressure-based reaction rate. I&G has been quite successful in modeling initiation and propagation of detonation and a large range of explosives have been calibrated and validated for this reactive model. However, its dependence on local pressure makes it unable to capture desensitization effects^{23,24}. The desensitization model by DeOliveira et al.²⁶ has showed promising results in capturing dead zone formation which enables the use of the extensive range of I&G parameter sets in modeling explosive applications that involve shock desensitization. This extension is included in the mathematical description of composition B to enable the study of the impact of shock desensitization in the initiation of the booster device.

A. The shock desensitization model

The model by DeOliveira et al.²⁶ is based on the classical view of desensitization which argues that two competing transformations are taking place when an explosive charge is shocked²⁹. One is the chemical transformation which turns reactants into products with the release of energy and the second is a mechanical transformation that activates the hotspots and progressively makes the explosive less sensitive. In this view, reactions and desensitization behave similarly which warrants similar treatment. The desensitization model introduces a desensitization parameter $\psi \in [0, 1]$ that is advected in the flow

$$\frac{\partial \psi}{\partial t} + \mathbf{u} \cdot \nabla \psi = \mathcal{C}, \quad (1)$$

where $\mathbf{u}$ is flow velocity, $\psi = 0$ corresponds to pristine explosive, $\psi = 1$ represents the completely desensitized state and a desensitization rate $\mathcal{C}$ determines the change from one state to the other.

The ψ variable is added to the hybrid model, presented in the first part of this work¹⁷, by combining it with the continuity equation for the reactive material which yields an addi-

tional equation

$$\frac{\partial z\rho_1\psi}{\partial t} + \nabla \cdot z\rho_1\psi\mathbf{u} = z\rho_1\mathcal{C}, \quad (2)$$

where ρ_1 is the explosive density and z is the volume fraction of the explosive. The form of the desensitization rate $\mathcal{C}$ as proposed by DeOliveira et al. is

$$\mathcal{C} = Ap(1 - \psi)(\psi + \varepsilon), \quad (3)$$

where p is local pressure, A is a constant representing the strength of the desensitization and ε is a small number required for the desensitization rate to produce non-trivial solutions at $\psi = 0$. The form of the desensitization rate is parabolic concave down which means that it has minima at the boundaries and a maximum at the midpoint of $\psi = 0.5$.

The desensitization model also modifies the reaction rate so that it depends on the desensitization parameter. The modifications aim to increase the ignition threshold and inhibit the growth terms. This is achieved by replacing the constant α in the I&G rate with the function

$$\alpha(\psi) = \alpha_0(1 - \psi) + \alpha_1\psi, \quad (4)$$

where α_0 is the original threshold and α_1 is a new constant that represents the ignition threshold of the completely desensitized explosive. In addition, it introduces a lower threshold for the first growth term by adding a minimum value of reaction progress before it is activated. This term is set to

$$\lambda_{G1}^{\min} = \lambda_c\psi, \quad (5)$$

where λ_c a constant. The original study suggests this restriction only for the first growth term because the second growth term usually has an already high threshold $\lambda_{G2}^{\min}$. However, our implementation also sets the lower threshold for the second growth term to be the maximum between the original I&G parameter and the value of equation (5) to ensure that no growth terms are activated below the desensitized threshold regardless of the original I&G parameters.

Overall, the desensitization model introduces four new parameters. Two relating to the desensitization rate and the two for the inhibition of the reaction rate. The rate parameters can be found using data of time to desensitization over input pressure for which experiments have been performed for a few explosives. The calibration usually concerns parameter A since ε is only required to be a small number. The parameters for the adjustment of the reaction rate are more arbitrarily deduced. Experiments investigating the increase in the threshold of initiation for completely desensitized explosive are used to determine parameter α_1 while the restriction of the growth terms is chosen so that experiments involving formation of dead zones are matched.

The expression of the desensitization rate (3) by DeOliveira et al.²⁶ is not supported by physical arguments but has been successful at producing dead zone formation numerically. However, considering that the closure of pores is assumed to be the strongest cause of desensitization and that the compression of a porous material requires the least energy at

the initial state of the material, then the desensitization rate should have a maximum when the explosive is in the pristine state and decrease as desensitization increases. Further, the linear dependence on pressure is contrary to experimental results. Campbell and Travis⁹ and later Mulford et al.³⁴ found that pressure p and time to desensitization τ are related by an expression of the form

$$p^m\tau = c \quad (6)$$

where m and c are constants. The exponent was found to be $m = 2.2$ for HMX-based polymer bonded explosive PBX9404 and is likely to deviate from unity for most explosives which suggests that the addition of an exponent on the pressure dependence will allow for more accurate calibration to experimental data as proposed by Hussain et al.⁶

Nonetheless, the parabolic form of the desensitization rate is useful numerically as it allows for the growth of reactions without interference from the desensitization model in cases where the shock wave is above the initiation threshold. The desensitization model is independent of reactions occurring in the explosive and desensitization can develop concurrently with reactions which will alter the reaction rate. The low value of the desensitization rate when the material is pristine ensures that the reaction progress variable λ increases faster than the desensitization variable ψ and thus, the desensitization model does not change the standard I&G detonation initiation and propagation characteristics in situations where reactions are occurring in the explosive. If instead, desensitization grew faster than the reaction variable, then the development of desensitization would hinder the growth of the reactions and influence detonation characteristics and even lead to initiation failure.

Another numerical advantage of the parabolic form is that the differential equation can be solved analytically which would allow for its quick and accurate numerical update without the need of calculating a numerical solution. The differential equation

$$\frac{dy}{d\tau} = Ap(1 - y)(y + \varepsilon) \rightarrow \int_{\psi_0}^{\psi} \frac{dy}{(1 - y)(y + \varepsilon)} = \int_0^t Apd\tau, \quad (7)$$

yields

$$\psi(t) = \frac{\exp(Apt(1 + \varepsilon)) + \varepsilon \frac{\psi_0 - 1}{\psi_0 + \varepsilon}}{\exp(Apt(1 + \varepsilon)) - \frac{\psi_0 - 1}{\psi_0 + \varepsilon}}, \quad (8)$$

which is used to update the desensitization variable at each time step.

