A full-scale hydrodynamic simulation of energetic component system

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A full scale hydrodynamic simulation that requires an accurate reproduction of shock-induced detonation was conducted for design of an energetic component system. A series of small scale gap tests and detailed hydrodynamic simulations were used to validate the reactive flow model for predicting the shock propagation in a train configuration and to quantify the shock sensitivity of the energetic materials. The energetic component system is composed of four main components, namely a donor unit (HNS-HMX), a bulkhead (STS), an acceptor explosive (RDX), and a propellant (BKN03) for gas generation. The pressurized gases generated from the burning propellant were purged into a 10 cc release chamber for study of the inherent oscillatory flow induced by the interferences between shock and rarefaction waves. The pressure fluctuations measured from experiment and calculation were investigated to further validate the peculiar peak at specific characteristic frequency ($\omega_c = 8.3$ kHz). In this paper, a step-by-step numerical description of detonation of high explosive components, deflagration of propellant component, and deformation of metal component is given in order to facilitate the proper implementation of the outlined formulation into a shock physics code for a full scale hydrodynamic simulation of the energetic component system.

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1. Introduction

The analysis of pyrotechnic mechanical actuation system requires a full-scale fully-integrated dynamic simulation of the fluid-solid interaction, combustion of explosives, and propellants arranged in a train configuration. The reaction of a solid-phase energetic material must be precisely calculated before transferring subsequent dynamic loading onto a contacting inert structure such as a metal or plastic that is commonly in contact with another energetic material in the train configuration. A pyrotechnical mechanical device (PMD) is typically devised with several energetic components together with inert gap materials that often play the role of shock pressure attenuator for various applications. Airbag inflator is a typical example that relies on this multi-material energetic-inert composite design that ultimately works as a single unit to achieve rapid release of high pressure gas intended for inflating the airbag for passenger safety.

The multi-material modeling and simulation is a daunting task for any single-phase hydrodynamic solver or Lagrangian structural code. Conventional multi-phase solvers also fall short in handling such tasks that require precise capturing of dynamic interface between the reacting energetic material and inert structure as well as resolving explosively fast time scale of chemical reaction associated with energetic substances which are typically experimentally calibrated and modeled to reproduce a series of calibration tests according to various military standards. In order to achieve this, a solver must be written in a fully integrated framework that strongly interacts with both fluid and solid. Furthermore, the reaction models must be built for each energetic material with unique composition and calorimetric properties. A high order numerical method must be utilized to track the rapid temporal transition during the chemical reaction which is also stable enough for smoothly linking the strain dynamics from the inert, elastic, and plastic neighboring structures.

One needs to adapt a stable multi-material interface handling algorithm based on a strongly-coupled fluid-structure interaction framework while accurately solving the chemical response of the involved high explosives, propellants, and reactive substances. In addition, the equations of state for each energetic material as well as the inert materials need to be modeled to reproduce the full scale dynamic behavior of the energetic system arranged in a train configuration.

In this paper, we have developed a multi-material hydrocode with a hybrid particle level set method for shock-to-detonation transition of energetic materials in a train configuration. A level set based reactive ghost fluid method that imposes physical boundary conditions at material interfaces is developed to reproduce the experimental data of the gap test and closed chamber test. The interface between two different materials is tracked through a hybrid particle level set method, and the flow properties near the interface is determined through the ghost fluid method. An integration with a 4th order scheme in space and 3rd order Runge-Kutta method in time is employed for precise calculations of the severely transient fluid-structure interaction problem.

The multi-material hydrodynamic simulation for a small-scale gap test (SSGT) considers an acceptor that is comprised of 97.5% RDX (cyclotrimethylene-trinitramine, C\textsubscript{3}H\textsubscript{6}N\textsubscript{2}O\textsubscript{6}), 0.5% polyisobutylene, 0.5% graphite, and 1.5% calcium stearate with initial density after pressing of 1.65 g/cm\textsuperscript{3}. Then the shock sensitivity of the explosive can be quantified. Then a full-scale simulation is conducted to analyze the performance characteristics of a pyrotechnic system in a closed chamber test, which requires a precise recreation of the shock-induced detonation processes. Test involves detonation of a composite donor consisting of HNS (hexanitrostilbene, C\textsubscript{8}H\textsubscript{12}N\textsubscript{6}O\textsubscript{12}) and HMX (cyclohexylenelene-tetrinitramine, C\textsubscript{8}H\textsubscript{8}N\textsubscript{6}O\textsubscript{8}), pressure attenuation in a stainless steel gap domain (STS), detonation of an acceptor (RDX), and ultimately a deflagration of a gas-generating propellant (boron potassium nitrate, BKN03). The purging gases into a 10cc dump chamber are subject to a subsequent monitoring of the flow oscillations due to the inherent shocks and rarefactions. The test results are used to validate the full-scale simulation results presented in this study.

2. Numerical approach

The massive analysis on the reactive system behavior during detonation of energetic components and their interaction with stainless steel containment demands a mathematical formulation that includes reactive flow models of detonation and deflagration, rupture model for metal casing, multi-material interface tracking, and hydrodynamic models for accurate capturing of various acoustic waves inherent to a globally hyperbolic system. When the external shock impact on a heterogeneous explosive is sufficiently large, the shock is enabled to further develop into a detonation through a process called shock-to-detonation transition (SDT). A shock that exceeds the minimum initiation pressure must be applied to an energetic material for this transition to occur. SDT for energetic materials occurs within a few microseconds, and relatively slower processes of thermal conduction and viscous dissipation are neglected. In effect, the time scale on the detonating chemical reaction is very fast in comparison to the hydrodynamic fluid time scale. Since detonation waves generally propagate at thousands of meters per second, the assumption that molecular diffusion, heat conduction, and viscous dissipation can be ignored in detonation dynamics is reasonable.