III. VALIDATION OF THE NUMERICAL SOLUTION

The numerical solution of the mathematical models representing each material and their interaction is obtained using the multiphysics methodology proposed by Michael and Nikiforakis²². The systems of equations of each model are formulated in the same hyperbolic form which enables their

independent solution on a common Eulerian grid using shock capturing Finite Volume Methods, as outlined in the first part of the study¹⁷. The interface of each material is tracked using a level set function and their interaction is captured using the Ghost Fluid Method and mixed Riemann solvers that have been specifically constructed for each pair of materials. The explosive materials are two-phase and are modeled with a reduced version of the MiNi16³³ multiphase model which provides a diffused interface between the reactants and products phases of the explosive and enables modeling of the reaction zone.

Validation of the models and methodology used in this study is restricted to the topic of shock desensitization which is the only extension to previous studies that employed and validated this simulation framework^{17,22}. The accurate representation of the shock desensitization process and dead-zone formation are particularly challenging to current reactive models. The physical process that govern the formation of dead zones is the result of the complex interactions between the rarefaction, shock, and detonation waves. The size and shape of the dead zone is heavily dependent on the relative timings and strengths of these interactions. As mentioned in the review article by Handley et al.⁷, detonation diffraction experiments are very sensitive to initial conditions and explosive composition and show significant variability between similar experiments. This sensitivity is observed in the numerical simulations as well which has made this class of experiments an ideal case for assessing the accuracy and capabilities of reactive models but also indicates the need for sufficient validation in the context of each study.

Adequate mesh resolution for the convergence of the numerical solution must also be determined for the case of the desensitization model. This follows from reactive models such as I&G which require finely resolved simulations to capture the phenomenology that is designed into the equations. Thus, the validation section also explores the resolution required to adequately capture the reaction and desensitization processes.

The experimental study of dead zone formation usually involves the diffraction of a detonation wave at a sharp edge, known as corner turning experiments. The desensitization model implemented for this study is validated through a series of test cases involving this geometry starting with the hockey puck geometry which was used in the study by DeOliveira et al.²⁶ that introduced the desensitization model. Two variations of the material of the corner are considered. One has rigid walls, as in the original study, and the second has steel, modeled as an elastic-plastic material. Lastly, the implementation is also assessed in the case of the Jack Rabbit experiments which provide a much more challenging configuration and for which there is useful experimental data.

The explosive composition B used in the booster device has not been previously modeled with the desensitization model by DeOliveira et al.²⁶ and the corresponding parameters are not available in literature. A procedure for the estimation of these parameters is presented in the last part of this section. It is based on experimental data on shock desensitization by Campbell and Travis⁹ which allows for the estimation of the

FIG. 1. A two-dimensional illustration of the axisymmetric hockey puck configuration. It involves a cylindrical disk of radius R and height L which is surrounded by explosive. The detonation is initiated by a hemispherical region of high pressure positioned in the middle of the top surface of the disk.

desensitization rate parameters whereas the remaining parameters are chosen so that the simulation replicates the formation of a dead zone observed experimentally by Held¹¹.

A. Detonation diffraction around a rigid corner

The hockey puck configuration considered here is shown in figure 1. It follows the experiment by Souers et al.³⁵ which used a cylindrical LX-17 explosive charge with a coaxial cylindrical cavity of $R = 19.05$ mm in radius and $L = 15$ mm in height. The equation of state and reaction parameters for the explosive are from the study of Tarver³⁶ and the desensitization parameters are obtained from DeOliveira et al.²⁶ and are both presented in the appendix. The LX-17 is initiated by a hemispherical TATB charge embedded within the LX-17 at the base of the cavity. The experimental study used streak cameras to record breakout times along the side and base of the charge as well as x-ray photography to examine the detonation front and showcased the formation of dead zones in LX-17.

Figure 2 shows numerical results for the hockey puck configuration using rigid walls, as done in the study by DeOliveira et al.²⁶. The setup is axisymmetric and the explosive is initiated by a hemispherical region of 7.68 mm in radius filled with products at the pressure of 31.46 GPa. This setup causes the formation of a hemispherical detonation that is well established when it reaches the corner.

The detonation is diffracted and weakened as it expands around the corner, while it continues to propagate undisturbed in the region above the corner. In the area shadowed by the corner, the reactions stop and a curved inert shock compresses and desensitizes the explosive as can be seen in the first frame of figure 2. The detonation continues to expand traveling faster than the inert shock and eventually impacts the vertical

FIG. 2. Density schlieren plots of the numerical solution for the hockey puck configuration with resolution $\Delta x = 10 \mu\text{m}$ at times (a) $2.6 \mu\text{s}$, (b) $3.3 \mu\text{s}$ and (c) $3.8 \mu\text{s}$. The weak lateral shock formed after the detonation reaches the corner leads to the desensitization of the explosive and the formation of a dead zone. The results are directly comparable to the original study of the desensitization model²⁶.

FIG. 3. Comparison of the dead zone formed in simulations of increasing resolution for the hockey puck configuration with a rigid corner at $t=4.8 \mu\text{s}$. The schlieren plot corresponds to a resolution of $10 \mu\text{m}$, the orange contour corresponds to $20 \mu\text{m}$ and the blue contour corresponds to $40 \mu\text{m}$. The detonation has sufficiently converged for a cell size of $20 \mu\text{m}$ but the shape of the dead zone requires increased resolution.

surface of the rigid body. This forms a region in the explosive where no reactions have taken place resulting in a dead zone that persists for the rest of the simulation.

The appropriate resolution of the computational mesh was determined by performing a convergence study. This validation test case has a base resolution of $160 \mu\text{m}$ and was adaptively refined using two levels of refinement of a factor of four each, resulting in an effective resolution of $10 \mu\text{m}$. Figure 3 shows the dead zone contour for solutions of increasing resolution. The shape of the dead-zone requires at least $10 \mu\text{m}$ to be adequately resolved while the position and shape of the

detonation front have converged at the $20 \mu\text{m}$ resolution. It should be noted that for resolutions of $80 \mu\text{m}$ or lower, the explosive is immediately desensitized, before the hemispherical detonation is established. This reinforces the notion that the effect of the desensitization model requires significant resolution to manifest and even more resolution to ensure convergence. The results agree with the original study by DeOliveira et al.²⁶ which validates the implementation used in the study.