The dynamic response of both energetic and inert components of the given system can be described by the compressible form of the governing equations. The stress tensor that describes the structural response of stainless steel is comprised of a deviatoric stress and a hydrostatic pressure [6]. The Mie–Grüneisen equation of state (EOS) defines the pressure attained by the gap between donor-acceptor pair, while the Jones–Wilkins–Lee (JWL) EOS determines the explosive pressure resulting from the hydrothermodynamic state. The rate of chemical reaction was based on the ignition and growth kinetics [8]. The interface between any two materials was tracked through a hybrid particle level set method, while material properties in the vicinity of an interface

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**Nomenclature**

- \( \vec{U} \) : vector for conserved variables
- \( \vec{E} \) : spatial fluxes in axial direction
- \( \vec{F} \) : spatial fluxes in radial direction
- \( \vec{S} \) : source term for multi-materials
- \( \sigma_{ij} \) : Cauchy stress tensor (Pa)
- \( s_{ij} \) : deviatoric stress tensor (Pa)
- \( \rho \) : density (kg/m\textsuperscript{3})
- \( t \) : time (s)
- \( u_r \) : r-axis velocity (m/s)
- \( u_z \) : z-axis velocity (m/s)
- \( p \) : pressure (Pa)
- \( \lambda \) : burned mass fraction
- \( E \) : total energy density (J/kg)
- \( e \) : specific internal energy (J/kg)
- \( \phi \) : distance level set function
- \( c \) : speed of sound (m/s)
- \( T \) : temperature (K)
- \( R \) : universal gas constant (J/mol-K)
- \( \sigma_Y \) : yield stress (Pa)
- \( \omega \) : reaction rate (s\textsuperscript{-1})
- \( r \) : burning rate (m/s)
- \( d \) : grid size (mm)
- \( \omega_{L} \) : characteristic frequency (kHz)
- \( Z \) : acoustic impedance (Pa s/m)
were determined through the ghost fluid method. Additional description of the method can be referred from Ref. [9].

2.1. Governing equations

The compressible Navier–Stokes equations in two-dimensional coordinate system reflect the conservations of mass, momentum and energy as shown in Eqs. (1)–(3), respectively.

\[
\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{E}}{\partial x} + \frac{\partial \mathbf{F}}{\partial y} = \mathbf{S}(\mathbf{U})
\]

(1)

\[
\hat{U} = \begin{bmatrix}
\frac{\rho}{\rho u_x} \\
\frac{\rho u_x}{\rho u_z} \\
\frac{\rho u_z}{\rho u_y}
\end{bmatrix}
\quad \hat{E} = \begin{bmatrix}
\rho u_x \\
\rho u_y \\
\rho u_z
\end{bmatrix}
\quad \hat{F} = \begin{bmatrix}
\rho u_x \\
\rho u_y \\
\rho u_z
\end{bmatrix}
\]

(2)

\[
\hat{S} = \begin{bmatrix}
\frac{-\rho u_x^2}{\rho} \dot{\phi} \\
\frac{-\rho u_y^2}{\rho} \dot{\phi} \\
\frac{-\rho u_z^2}{\rho} \dot{\phi} + \eta \left( \frac{\dot{\rho}}{\rho} + \frac{\dot{\rho}}{\rho} \right)
\end{bmatrix}
\]

(3)

where, \(\rho = 0\) for rectangular and \(\rho = 1\) for cylindrical coordinates. Also, \(\eta = 0\) for energetic materials while \(\eta = 1\) for inert materials. Here, \(r, \theta, z\) are the cylindrical coordinate variables and \(\rho\) is density, \(u_x, u_y, u_z\) are velocity components in axial and radial coordinates. \(E = e + (u_x^2 + u_y^2)/2\) is the total energy per unit mass with the specific internal energy \(e\) and \(p\) is the hydrostatic pressure, respectively. The temperature is derived from the relationship, \(e = \frac{1}{2}(u_x^2 + u_y^2) = \frac{1}{2}\). Reaction rate, \(\dot{\phi} = \frac{\partial \lambda_i}{\partial t} + \dot{\lambda}_i\), can be described by the temperature-dependent Arrhenius model of deflagration to detonation transition or by the pressure-based ignition and growth model from the shock to detonation transition data.

The resulting hyperbolic system of equations was solved by a third-order Runge–Kutta and essentially non-oscillatory (ENO) methods [10] for temporal and spatial discretization, respectively. Here, any stress effect in the unreacted high explosives or propellant was ignored in comparison to a dominantly high hydrostatic pressure resulting from the reacted product gases. However, to capture the drastic change in deformation of the inert material boundary, the Cauchy stress tensor \(\sigma_{ij}\) was formulated into a deviatoric stress tensor and a hydrostatic pressure as shown in Eq. (4).

\[
\sigma_{ij} = \sigma_{ij} - p \delta_{ij}
\]

(4)

\[
I_1 = \sigma_{kk} = \sigma_{11} + \sigma_{22} + \sigma_{33} - 3p,
\]

\[
J_1 = \sigma_{kk} = \epsilon_{11} + \epsilon_{22} + \epsilon_{33} - 3p
\]

(5)

Here, \(I_1\) and \(J_1\) are the first scalar invariants of the Cauchy stress and the deviator stress tensors, respectively. Deviatoric stress tensor, \(\sigma_{ij}\), and the hydrostatic pressure, \(p\), are taken to be positive in compression.

\[
\varepsilon = \varepsilon^e + \varepsilon^p, \quad \varepsilon^p_{ij} = \varepsilon^p_{ij} - \frac{1}{3} \varepsilon^p_{kk} \delta_{ij} = \varepsilon^i_j,
\]

\[
\tilde{D}_{ij} = D_{ij} - \frac{1}{3} \delta_{kk} \delta_{ij}, \quad D_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)
\]

(6)

where, \(\varepsilon\) is the strain tensor, \(\varepsilon^e\) and \(\varepsilon^p\) are the elastic strain tensor and the plastic strain tensor, respectively. \(\varepsilon^p\) is the plastic deviatoric strain tensor, \(D_{ij}\) and \(\tilde{D}_{ij}\) are the strain rate tensor and the deviatoric strain rate tensor, respectively. Components of the strain tensor are used to derive the yield stress depending on the shear rate in the form of Johnson–Cook flow stress model.

A Huber–von Mises yield function for von Mises material with isotropic hardening is given by Eq. (7).

\[
f = f(\sigma, \sigma_r) = f(\sigma_{ij}, \tilde{\sigma}) = \sqrt{2\sigma_{ij} \sigma_{ij} - \sigma_r} = \sigma_{ij} - \sqrt{2\sigma_{ij} \sigma_{ij} - \sigma_r} \leq 0
\]

(7)

where \(\tilde{\sigma}\) is the effective stress and \(\sigma_r\) is the current yield stress. The effective stress \(\tilde{\sigma}\) and the effective plastic strain \(\tilde{\sigma}\) are defined as Eqs. (8) and (9), respectively.

\[
\tilde{\sigma} = \sqrt{2\sigma_{ij} \sigma_{ij}} = \sqrt{\frac{3}{2} (s_{11}^2 + s_{22}^2 + s_{33}^2 + 2(s_{12}^2 + s_{23}^2 + s_{31}^2))}
\]

(8)

\[
\tilde{\sigma}_p = \sqrt{\frac{2}{3} D_{ij} D_{ij}} = \frac{1}{\sqrt{3}} \Lambda
\]

(9)

Here, \(\Lambda\) is a positive parameter called the consistency parameter and \(D_{ij}\) the plastic strain rate tensor.

In the cases of cylindrical coordinate or axisymmetric problem, the effective plastic strain is expressed as Eq. (10) with \(s_{00} = -s_{rr} - s_{zz}\).

\[
\tilde{\sigma}_p = \sqrt{\frac{2}{3} (s_{rr}^2 + s_{zz}^2 + 2s_{rzz}^2)} = \sqrt{3 (s_{rr}^2 + s_{zz}^2 + s_{rzz}^2)}
\]

(10)

Deviatoric stresses of evolution equation are shown in Eqs. (11)–(13).

\[
\dot{s}_{rr} = \Omega_{rr} s_{rr} - s_{rr} \Omega_{rr} + 2G(\frac{\dot{\rho}}{\rho} - \Sigma - D_{rr}^p)
\]

(11)

\[
\dot{s}_{zz} = \Omega_{zz} s_{zz} - s_{zz} \Omega_{zz} + 2G(\frac{\dot{\rho}}{\rho} - \Sigma - D_{zz}^p)
\]

(12)

\[
\dot{s}_{rz} = \Omega_{rz} s_{rz} - s_{rz} \Omega_{rz} + 2G(\frac{\dot{\rho}}{\rho} - \Sigma - D_{rz}^p)
\]

(13)

where, the spin tensor \(\Omega_{ij}\) and the volume strain \(\Sigma\) are calculated by Eqs. (14) and (15), respectively.

\[
\Omega_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)
\]

(14)

\[
\Sigma = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)
\]

(15)

The rate of deviatoric stress change follows the first order ordinary differential equation given in Eq. (16).

\[
\dot{s}_{ij} = \dot{s}_{ij,rr} + \dot{s}_{ij,zz} - \Omega_{ik} s_{kj} - s_{ik} \Omega_{kj} + 2G(\tilde{D}_{ij} - D_{ij}^p)
\]

(16)

where each operator is defined as

\[
\dot{s}_{ij,rr} = \Omega_{ik} s_{kj} - s_{ik} \Omega_{kj} + 2G \tilde{D}_{ij}
\]

(17)

\[
\dot{s}_{ij,zz} = -H : D_{ij}^p = -2G A N_{ij,rr}
\]

(18)

The plastic strain rate tensor is given as

\[
D_{ij}^p = \Lambda \frac{\partial f}{\partial \sigma} = \Lambda N_{ij}
\]

(19)

\[
N_{ij} = \frac{\dot{s}_{ij}}{\sqrt{3} s_{kk} \delta_{ij}}
\]

(20)

With the consistency condition defined by

\[
\dot{f}(\sigma, \sigma_r) = \frac{\partial f}{\partial \sigma} \tilde{\sigma} + \frac{\partial f}{\partial \sigma_r} \tilde{\sigma}_p = 0
\]

(21)
The hardening law is given by Eq. (22).
\[
\dot{\sigma}_p = \sqrt{\frac{2}{3}} h \Lambda = h \dot{e}_p
\]  
(22)
where \( h \) which is the hardening coefficient and corresponds to the slope of the effective stress versus effective plastic strain curve under uniaxial loading conditions.

2.2. Level set method

To obtain sharp interface between two different materials, hybrid particle level set method [11] is applied. The motion of the level set follows the method given in [12] and [13] as shown in Eq. (23).
\[
\frac{\partial \phi}{\partial t} + V \cdot \nabla \phi = 0
\]  
(23)
Here, the interface of each substance is a zero level set \( \phi = 0 \). \( \phi < 0 \) indicates the inner and \( \phi > 0 \) indicates the outside of a material. This equation is integrated with a 4th order scheme in space and 3rd order Runge-Kutta method in time.