B. Detonation diffraction around a solid corner

We consider the same configuration as used in section III A but with a solid material replacing the rigid corner. The material is steel and is governed by the elastic-plastic formulation along with the hyperelastic EOS from Barton and Drikakis³⁷ and the perfect plasticity model of constant yield stress³⁸ (material parameters are presented in the appendix). The addition of a high sound speed and high impedance material will introduce a fast shock wave that propagates in the confining material and reaches the explosive region shadowed by the corner ahead of the weak lateral shock that forms from the diffraction of the detonation. This has the potential to desensitize a larger portion of the explosive and produce a bigger dead zone.

The explosive is initiated by a hemispherical region of high pressure products. Figure 4 plots the numerical solution of the detonation diffracting around the solid corner at selected times. Initially, the propagation of the detonation along the steel disk generates a shock wave in the solid. This shock propagates within the solid to reach the vertical side of the corner and transmit a shock into the explosive. This is in addition to the lateral shock formed by the diffraction of the detonation. These two shock waves are not strong enough to induce reactions in the explosive and they jointly desensitize the explosive.

In subsequent times, the detonation expands and propagates

FIG. 4. Density schlieren plots of the numerical solution of the hockey puck configuration with a solid corner and resolution $\Delta x = 10 \mu\text{m}$ at times (a) $2.6 \mu\text{s}$, (b) $3.3 \mu\text{s}$ and (c) $3.8 \mu\text{s}$. The shock wave formed in the solid material is transmitted into the explosive along the vertical side of the corner. This desensitizes the explosive region and leads to the formation of a dead-zone.

FIG. 5. Comparison of the dead zone formed in simulations of increasing resolution for the hockey puck configuration with a solid corner at $t=4.8 \mu\text{s}$. The schlieren plot corresponds to a resolution of $10 \mu\text{m}$, the orange contour corresponds to $20 \mu\text{m}$ and the blue contour corresponds to $40 \mu\text{m}$. The solution has sufficiently converged even for the resolution of $40 \mu\text{m}$.

round the corner. It does not penetrate the desensitized region where it is quenched and degenerates into an inert shock wave. Plot 4b illustrates the complex wave structures formed after the diffraction of the detonation. The shock wave transmitted from the solid formed an oblique shock in the explosive that has propagated farthest from the corner. This is followed by the curved inert shock generated at the corner and forms a Mach stem as it interacts with the oblique shock. The pressure generated in the region traversed by these shocks does not exceed the initiation threshold and no reactions have occurred. However, the region is completely desensitized and the expanding detonation upstream is quenched as it encoun-

ters this region. The locus of interaction between the Mach stem formed by the two inert shock waves and the detonation is approximately the boundary of the formed dead zone.

The configurations of rigid and solid corner show differences in both the diffraction of detonation and the formed dead-zone. The detonation in the case of the solid hockey puck is slightly slower in reaching the corner because of some energy lost in deforming the solid. However, the detonation around the solid corner expands faster than around the rigid corner because the solid corner has become more rounded by the passage of the detonation. Already at $2.6 \mu\text{s}$ after initiation, the detonation in the solid corner configuration has acquired significant curvature while in the rigid case, detonation has not been established below the height of the corner. Consequently the dead zone formed next to the solid corner is smaller than in the case of the rigid corner. However, the dead zone of the solid corner is longer in height due to desensitization by the oblique shock wave transmitted from within the solid. Overall, the shape of the dead zone is determined by the interaction between the detonation wave, the lateral shock that is formed by the diffraction of the detonation at the corner and the shock traveling through the solid and into the explosive region shadowed by the corner. A faster diffraction of the detonation which occurs due to the deformation of the solid corner or alternatively by increasing the radius of the puck and producing a stronger detonation, will lead to the formation of a smaller dead zone.

A convergence study was performed for the configuration of the solid corner and can be seen in figure 5. The numerical solution of this configuration has adequately converged for a resolution of $40 \mu\text{m}$ even in terms of the shape of the dead zone. This indicates that the resolution required for convergence depends on the shape complexity of the dead zone. As this can not be determined a priori, appropriate resolution studies are required for each application.

FIG. 6. Illustration of the axisymmetric configuration used in the Jack Rabbit experiments. It involves a hemispherical ultra-fine TATB charge placed on top of a steel disk. These are embedded in a cylindrical LX-17 charge with aluminum plates at its bases (only the bottom one is shown). The uTATB is initiated by a detonator housed in the steel plate which is represented in the simulations by a high pressure region (gray area). The points on the outer surface of the aluminum disk indicate the positions where the speed of the plate is measured. The distances correspond to the PT5 variation.

C. The Jack Rabbit experiments

The desensitization model is further validated against the “Jack Rabbit” experiments performed at Lawrence Livermore National Laboratory³⁹. These are a series of five experiments (named PT3-7) with a complex setup that have been specifically designed to assess mathematical models of detonation in terms of detonation diffraction and desensitization. Several studies have considered the numerical simulation of these experiments using the most popular reactive models, including the one used in this study¹⁰ as well as CREST³⁰ and more recently WSD(T)⁴⁰. These studies have shown reasonable agreement with the experiment but neither has demonstrated a complete match and the discrepancies vary to different degrees for each configuration. It is generally accepted that the numerical results are very sensitive to EOS and reaction rate parameters and that careful calibration is required for a more accurate match.

The configuration of this experiment can be seen in figure 6. The detonation is initiated at the center of the uTATB charge and develops a hemispherical detonation front that is transferred to the LX-17 charge. The existence of the steel plate forces the detonation to diffract around it while a shock propagates through the steel plate and into the explosive region between the two plates. The shock is designed to be weak enough to desensitize the explosive in that region and lead to

the formation of a dead zone. The experimental setup used photon Doppler velocimetry (PDV) to measure the axial velocity along the lower aluminum plate in addition to x-ray photography.

The simulations were performed using explosive material parameters from the study of Tarver³⁶ for both uTATB and LX-17 and from the work of Barton and Drikakis³⁷ for the metals which are provided in the appendix. Air is modeled as an ideal gas with $\gamma = 1.4$. Figure 7 shows the numerical solution at selected times for the PT5 configuration. The first plot shows the detonation wave establishing in the ultra-fine TATB. It is then transmitted into the LX-17 and propagates along the steel disk. At the same time, a shock propagates in the steel plate and is transmitted into the lower explosive region. It does not induce any reactions in the explosive but completely desensitizes a large region of the explosive between the two disks.