While calculating the interface level-set function, a drastic change in the material property may give rise to distortion of the interface. In order to remedy this, a periodic re-initialization was adopted by solving the Eq. (24) until steady state.
\[
\phi_i + S(\phi)(|\nabla \phi| - 1) = 0
\]  
(24)
Here \( S \) is given by Eq. (25).
\[
S = \frac{\phi}{\sqrt{\phi^2 + (1 - |\nabla \phi|)^2}}
\]  
(25)
with \( d \) being the grid size. The unit normal vector and curvature are obtained as

Unit normal vector : \( \vec{n} = \frac{\nabla \phi}{|\nabla \phi|} \)
(26)
Curvature : \( \kappa = \nabla \cdot \vec{n} = \nabla \cdot \left( \frac{\nabla \phi}{|\nabla \phi|} \right) \)
(27)

The dissipation characteristics of ENO scheme and re-initializations of level set lead to interface round off errors and violation of mass conservation. In order to correct these issues for precise interface tracking, a hybrid particle level set method was applied [12,13]. Here, two types of massless particles, positive and negative particles, were placed in the region of \( \phi > 0 \) and \( \phi < 0 \). These particles are allowed to advect following the Eq. (28).
\[
\frac{d\vec{x}_p}{dt} = \vec{u}(\vec{x}_p)
\]  
(28)
Here, \( \vec{x}_p \) is the position of the particles and \( \vec{u}(\vec{x}_p) \) is their velocity vector. The characteristic information of the flow is preserved due to deletion of the dissipation from the evolution equation. The third order TVD Runge-Kutta method is used to solve the temporal derivative for the evolution equation.

Each particle has zero mass but has a non-zero volume. The radii of those particles were determined from the size of the grid as such, the maximum and minimum values are given by Eqs. (29) and (30).
\[
r_{\text{min}} = 0.1 \min(\Delta r, \Delta z)
\]  
(29)
\[
r_{\text{max}} = 0.5 \min(\Delta r, \Delta z)
\]  
(30)
Initially, the particles were randomly placed and then directed to the correct path. Then the final radii for particles follow Eq. (31).
\[
r_p = \begin{cases} 
  r_{\text{max}} & \text{if } S_p \phi(\vec{x}_p) > r_{\text{max}} \\
  S_p \phi(\vec{x}_p) & \text{if } r_{\text{min}} \leq S_p \phi(\vec{x}_p) \leq r_{\text{max}} \\
  r_{\text{min}} & \text{if } S_p \phi(\vec{x}_p) < r_{\text{min}} 
\end{cases}
\]  
(31)
where, \( S_p \) is the sign of the particle and sets to +1 if \( \phi(\vec{x}_p) > 0 \) and -1 if \( \phi(\vec{x}_p) < 0 \) respectively. Here, if an error by the particles to move in the wrong direction with respect to the interface is detected, error correction through the local level set reconstruction is performed.

In the well-resolved regions, the interface tracked by a level set is quite precise and the particles do not drift farther from the interface. In the under-resolved regions, however, the calculation of level set generates mass loss and particles tend to escape quietly across the interface. In the pure Eulerian based approach, drastic physical phenomena sometimes result in level set warping, which incurs numerical problems. One of the major problems is related to level set normal vector determination. In this case, the physical variables calculated based on the information of the orthogonal vector may not converge or converge into nonphysical values. The correction of the level set value is achieved by the comparison of the values from grid based-level set and the escaped particles' localized level set. The main idea of level set correction is to eliminate the center grid point around where level set warping is occurred. In other words, level set values are artificially designated so that the configuration of the level set does not form a singularity. This kind of artificial treatment is expected to have negligible effect on the whole physical process provided that grid size is sufficiently small. Here, the conservative variables at the center grid point are re-calculated through a distance based interpolation using the same material grid points around the center grid.

2.3. Ghost fluid method

The material properties change drastically across the interface between any two dissimilar materials. This is mainly due to the discontinuous entropy distribution at the interface that results in numerical truncation errors, which can be quite significant if not properly treated. In the present method, the ghost cells were populated opposite of the real material of interest using the extrapolation while having the continuous entropy distribution. Here, the real discontinuous entropy distribution was merged with the entropy distribution of ghost cells and generates proper boundary conditions. The physical conditions were used in the ghost band where pressure and velocity were the same as the interface conditions. Then the entropy in the ghost band was assigned the value of the real material. All other remaining variables were determined through the entropy relation and the proper EOS [14].

As shown in Fig. 1, if the material interface is located between \( i \) and \( i + 1 \) nodes, that the level set function has a value of 0, the left (subscript \( l \) ) side becomes the area of material 1, and the material 2 takes the opposite side. In order to update information of material 1, we use the information of the right (subscript \( r \) ) area including the \( i + 1 \) node to specify the ghost values. Entropy is extrapolated from the value of the region of material 1, while pressure and velocity of region 2 are directly used for the ghost nodes. Also, to update the area of material 2, the method is repeated.

Once the location of \( P \) corresponding to the ghost phantom point is specified, a normal vector is drawn from the interface to \( P \) and the interpolated node 1 is generated. Then, the point \( P \) and interpolated node 1 are connected to calculate the position of the interpolated node 2 which is at the same distance. Next, the value of node 1 is interpolated using the information at the nearest four nodes, and the value of node 2 is also defined using the informa-
tion at the four nodes closest to it. Following these steps, all values of the fluid ghost are determined.

Two nonlinear characteristics that intersect at the interface are given by Eqs. (32) and (33).

\[
\frac{dp_l}{dt} + \rho_{IL}c_l \frac{du_l}{dt} = 0 \quad \text{along} \quad \frac{dx}{dt} = u_l + c_l
\] (32)

\[
\frac{dp_r}{dt} - \rho_{IR}c_r \frac{du_r}{dt} = 0 \quad \text{along} \quad \frac{dx}{dt} = u_r - c_r
\] (33)

With the interface characteristics, we have the following linearized relations

\[
u_l = u_l - \frac{p_l - p_1}{\rho_1 c_l}, \quad \nu_r = u_r - \frac{p_l - p_r}{\rho_1 c_r}
\] (34)

The modification to the ghost method is directly expressed in Eqs. (35) and (36).

\[
u_l = \frac{\rho_1 c_l}{\rho_1 c_r} \nu_r + \rho_1 c_r u_r + (p_1 - p_r) = \frac{w_l u_l + w_r u_r + (p_1 - p_r)}{w_l + w_r}
\] (35)

\[
p_l = \frac{\rho_1 c_1 p_1 + \rho_1 c_1 p_r + \rho_1 c_r (p_1 - p_r)}{\rho_1 c_1 + \rho_1 c_r} = \frac{w_l p_l + w_r p_r + w_l w_r (p_1 - p_r)}{w_l + w_r}
\] (36)

2.4. Interface conditions

At the interface, the velocity components in the normal direction and stress fields must remain continuous following the conservation law expressed in Eqs. (37) and (38).

\[
\rho_r = \rho_1, \quad u_r = -u_l, \quad v_r = v_l
\] (37)

\[
u_l = 0, \quad p_l = 2 p_1
\] (38)

The particle velocity at the surface is zero as shown in Eq. (39).

\[
\alpha_{ms}^{\text{solid}} = -p_\text{fluid}, \quad \alpha_{nt}^{\text{solid}} = 0, \quad v_n^{\text{solid}} = v_0^{\text{fluid}}
\] (39)

2.5. Discretization

The third order Runge–Kutta method for time marching is given by Eqs. (40) and (41).

\[
U^{n+1} = U^n + \sum_{j=1}^{r} w_j k_j
\] (40)

\[
\begin{align*}
I - \Delta t \delta \left( \sum_{j=1}^{r} c_j k_j \right) k_i \\
= \Delta t \left[ E \left( U^n + \sum_{j=1}^{r} b_j k_j \right) + F \left( U^n + \sum_{j=1}^{r} b_j k_j \right) \right] (i = 1, ..., r)
\end{align*}
\] (41)

Here, the implicit Runge–Kutta coefficients (\(c_j\)) are used for integrating the source term and the explicit Runge–Kutta coefficients (\(b_j\)) are used for the convective process of the Euler equation where the spatial derivative was replaced by a set of discretized fluxes. The fluxes of a hyperbolic equation will determine the order of spatial accuracy. For a high-order ENO flux construction, a combination of upwind and downwind fluxes are given by Eqs. (42) and (43).

\[
f_{j+1/2}(U) = \frac{1}{2} \left( f(U) + \alpha_{j+1/2} U \right)
\] (42)

\[
f_{j+1/2}(U) = \frac{1}{2} \left( f(U) - \alpha_{j+1/2} U \right)
\] (43)

where \(\alpha_{j+1/2}\) is the largest eigenvalue of the flux Jacobian, and the local Lax–Friedrichs flux is defined by Eq. (44).

\[
\hat{f}_{j+1/2} = f_{j+1/2}(U_j) + f_{j-1/2}(U_{j+1})
\] (44)

The control of the time step increment is determined automatically, where the step size is given by Eq. (45).

\[
\Delta t_{\text{ CFL}} = \frac{\min(\Delta z, \Delta r)}{\max[u + c, u, u - c]}
\] (45)

2.6. Equation of state

In order to describe both the unreacted and the product state of an energetic material, the equations of state defining the pressure are necessary. The Jones–Wilkins–Lee (JWL) form of equations [15] are shown in Eqs. (46) and (47) for unreacted reactant and gaseous product of high explosives.

\[
p_{\text{unreacted}} = \frac{\omega}{R_1 (\rho_0 / \rho)} e^{-R_1 (\rho_0 / \rho)} + \frac{\omega e_0}{(\rho_0 / \rho)^{\omega+1}}
\] (46)

\[
p_{\text{reacted}} = \frac{\omega e_0}{(\rho_0 / \rho)^{\omega+1}} + \frac{C}{(\rho_0 / \rho)^{\omega+1}}
\] (47)
Here, $\rho_0$ and $\rho$ are the initial and current densities respectively. A, B, C, $R_A$, and $R_B$ are the material dependent JWL parameters with $\omega$ being the Gruneisen coefficient of the explosive. These parameters were obtained by fitting the JWL EOS to the cylinder expansion test results or thermodynamic equilibrium calculation of CHEETAH [16], where $\epsilon_0 = \rho_0 C_v T$ refers to the thermodynamic energy in GPa. In particular, Eq. (47) is an isentropic JWL C-term form of EOS used for gaseous products, and is derived according to the thermodynamics 1st law argument for isentropic process as shown in Eq. (48).

$$de = \delta q - \delta w = Tds - pdv = -pdv$$

(48)

Integrating Eq. (48) returns the expression given in Eq. (49).

$$\epsilon_0 = -\int pd(\rho_0/\rho)$$

$$\int \left( A e^{-R_A(\rho_0/\rho)} + B e^{-R_B(\rho_0/\rho)} + C (\rho_0/\rho) \right) d(\rho_0/\rho)$$

$$= \frac{A}{R_A} e^{-R_A(\rho_0/\rho)} + \frac{B}{R_B} e^{-R_B(\rho_0/\rho)} + \frac{C}{\alpha_0(\rho_0/\rho)^{\alpha_1}}$$

(49)

When Eq. (49) is substituted into JWL EOS in Eq. (46), we arrive at Eq. (50).

$$P_{\text{unreacted}} = A \left( 1 - \frac{\omega}{R_A(\rho_0/\rho)} \right) e^{-R_A(\rho_0/\rho)}$$

$$+ B \left( 1 - \frac{\omega}{R_B(\rho_0/\rho)} \right) e^{-R_B(\rho_0/\rho)}$$

$$+ A \frac{\omega}{R_A(\rho_0/\rho)} e^{-R_A(\rho_0/\rho)} + B \frac{\omega}{R_B(\rho_0/\rho)} e^{-R_B(\rho_0/\rho)}$$

$$+ C \frac{\omega}{\alpha_0(\rho_0/\rho)^{\alpha_1}}$$

Thus, the C-term JWL EOS is the isentropic form of the original JWL equation.