The detonation is diffracted when it reaches the end of the steel disk and forms a weak shock which desensitizes a small pocket of explosive next to the disk, similar to the cases discussed in sections III A and III B. This is in addition to the larger region of desensitized explosive between the two metal disks. As the detonation turns around the steel plate and moves into the desensitized region, the reactions stop and it is reduced to an inert shock propagating in the reactant. The inert shock wave moves towards the axis of symmetry of the configuration while a detonation propagates radially outwards into the undisturbed explosive. This is evident by the curved shape of the lower aluminum plate caused by the difference between the forces applied by the detonation and the inert shock. The point where there is a change in the curvature of the aluminum disk indicates the approximate radial extent of the dead zone. Meanwhile, the inert shock propagating in the desensitized region is focused on the axis of the configuration which strengthens it and initiates reactions in that region. However, it is promptly extinguished as it begins to propagate outwards and degenerates into an inert shock once again as seen in the last plot of figure 7.

The comparison between the numerical and experimental axial velocity values and resulting dead zone for the PT5 experiment is shown in figures 8 and 9. Our results show good agreement with the experiment in terms of peak axial speeds and resulting dead zone. The detonation first impacts the aluminum plate somewhere between the 45 mm – 55 mm as in the experiment. In terms of jump off times, best agreement is seen for positions outside the point of first impact, where the detonation propagates. However, the numerical solution shows a slightly slower propagation of the detonation as indicated by the increasing discrepancy in larger radial distances. This fact, in conjunction with the somewhat bigger dead zone of the numerical solution indicate that the desensitization parameters should be adjusted to produce less desensitization, as is also mentioned by Tarver¹⁰. In the region where the inert shock propagates (inside the point of first impact), the numerical solution predicts a faster traveling shock wave than seen in the experiment which suggests that the reactants EOS require minor calibration. Last, it is important to note that the ignition seen at the region near the axis of the plate caused a rapid in-

FIG. 7. Plots of the numerical solution of experiment PT5 of the Jack Rabbit experiments³⁹ at times (a) 2 μ s, (b) 4 μ s, (c) 7 μ s, (d) 12 μ s, (e) 17 μ s and (f) 19 μ s. As the spherical detonation propagates along the steel disk, an inert shock is transmitted into the explosive on the other side of the disk. This desensitizes a large region of the explosive which remains unreacted as was seen in the experiment.

crease of the velocity at the center of the plate which is also seen in the experimental results.

A final distinction between the numerical and experimental results is seen in the speed of the aluminum plate after the initial peaks. The experimental data show constant velocity for the plate whereas the numerical results predict oscillating values. The oscillations of the numerical simulation are caused by the consecutive reflections of the shock wave inside the aluminum plate. The lack of oscillations in the case of the experiments is probably due to spallation. As the plate is bent, fragments break off and interfere with the velocimeter which registers the constant velocity of the fragments instead of the plate velocity.

D. Desensitization model parameters for composition B

The most common explosive used in mining boosters has been composition B (RDX,TNT) which is progressively being replaced by pentolite (PETN,TNT). For both of these explosives there exist validated parameter sets for the regular I&G reactive model. However, the desensitization model of DeOliveira et al.²⁶ has only been used for the TATB-based explosive LX-17 and no parameters exist for either of these explosives. Fortunately, one of the original studies on shock desensitization had used composition B⁹ and includes the necessary experimental data to determine the parameters for the desensitization model. Furthermore, dead zone formation in

FIG. 8. Comparison of experimental (solid lines) and numerical results (dashed lines) for the Jack Rabbit experiment PT5. The plot shows axial velocity measured at given radial distances from the center of the aluminum plate.

composition B has been observed experimentally which allows for the validation of the selected parameters. For these reasons the study of the booster configuration considers composition B as the booster explosive instead of pentolite.

The desensitization rate requires two parameters, A and ε . These were determined based on the experimental data on desensitization time over shock pressure taken from the study of composition B-3 (60/40 RDX/TNT)⁹ of initial density 1.737 g cm^{-3} . The study provides just two data points but the form of the desensitization rate does not allow for both to be satisfied as discussed in section II A. Parameter ε is only required to be a small number, so $\varepsilon = 10^{-3}$ is chosen as in the original study. Parameter A is determined using the analytical solution of the desensitization source term (8) where we require that the desensitization variable ψ increases from 0 to 0.98 for the desensitization time and applied pressure that are provided by the experimental study. The two experimental measurements provide two values for A and their average is selected so that it is equally close to both data points. This yields a value of $A = 3.5 \times 10^{-3} \text{ Pa}^{-1} \text{ s}^{-1}$.

Parameters for the equation of states and reaction rate for composition B are taken from the study of Urtiew et al.⁴¹ which considered a 63/36/1 RDX/TNT/wax variant of composition B with initial density 1.717 g cm^{-3} . The density threshold for initiation was set so that it can be ignited by shock waves of 0.5 GPa or stronger. This does not agree with the study of Campbell and Travis⁹ in which shock waves up to 2.4 GPa did not ignite the explosive. The discrepancy is attributed to the different composition B variant used for each study. To ensure that the desensitization behavior is replicated, the density threshold of the pristine explosive was raised to $\alpha_0 = 0.1$ so that shock waves of approximately 2 GPa do not ignite it.

Two additional parameters are required by the desensitiza-

tion model which relate to the change of the reaction rate when the explosive is desensitized. These are α_1 which represents the increased density threshold for initiation and λ_c which restricts the growth terms until some reactions have occurred. There is no standard method for determining these parameters and following the example of DeOliveira et al.²⁶, they are determined by exploring the range of valid values $[0, 1]$ and selecting the set of values that reproduces a dead zone with dimensions that have been experimentally observed.

An experimental study on dead zone formation in composition B was performed by Held¹¹. The author used a semi-cylindrical charge of composition B with RDX/TNT ratio of 65/35 that had an average density of 1.72 g cm^{-3} . The charge had a radius of 29 mm and was initiated by a cylindrical charge of 95/5 RDX/wax and a radius of 4 mm. The detonation from the small charge passed into the semi-cylindrical charge where it was diffracted and was recorded using a streak mask positioned on the flat surface of the semi-cylindrical charge. The results confirmed the formation of a dead zone located in a zone that extends up to 20 mm in radial distance from the initiation axis.