The sound speed can be defined by Eq. (51).

$$c^2 = \left( \frac{\partial p}{\partial \rho} \right)_s = \left( \frac{\partial p}{\partial \rho} \right)_e + \frac{p}{\rho^2} \left( \frac{\partial p}{\partial e} \right)_\rho$$

(51)

Here, the sound speeds for JWL EOSs (unreacted and reacted) are given by Eqs. (52) and (53).

$$c^2_{\text{unreacted}} = -\frac{\rho_0}{\rho^2} \left[ \frac{\omega}{R_A(\rho_0/\rho)} e^{-R_A(\rho_0/\rho)} + B \frac{\omega}{R_B(\rho_0/\rho)} e^{-R_B(\rho_0/\rho)} \right.$$  

$$- \frac{\omega \epsilon_0}{(\rho_0/\rho)} - AR_A \left( 1 - \frac{\omega}{R_A(\rho_0/\rho)} \right) e^{-R_A(\rho_0/\rho)}$$

$$- BR_B \left( 1 - \frac{\omega}{R_B(\rho_0/\rho)} \right) e^{-R_B(\rho_0/\rho)} \right]$$

$$c^2_{\text{reacted}} = \frac{\rho_0}{\rho^2} \left[ \lambda AR_A e^{-R_A(\rho_0/\rho)} + B R_B e^{-R_B(\rho_0/\rho)} - C \right]$$

(52)

The unreacted and reacted EOS were combined into a single expression, Eq. (54), using the product mass fraction ($\lambda$) and reactant depletion ($1 - \lambda$).

$$\rho = (1 - \lambda) \rho_{\text{unreacted}} + \lambda \rho_{\text{reacted}}$$

(54)

The combined sound speed is then calculated by using Eq. (55).

$$c^2 = (1 - \lambda) c^2_{\text{unreacted}} + \lambda c^2_{\text{reacted}}$$

(55)

Meanwhile, a thermo-chemical equilibrium code, CHEETAH incorporates a fitting program to an optimal parameters of JWL EOS. It works based on the cylinder test data that provides detailed information on the theoretical C-J states including pressure, volume, energy, temperature, and detonation velocity. Parameterization of JWL EOS was done by multiple CHEETAH runs to use in the empirical fitting procedure. Table 1 shows the C-J conditions for the energetic components of this work.

As for the gap and bulkhead materials, Mie–Grüneisen EOS is adopted to calculate the pressure of non-reactive materials [17] shown in Eq. (56).

$$P_{\text{non-reactive}} = \Gamma_0 \rho_0 + \left\{ \begin{array}{ll}
\rho_0 \rho_0 \mu \left[ 1 + (1 - \frac{\Gamma_0}{\Gamma_1}) \mu \right] / \mu & \text{if } \mu > 0 \\
\frac{c_0^2 \rho_0 \mu}{\epsilon} & \text{if } \mu < 0
\end{array} \right.$$  

(56)

Where, $\mu = \rho/\rho_0 - 1$.

Assuming that $\rho \Gamma = \rho_0 \Gamma_0$, the sound speed of Mie–Grüneisen EOS is given by Eq. (57).

$$c^2_{\text{non-reactive}} = \rho_0 \Gamma_0 \frac{p - p_0}{\rho^2} + \left\{ \begin{array}{ll}
\frac{\rho^2_0 \epsilon_0}{\rho^2_0 - \rho_0^2} & \text{if } \rho > \rho_0 \\
\frac{\rho_0 \epsilon_0}{\rho_0 - \rho} & \text{otherwise}
\end{array} \right.$$  

(57)

The Johnson–Cook model was applied for flow stress or the minimum outer force needed to deform plastically. This model makes use of the equivalent plastic strain, strain rate, and melting temperature [18] as shown in Eq. (58).

$$\sigma_{\gamma}(\varepsilon_p, \dot{\varepsilon}_p, T) = [A_0 + B_0 \dot{\varepsilon}_p^n] \left[ 1 + C_0 \ln \left( \frac{\dot{\varepsilon}_p}{\varepsilon_p^0} \right) \right] \left[ 1 + \left( \frac{T - T_0}{T_m - T_0} \right)^m \right]$$

(58)

Here, $\sigma_{\gamma}$ is the yield stress and $\varepsilon_p$, $\dot{\varepsilon}_p$, and $\dot{\varepsilon}_p^0$ are the effective plastic strain, the effective plastic strain rate, and the effective plastic strain rate of the quasi-static state, respectively. The normalized temperature is defined according to reference room temperature ($T_0$) and reference melt temperature ($T_m$). For conditions where $(T - T_0) < 0$, we assume that $m = 1$. The strength model that accounts for the effects of strain hardening, strain-rate hardening, and thermal softening were adopted to describe the dynamic response of the steel. In addition, the strength model constants, namely, $A_0$, $B_0$, $C_0$, $m$, and $n$ are used for PMMA, Brass, and STS. As strain rate approaches zero, the natural log approaches negative infinity, and therefore the Johnson-Cook model sets $C_0$ to a zero if strain rate reaches a certain minimum value, usually $1 \text{s}^{-1}$, $\dot{\varepsilon}_p^0$ is commonly set to unity. The material properties and Mie–Grüneisen EOS constants are summarized in Table 2 [17].

2.7. Chemical reaction

The rate of burnt mass production is governed by

$$D \frac{\partial \rho_i}{\partial t} = -\nabla \cdot w_i$$

(59)
where \( w_i \) is the reaction rate and \( \lambda_i \) is the reaction progress variable or burned mass fraction. The mathematical closure is enforced by introducing the equation of state and the rate law. Both pressure based and temperature based chemical kinetics are utilized depending on the reaction characteristics of the energetic components.

The reactive flow model is described by the rate law that consists of both ignition and growth steps suggested by Kim et al. [8] as shown in Eq. (60).

\[
\frac{d\lambda}{dt} = I(1 - \lambda)\mu^a + G(1 - \lambda)\rho^b\mu = \frac{\rho}{\rho_0} - 1 \tag{60}
\]

Here, \( p \) is pressure, \( t \) is time, while \( \rho_0 \) and \( \rho \) denote the initial and current density respectively. Constants \( I, a, G, \) and \( b \) are the unknown parameters while \( \lambda \) is the burned mass fraction that represents reaction progress such that \( \lambda = 0 \) is unreacted and \( \lambda = 1 \) is reacted state. The compression was defined as \( \mu = \rho/\rho_0 - 1 \). Four unknown parameters of major significance in view of detonation were determined by a series of standardized unconfined rate stick experiment performed [8].

For the RDX, the constants of ignition \( I \) and growth \( G \) were set to \( 5.8 \times 10^5 \) s\(^{-1}\) and \( 3.8 \times 10^8 \) s\(^{-1}\) Mbar\(^{-b}\) respectively. The pressure sensitivity \( b \) was 1.1, and the compression sensitivity \( a \) was 4.0. The rate law of HMX was modeled by Eq. (61), with the rate parameters of \( I = 4.4 \times 10^7 \) s\(^{-1}\), \( a = 4.0 \), \( G = 8.5 \times 10^8 \) s\(^{-1}\) Mbar\(^{-0.666}\), and \( b = 2.0 \).

\[
\frac{d\lambda}{dt} = I(1 - \lambda)0.222\mu^a + G(1 - \lambda)0.666\rho^b \tag{61}
\]

BKNO3 is a pyrotechnic propellant used in the solid fuel igniters, thermites, and gas generators, etc. The chemical reaction of BKNO3 is classified as a deflagration as opposed to a detonation, and the reaction rate [19] is calculated using Eqs. (62) and (63) can be directly used to track the burning BKNO3.

\[
\dot{w} = \frac{d\lambda}{dt} = \rho_0 Z\lambda \exp(-E_a/(RT)) \tag{62}
\]
3. Results and validations

3.1. Riemann test for checking the discontinuity capturing precision

Precise handling of the subtle motion between gap (STS) and acceptor (RDX) is critical in this work. One-dimensional Riemann test, in which initial condition is given in Table 4, was performed and compared against the exact solution. The result with mesh size of 0.5 mm at 7 μs is shown in Fig. 3. The initial position of the interface between STS and RDX at x = 0.05 m is moved to x = 0.062 m while retaining a sharp discontinuity, thanks to the hybrid particle level set method implemented in the solver. Although a minor undershoot showed near the contact line, two shocks propagating into acceptor and gap are captured, precisely.

3.2. SDT test for checking the grid convergence

The numerical simulation requires a large number of meshes through the reactive area of the explosive material, in order to resolve the sharp detonation structure and to attain the theoretical CJ equilibrium properties. The SDT calculation is both mesh and time intensive as the velocity on the order of several thousand meters per second and few tens of GPa in pressure are generated within microscale widths of RDX and HMX reaction zones. Specifically, the reaction zone width is approximately 0.1 mm for HMX and 0.5 mm for RDX. The time evolution graphs for pressure are shown in Fig. 4. Here, four different sizes of meshes viz. 0.10 mm, 0.05 mm, 0.02 mm and 0.01 mm were used. While detonation velocities were quite close to the theoretical values (6.9 mm/μs) for all three cases (6.0 mm/μs – 7.0 mm/μs), von Neumann spike pressure varies in each case. However, as mesh becomes finer, the von Neumann spike pressure approaches the experimental value of 35 GPa. As von Neumann spike pressure became close enough to the experimental value in grid size of 0.01 mm, we selected the mesh size of 0.01 mm × 0.01 mm for the integrated system simulation in the rest of the study.

3.3. Small-scale gap test

A small-scale gap test (SSGT) can be performed with a small amount of sample about 1/10 of the amount used for large-scale gap test (LSGT) [20] with a reduced sample diameter of 5 mm, filled into a 10 mm thick cylindrical Brass shell. LSGT is tested unconfined (no metal walls) while SSGT uses confined rate sticks. Therefore, it is possible to obtain a more precise judgement of the shock sensitivity of the acceptor when considering the composite interactions between reactant and inert material such as shock pressure attenuation in the gap and deformation of the inert materials.

Price et al. [21] compared the measured results of SSGT and LSGT to allow mutual calibration of the initiating threshold pressure. Sowers et al. [22] analyzed the trends of initiating threshold pressure derived from flyer impact and gap tests for various energetic materials. However, the demand for numerical methodology has been steadily increasing because of high cost and high risk associated with explosion experiments. In view of the experimentalist, numerical models would contribute to the better understanding of the internal flow dynamics for shock wave generation and

\[ \frac{dl}{dt} = \sqrt{\frac{Z \cdot e^{E_a/RT} \cdot k \cdot RT^2}{c_p \cdot E_a \cdot (T_f - T_0)}} / \rho_0 \]  

(63)

Here, the thermal response of BKN03 is simulated using the Arrhenius law, and related parameters are quantified by the DSC (Different Scanning Calorimetry) analysis which measures the calorific heat of chemical reaction. The reaction parameters of BKN03 are \( Z = 9.2 \times 10^3 \text{s}^{-1}, E_a = 1.8 \times 10^2 \text{kJ/mol}, \) and \( k = 3.2 \times 10^{-3} \text{kJ/m – sec – K}. \) The reaction rate and regression rate of BKN03 with temperature are shown in Fig. 2.

The rate parameters used in the calculation are summarized in Table 3. The JW L EOS parameters of product gas of energetic materials are calculated with a thermo-chemical equilibrium code [16].