The parameter values $\alpha_1 = 0.5$ and $\lambda_c = 0.2$ were found to reproduce the formation of a dead zone for the configuration used in the experimental study by Held¹¹. The dead zone formed in the simulation is shown in figure 10 for solutions of increasing resolution. It should be noted that the simulation is performed in a two-dimensional axisymmetric domain and thus the explosive charge is a complete cylinder instead of a semi-cylinder as in the experiment. Thus, it is expected that the resulting dead zone will be smaller than reported in the experimental study due to additional release waves that weaken the detonation in a semi-cylindrical charge.

IV. RESULTS

We perform numerical simulations of the initiating system that includes a detonator and a booster for the purpose of assessing the initiating capability of different types of detonators in this configuration. In particular, we examine the impact of the material and thickness of the shell of the detonator on the amount of booster explosive that is ignited and consumed. Three metal materials are considered: aluminum, copper and steel with thicknesses of 0.5 mm and 1 mm, as in the first part of the study. The three materials vary in terms of density and impedance. Aluminum has the lowest density (2.71 g cm^{-3}) and impedance which is closest to the impedance of the booster explosive composition B. The density of copper (8.93 g cm^{-3}) and steel (8.03 g cm^{-3}) is approximately three times larger than aluminum with steel having a higher speed of sound which translates to the highest impedance of the materials considered.

The details of the detonator and booster configuration used in the simulations are presented first. Then, the initiation of the booster is examined without the use of a desensitization model in order to establish an understanding of the initiation process in the absence of desensitizing effects. The simulations are repeated with the inclusion of the desensitization

FIG. 9. Comparison of dead zone formed in (a) experiment and (b) numerical simulation for the Jack Rabbit experiment PT5.

FIG. 10. Contour plot of the dead zone formed in composition B after the detonation diffracts into the wider cylindrical charge for simulations of increasing resolution starting with $\Delta x = 40 \mu\text{m}$ (blue), $\Delta x = 20 \mu\text{m}$ (orange) and $\Delta x = 10 \mu\text{m}$ (green).

model which enables the assessment of the impact of desensitization on booster initiation as well as the comparison of the initiating capability of the different types of detonators considered. Following this analysis, an adjusted configuration of the initiating system featuring a shorter detonator is examined which is less susceptible to shock desensitization effects.

A. The configuration of the initiating system

The design considered in this study is based on the Global Booster device produced by Orica. This device consists of multiple parts and has a complex design that enables the use of different types of detonators, detonator cord and even a sensitizing PETN bottle. The design adopted here, shown in figure 11, is simpler and axisymmetric to allow for a two-dimensional representation and enable high resolution simulations of the whole initiating system.

The booster is made out of an outer shell filled with the ex-

plosive and a cap on top. There is a cylindrical cavity along its axis for placing the detonator. The shell has a cylindrical shape of 25 mm in radius and 130 mm in length with a rounded lower corner of 20 mm in radius and is made from a thermo-plastic polymer of 1 mm in thickness. It is modeled as a fluid using the shock Mie-Grüneisen EOS with parameters corresponding to Polymethyl Methacrylate (PMMA) from the work of Hamada et al.⁴². The high pressures imparted on the plastic shell by detonation waves justify the assumption of purely fluid behavior given the low yield strength of plastics.

The booster explosive is composition B which has been widely used in mining and for which there exist validated I&G parameter sets and extensive experimental studies. The parameter set is taken from the study of Urtiew et al.⁴¹ and the desensitization model parameters were determined as described in section III D. The initial density of composition B is 1.717 g cm^{-3} and the volume of the booster is 233.36 cm^3 which translates to approximately 400 g as in the Global Booster.

The design of the detonator also follows the specifications of an industrial detonator and specifically of the i-kon II by Orica. This has a copper shell of 3.3 mm in radius and 89 mm in length with a thickness of 0.5 mm. It is filled with 780 mg of the explosive PETN which is placed at the base of detonator, deep inside the booster explosive. The PETN is modeled as a two phase explosive with the I&G reactive model and parameters from the study by Tarver et al.⁴³. The explosive charge is sealed with a copper cup of 6.2 mm in length. The metal shell and cup of the detonator are both modeled with the elastic-plastic formulation.

The detonator and booster configuration is initiated by a small hemispherical region of high pressure PETN products as shown in figure 11 (with red). The expansion of the products leads to a prompt detonation of the PETN base charge which generates a shock in the detonator shell and subsequently in the explosive of the booster. The material surrounding the booster is water which emulates the aquarium tests commonly used in the study of explosive devices. The water is modeled with the stiffened gas EOS as in the first part of the study¹⁷. The numerical solution is computed with a resolution of $40 \mu\text{m}$ which was found adequate for the convergence of the detonation front and of the size and shape of the dead zones formed.

FIG. 11. The booster and detonator configuration have an axisymmetric design which is based on actual devices used in the mining industry. The booster has a plastic shell (shown in gray) and is filled with approximately 400 g of composition B (shown in beige). The detonator is placed inside the booster charge and has a metal shell (shown in purple). It contains a base charge of 780 mg of PETN (shown in blue) which is sealed with a copper cup (shown in green). The detonator is initiated by a high pressure region (shown in red).

B. Initiation of the booster without desensitization

We initially examine the booster initiation process without accounting for desensitization effects and modeling the explosive with the regular pressure-based I&G reaction rate. The aim is to investigate the intricate processes involved in the initiation and propagation of a detonation in the booster and to provide a basis for evaluating the impact of desensitization.

The successful initiation of the explosive in the booster depends on several factors in addition to potential desensitization effects. Initially, the shock generated by the detonator must lead to a run to detonation distance that is well inside the boundaries of the explosive. Furthermore, the established detonation should have curvature that does not exceed the limits for a self-sustained detonation and be able to expand and propagate in the entire booster explosive, including the region above the detonator. Lastly, the detonation wave must not be critically disturbed by any of the waves generated from the interaction of the detonation with the material boundaries of the detonator and the booster shell which can affect the flow in the reaction zone and influence the propagation of the detonation wave.

The initiation of the booster by the 0.5 mm aluminum detonator is shown in figure 12. The impulse produced by the detonator leads to the formation of an extensive detonation front mainly downstream of the detonator while a shock of approximately 1 GPa – 3 GPa (at 3 μ s) is transmitted from the sides of the detonator and propagates upwards without inducing reac-

tions. The detonation quickly expands and increases its curvature. When it first impacts the outer shell of the booster, the detonation is divided into two fronts, one propagating downwards and one upwards as seen in plot 12b. Both fronts continue to propagate undisturbed until all of the explosive is consumed. A curved shock front is transmitted into the surrounding water which expands outwards and is supported by the expansion of the explosive products.

In the configuration featuring the 0.5 mm copper detonator shell, the ignition of the detonator induces a weaker pulse in the explosive of the booster. This is due to the larger impedance difference between copper and composition B which leads to a reduced wave transmission coefficient. The buildup to detonation is slower and the run to detonation distance is longer. Nevertheless, a detonation is established in the region below the detonator which progressively expands leading to upwards propagation (figure 13). The detonation propagates through a large region of explosive that has been compressed by the passage of the shock emanating from the side of the detonator. The shock strength is slightly lower than in the configuration with the aluminum detonator and in the range of 1 GPa – 2 GPa. However, the detonation is not affected by desensitization effects since the pressure-based reactions are activated regardless of the state of the explosive ahead. The configuration featuring the steel detonator showed an almost identical behavior to the case of the copper detonator.

In all considered configurations, the initiation and propagation of detonation in the explosive of the booster follows the same pattern. The ignition of the detonator transmits an elliptic blast wave into the booster. Initially, detonation is only established in the region below the detonator and subsequently diffracts and attains upwards propagation until the explosive is completely consumed. The copper and steel detonators showed slower formation of the detonation but apart from a time delay, the detonation progressed in the same way and generated a similar wave in the surrounding water. The shock wave transmitted from the side surface of the detonator was too weak to directly initiate the explosive in that region and resulted in the pre-shocking of a portion of the booster explosive in all configurations of the 0.5 mm detonator shells.

C. The effect of detonator shell material

The initiating capability of detonators placed within a booster is examined using the reactive model that includes shock desensitization. An ideal initiation of the booster would lead to the detonation of the entire explosive of the booster and extract the maximum energy from the device. However, the variable strength of the blast wave generated by the detonator has been seen to compress parts of the explosive of the booster without initiating reactions which has the potential to desensitize the explosive and lead to the formation of regions of unreacted explosive.

Figure 14 shows plots of the initiation of the booster by the 0.5 mm aluminum detonator. The impulse generated by the detonator in the booster leads to the formation of a deto-

FIG. 12. Plots of pressure (left) and density (right) depicting the initiation of the booster explosive by the 0.5 mm aluminum detonator without accounting for desensitization at times (a) 3 μ s, (b) 6 μ s and (c) 9 μ s. A detonation is promptly established and propagates through the entire charge.

nation that is virtually indistinguishable from the case of no desensitization in the times up to 3 μ s. Even at later times, the detonation of the explosive in the region below the detonator is the same as in the case of no desensitization. However, the region above the base of the detonator shows distinct behavior as is evident 6 μ s after initiation, in figure 14b. The inert shock transmitted from the side of the detonator has desensitized part of the explosive which prevents it from reacting. Nevertheless, the expansion of the detonation front is fast enough to overtake the desensitizing shock wave which gets slower and weaker as it expands and the detonation manages to propagate around the desensitized region. Inside this region, the detonation is quenched and reduced to an inert shock.

Once the detonation moves ahead of the desensitized region, it propagates steadily in the booster area above the detonator charge and consumes the remaining explosive. The unreacted region persists throughout the rest of the simulation and is slightly compressed by subsequent pressure waves arising in the flow field. The explosive products expand and support the shock generated in the water.

The initiating system with the 0.5 mm copper detonator shows more profound differences from the case of no desensitization. The detonation front established in the region below the detonator is smaller and restricted close to the axis of the configuration. The weaker pulse transmitted from the

sides of the detonator is not able to induce reactions similar to the previous cases. The detonation expands into the pristine explosive downstream and attains enough curvature to begin upstream propagation. However, this process is slower than in the configuration with the aluminum detonator which allows the inert shock to desensitize a large region of the explosive next to the detonator. Once the detonation encounters this region, it is quenched and degenerates into an inert shock (figure 15). This leaves the majority of the explosive of the booster in the unreacted state.

The configuration featuring the steel detonator has largely similar results to the copper detonator. The detonation in the booster is only established in the region below the detonator whereas a large region above is desensitized which prevents the detonation from propagating upwards. The resulting dead zone has very similar shape but is slightly smaller due to the detonation wave establishing marginally faster and propagating further upwards before encountering the desensitizing shock.

The desensitization observed in the case of the copper and steel detonator is critically extensive. The majority of the explosive has not been consumed as the formation of a dead zone blocked the propagation of the detonation in the region above the detonator base charge. In the configuration of the 0.5 mm copper detonator, the remaining explosive has a mass

FIG. 13. The configuration with the 0.5 mm copper detonator and without desensitization leads to the complete detonation of the booster ($t = 9 \mu$ s).

FIG. 14. Plots of pressure (left) and density (right) depicting the effect of desensitization on the initiation of the booster explosive by the 0.5 mm aluminum detonator at times (a) 6 μ s, (b) 9 μ s and (c) 12 μ s. Part of the explosive is desensitized and remains unreacted while the detonation propagates around it and consumes most of the booster charge.

of 318(1) g which amounts to 80% of the explosive whereas the 0.5 mm aluminum detonator produced a 24(1) g dead zone which is only 6% of the booster explosive. As a consequence, the shock produced by the booster with the copper or steel detonator is weaker and will decay faster because of the lower support from the expansion of the explosive products. This will inhibit the ability of initiating system to ignite the surrounding explosive and potentially lead to failure in the initiation of the blasthole.

D. The effect of detonator shell thickness

We examine the effect of increasing the thickness of the detonator shell to 1 mm. The increased thickness will weaken the impulse produced by the detonator leading to slower establishment of the detonation. At the same time, the desensitizing shock wave transmitted from the side of the detonator will also be weaker and thus, the desensitization will be slower as well. The combined result of these processes will depend on their relative timings and strengths and will determine the extent of dead zone formation.

The initiation of the configuration with the 1 mm aluminum shell, shown in figure 16, leads to the formation of a curved detonation front below the detonator by the time mark of 5 μ s.

FIG. 15. Plot of the desensitization of the booster explosive initiated by the 0.5 mm copper detonator ($t = 9 \mu$ s).

Compared to the case of the 0.5 mm aluminum detonator, the expansion of the detonation front is slower but attains enough curvature to begin upwards propagation. The shock transmitted from the sides of the detonator has desensitized a larger region which is rendered unable to detonate. Thus, the detonation can only propagate into an increasingly narrower region of pristine explosive. However, a sufficient portion of the explosive remains able to detonate which allows the detonation to propagate around the completely desensitized and non-reacting region. The detonation continues to propagate upwards and the majority of the explosive in the booster is consumed. The resulting dead zone has a mass of 68(1) g which is approximately three times larger than in the case of the thin aluminum detonator and 17% of the total explosive mass.

The copper and steel detonators with a thickness of 1 mm do not ignite the explosive in the booster at all. The thicker shell absorbs much of the energy from the explosion of the detonator and the generated blast wave is too weak to lead to a shock to detonation transition. Figure 17 shows the inert shock propagating in the explosive for the configuration with the copper detonator which is similar for steel as well. The shock is desensitizing the explosive but its effect is of no importance since a detonation has not been established.

FIG. 16. Plots of pressure (left) and density (right) depicting the initiation of the booster explosive by the 1 mm aluminum detonator at times (a) 6 μ s, (b) 9 μ s and (c) 12 μ s. The generated blast wave is weaker compared to case of the thinner detonator and the detonation is slow to establish leading to the formation of a more extensive dead zone in the explosive.

E. The effect of detonator positioning

The outcomes of the previous sections indicate that the initiation process of the booster is influenced by the desensitization of the explosive region next to the detonator which hinders the upwards propagation of the detonation. On the other hand, most configurations do manage to establish detonation in the region below the detonator which propagates into pristine explosive undisturbed by desensitization effects. This motivates the examination of whether the positioning of the detonator can be adjusted to reduce the impact of shock desensitization and lead to more efficient initiation of the booster.

We consider a configuration where the detonator is withdrawn by 60 mm towards the top of the booster and has a length of 30 mm. The base charge of the detonator remains the same as it is only 13 mm in length. This design leaves the majority of the booster explosive below the base charge of the detonator and has the potential to increase the efficiency of the booster for the configurations that are able to initiate the booster explosive but are prone to extensive desensitization such as the 0.5 mm copper and steel shell. However, the construction of a short detonator might be challenging from a

design and manufacturing point of view as it makes it difficult to fit the additional components and circuitry required.

Figure 18 shows plots for the configuration of the withdrawn detonator with a 0.5 mm thick copper shell and similar results are observed for the case of the steel shell as well. The detonation is established downstream while the region next to the detonator is being desensitized. Similar to the configuration of the longer detonator, the detonation does not manage to propagate upwards before the explosive is desensitized. However, the detonation downstream propagates as a single front and consumes all of the explosive below the detonator. The resulting dead zone has mass of 71(1) g which is 17% of the total mass of the booster. This will have an impact on the impulse generated by the booster but since the majority of the charge has detonated, the performance of the initiating system is greatly increased compared to the configurations of the long detonator in which all of the explosive above the detonator base charge did not react.

FIG. 17. The configuration with the 1 mm copper detonator fails to initiate the booster explosive ($t = 9 \mu$ s).

FIG. 18. Plots of the booster configuration with a withdrawn copper detonator at times (a) $6\mu\text{s}$ and (b) $10\mu\text{s}$. The explosive upstream is desensitized and remains unreacted but the detonation propagates downstream undisturbed, consuming most of the explosive.

V. CONCLUSIONS

The study presented in this article uses numerical simulations to investigate the initiating capability of detonators placed within a booster device, as used in initiating systems for mining blastholes. The mathematical representation follows a multiphysics methodology which makes use of several mathematical models including the Euler equations for the fluid materials, a two phase reactive model for the explosive and an elastic-plastic formulation for the metal shell of the detonator.

The reactive model is an extension of the I&G formulation which accounts for shock desensitization and enables the study of the impact of this phenomenon on the initiation of the booster explosive. The implementation of the model is validated against a test case which involves detonation diffraction around a rigid corner as in the original article on the desensitization model²⁶. This is extended to the case of a solid corner and even further by examining the configuration of the Jack Rabbit series of experiments³⁹.

The design of the detonator and booster initiating system is based on actual industrial devices. The explosive used in booster devices is composition B, for which a calibrated I&G parameter set exists in literature⁴¹. However, the desensitization model has not been previously applied to this explosive and no parameters exist. Following the example of DeOliveira et al.²⁶, a set of desensitization model parameters for composition B were determined based on experiments by Campbell and Travis⁹ and Held¹¹.

The validated computational implementation is used to perform simulations of the initiation process of the booster by different types of detonators. The considered detonators have three different shell materials: aluminum, copper and steel and two thickness values of 0.5 mm and 1 mm. Results show that all configurations that are able to initiate the explosive in the booster are affected by shock desensitization which leads to the formation of dead zones, even though their size varies greatly depending on the type of detonator, from 6% to 80% of the total explosive mass.

The observed shock desensitization and dead zone formation process is a result of the variable strength of the blast wave produced by the detonator which was demonstrated in the study of the isolated detonators in the first part of this work¹⁷. The shock in the axial direction is stronger and leads to the establishment of a detonation in the region below the detonator whereas the section of the blast wave transmitted from the side of the detonator is weaker and does not initiate reactions. The weak shock progressively desensitizes an expanding region of the explosive next to the detonator. The extent of the resulting dead zone depends on the overall rate of detonation formation and expansion compared to the desensitizing shock.

In the case of the 0.5 mm detonators, the aluminum shell configuration exhibits the quickest formation of the detonation wave which expands and propagates upwards. The detonation intercepts the expansion of the desensitizing shock resulting in a limited dead zone that has the smallest size of all configurations. In contrast, the detonation in the copper and steel shell configurations take longer to establish which allows the desensitizing shock to expand all the way to the boundary of the booster. The detonation is quenched when it encounters the desensitized region leaving the majority of the explosive unreacted. In configurations with thicker shells, the aluminum detonator leads to the formation of a larger dead zone compared to the thinner shell but the detonation still manages to propagate in the region above the detonator base charge and consume the majority of the explosive of the booster. The detonators with the thick copper and steel shell did not ignite the booster explosive at all and only a weak inert shock was formed in the booster device.

The differences in the initiating capability of detonators, as determined by the proportion of the booster explosive remaining unreacted, is caused by the difference in the strength of the impulse produced by the detonator. The detonation of the detonator base charge generates a shock wave in the metal shell of the detonator which is transmitted into the booster explosive. The ratio of the transmitted over the incident wave is determined by the impedance difference between the material of the shell and the explosive of the booster. Aluminum has the smallest impedance difference to composition B leading to the transmission of a stronger blast wave and the prompt formation of a detonation wave compared to the other materials considered. Copper and steel have higher impedance differences to composition B resulting in a reduced transmission coefficient. Further, increasing the thickness of the shell also leads to a weaker impulse due to the increased distance traveled inside the metal shell in which the shock wave attenuates.

The blast wave produced by each type of detonator determines the fine balance between detonation and desensitization which governs the formation of the dead zone in the booster. This highlights the importance of the near field characteristics of the blast wave in the initiating capability of detonators. As was shown in the study on isolated detonators¹⁷, the blast wave generated in water varies significantly depending on the shell of the detonator but the differences do not persist in the far field of the detonator. In particular, the aluminum detonator exhibits significantly larger blast wave magnitude in both the axial and normal direction compared to the copper and steel detonators despite the similar blast waves recorded in the far field for all detonators. These differences correlate well with the differences in the initiating capability observed in this study and strengthen the argument that assessing the initiating capability through the underwater test should consider the near field properties of the blast wave whereas the far field properties are not able to capture these variations.

The critical influence of shock desensitization on the initiation of the booster warrants its consideration in the design of initiating systems. The use of lighter materials for the detonator shell with similar impedance to the explosive of the booster should be preferred since they allow the transmission of a stronger impulse into the explosive and lead to prompt reactions. In addition, this study considered an alternative design which features a short detonator placed higher in the booster. This was shown to lead to the detonation of a larger portion of the explosive in configurations where a detonation is established but is unable to propagate upwards due to extensive desensitization in the area neighboring the detonator. Further investigations may consider alternative solutions such as damping the shock transmitted from the sides of the detonator using a specialized material or an air gap.

The work presented in this study also showcases the capabilities of the employed numerical methodology and its potential to aid in the design and assessment of initiating devices. However, experiments involving configurations of initiating systems, such as the one considered here, do not exist in literature and are highly needed in order to establish the actual impact of shock desensitization and the extent of the agreement with the numerical results. In addition, the use of a desensitization model is still a novel development and there exist several alternative reactive models that have shown promising results in capturing shock desensitization using different approaches. The explosives community is showing an active interest in the development of these models which is supported by a range of new experiments using improved diagnostic techniques. The high quality experimental data are expected to provide valuable insight for the advancement of high-fidelity reactive models which will directly benefit the use of computational techniques for the study of initiating systems.

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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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Appendix: Material Parameters

The parameter sets for the equations of state and reaction rates for the materials used in the simulations of this study are presented in tables I-V.

Parameters	LX-17 ³⁶		uTATB ³⁶		PETN ⁴³		Composition B ⁴¹	
	Reactants	Products	Reactants	Products	Reactants	Products	Reactants	Products
Γ_0	0.8938	0.5	0.8938	0.5	0.5675	0.57	0.8938	0.5
A [10^{11} Pa]	778.1	14.8105	632.07	12.05	202.8	10.32158	778.1	5.242
B [10^{11} Pa]	-0.05031	0.6379	-0.04472	0.6025	-0.03752	0.9057	-0.05031	0.07678
R_1	11.3	6.2	11.3	6.2	10	6	11.3	4.2
R_2	1.13	2.2	1.13	2.2	1	2.6	1.13	1.1
Q [10^6 m ² s ⁻²]	0	3.94	0	3.69	0	6.343	0	0
c_V [m ² s ⁻² K ⁻¹]	1305.5	524.9	1381.7	555.6	1528.4	562.4	1448	582.4
ρ_0 [kg m ⁻³]	1905	1905	1800	1800	1778	1778	1717	1717

TABLE I. JWL equations of state parameters for the explosives.

Parameters	LX-17 ³⁶	uTATB ³⁶	PETN ⁴³	Composition B ⁴¹
I [μs^{-1}]	4×10^6	4×10^6	400	4×10^6
α	0.22	0.22	0	0.1
b	0.667	0.667	0.667	0.667
x	7	7	9	7
$\lambda_{ig}^{\max}$	0.02	0.071	0.01	0.022
G_1 [GPa ^{-y} μs^{-1}]	0.0045	0.22	0.001	0.014
c	0.667	0.667	0.667	0.667
d	1	1	0.01	0.33
y	3	2	1	2
$\lambda_{G_1}^{\max}$	0.8	1	0.01	0.7
G_2 [GPa ^{-z} μs^{-1}]	0.3	0.6	0.15	0.001
e	0.667	0.667	0.667	0.222
g	0.667	0.667	0.667	1
z	1	1	2	3
$\lambda_{G_2}^{\min}$	0.8	0.8	0.01	0

TABLE II. Ignition and Growth parameters for the reaction rates of the explosives.

Parameters	LX-17 ²⁶	Composition B
A [10^{-3} Pa ⁻¹ s ⁻¹]	8.9	3.5
ε	0.001	0.001
α_1	0.5	0.5
λ_c	0.01	0.2

TABLE III. Desensitization model parameters for the explosives.

Parameters	Al	Cu	Steel
ρ_0 [kg m ⁻³]	2710	8930	8030
c_0 [m s ⁻¹]	6220	4600	5680
c_V [m ² s ⁻² K ⁻¹]	900	390	500
T_0 [K]	300	300	300
b_0 [m s ⁻¹]	3160	2100	3100
α	1	1	0.596
β	3.577	3	2.437
γ	2.088	2	1.563

TABLE IV. Equation of state parameters for the metals³⁷.

Parameters	PMMA
ρ_0 [kg m ⁻³]	1180
c_0 [m s ⁻¹]	2260
s	1.82
Γ	0.75

TABLE V. Shock Mie Grüneisen equation of state parameters for PMMA⁴².