### Table 4

<table>
<thead>
<tr>
<th>Working mediums</th>
<th>STS (gap)</th>
<th>RDX (acceptor)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density (kg/m³)</td>
<td>7800</td>
<td>2100</td>
</tr>
<tr>
<td>Pressure (GPa)</td>
<td>0</td>
<td>12</td>
</tr>
<tr>
<td>Velocity (mm/μs)</td>
<td>0</td>
<td>2.0</td>
</tr>
<tr>
<td>Initial yield stress (GPa)</td>
<td>0.34</td>
<td>none</td>
</tr>
<tr>
<td>Shear modulus (GPa)</td>
<td>77</td>
<td>none</td>
</tr>
<tr>
<td>Strength model</td>
<td>Constant yield stress</td>
<td>none</td>
</tr>
</tbody>
</table>

### Table 3

<table>
<thead>
<tr>
<th>Parameter</th>
<th>HNS</th>
<th>HMX</th>
<th>RDX</th>
<th>BKN03</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reactant</td>
<td>( \rho_0 ) (kg/m³)</td>
<td>1430</td>
<td>1700</td>
<td>1640</td>
</tr>
<tr>
<td></td>
<td>A (GPa)</td>
<td>–</td>
<td>952.200</td>
<td>77.810</td>
</tr>
<tr>
<td></td>
<td>B (GPa)</td>
<td>–</td>
<td>–5.944</td>
<td>–5.031</td>
</tr>
<tr>
<td></td>
<td>R₁</td>
<td>–</td>
<td>14.1</td>
<td>11.3</td>
</tr>
<tr>
<td></td>
<td>R₂</td>
<td>–</td>
<td>1.41</td>
<td>1.13</td>
</tr>
<tr>
<td></td>
<td>ω</td>
<td>–</td>
<td>0.89</td>
<td>0.89</td>
</tr>
<tr>
<td>Product</td>
<td>A (GPa)</td>
<td>250.05</td>
<td>333.88</td>
<td>311.19</td>
</tr>
<tr>
<td></td>
<td>B (GPa)</td>
<td>4.00</td>
<td>5.92</td>
<td>5.69</td>
</tr>
<tr>
<td></td>
<td>C (GPa)</td>
<td>1.00</td>
<td>1.35</td>
<td>1.36</td>
</tr>
<tr>
<td></td>
<td>R₁</td>
<td>4.14</td>
<td>3.63</td>
<td>3.61</td>
</tr>
<tr>
<td></td>
<td>R₂</td>
<td>1.05</td>
<td>1.02</td>
<td>1.01</td>
</tr>
<tr>
<td></td>
<td>α</td>
<td>0.32</td>
<td>0.37</td>
<td>0.36</td>
</tr>
<tr>
<td>Chemical kinetics</td>
<td>I (s⁻¹)</td>
<td>–</td>
<td>4.4 × 10⁷</td>
<td>5.8 × 10⁷</td>
</tr>
<tr>
<td></td>
<td>a</td>
<td>–</td>
<td>4.0</td>
<td>4.0</td>
</tr>
<tr>
<td></td>
<td>G (s⁻¹ Mbar⁻³)</td>
<td>–</td>
<td>8.5 × 10⁸</td>
<td>3.8 × 10⁸</td>
</tr>
<tr>
<td></td>
<td>b</td>
<td>–</td>
<td>2.0</td>
<td>1.1</td>
</tr>
<tr>
<td></td>
<td>Z (s⁻¹)</td>
<td>–</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td></td>
<td>E_v (kJ/kmol)</td>
<td>–</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td></td>
<td>k (kJ/m-sec-K)</td>
<td>–</td>
<td>–</td>
<td>–</td>
</tr>
</tbody>
</table>
transfer processes, both of which are impossible to evaluate via experiments.

We tested a combination of PMMA gap and RDX explosives to verify the shock sensitivity and attenuation characteristics. The length of gap substance was varied to observe the critical gap thickness until acceptor charge detonated in 50% of the trials. The donor charge was RDX whose initial density is 1.57 g/cm³, while the acceptor was 97.5% RDX with initial density 1.64 g/cm³. Fig. 5 shows a SEM image utilized for particle size analysis of RDX. The particle diameter ranged from 100 to 500 μm and the average particle size was found to be about 300 μm, as uniform particle size is assumed in the simulation. The explosive as well as the gap material were confined within a circular Brass container with an inner diameter of approximately 5.11 mm and a thickness of 10.145 mm. The heights of donor and acceptor were kept the same at 38.1 mm, while the gap thickness was varied by stacking PMMA discs. The gap test specimen and configuration are shown in Fig. 6. Fifteen trials were conducted with thickness variations from 9.84 mm to 11.85 mm. Go/No-go criterion was obtained based on the witness plate breakage.

Brass container was filled with the test explosive using a dedicated pneumatic press to obtain the initial density. Initiation was achieved by an electronic bridge wire connected to the center of the upper surface of the donor. The thickness of the attenuator can be reduced by observing alternating positive (Go) and negative (No-go) responses. A total of 15 tests were carried out to a precision of ± 0.05 mm thickness. A witness plate of mild steel material was installed at the bottom of the acceptor to facilitate the Go/No-go judgment by observing the breaking of the plate according to whether or not detonation occurred. Table 5 lists the SSGT experimental results. The critical thickness was found to be between 11.51 to 11.56 mm based on the experimental data. A thicker gap material resulted in undamaged witness plate. Therefore, the critical gap thickness of PMMA for the initiation of 97.5% RDX was defined to be around 11.5 mm, and the incident pressure delivered to...
to the acceptor can be considered as the minimum value for initiation. Go (broken) and No-go (preserved) results of small scale gap test are shown in Fig. 7. If the acceptor charge is initiated by shock to detonate, the Brass confinement is broken like sample number 1 or 2 on the left side case only in case of detonation. The schematic of the gap test simulation is shown on the right side of Fig. 6. In order to precisely simulate shock-to-detonation transition and pressure attenuation in the gap test, we constructed a dense grid system \( d = 0.01 \) mm in order to ensure the resolution of the reaction length of 0.5 mm for both shock wave front and the C-J properties.

The gap sizes were varied from 10 mm to 12 mm with 1 mm interval. The computational results of Go/No-go response when shock wave passes through the PMMA of 11 mm and 12 mm thickness and reaches the acceptor (97.5% RDX) is shown in Fig. 8. The contours indicate the reaction progress variable where 0 indicates reactant and 1 indicates product to distinguish Go/No-go response. The non-reactive materials, PMMA and Brass, show pressure (left) and density (right) to observe the generation of transmitted and reflected waves. Six cross-sectional views are shown from 2.0 \( \mu \)s at the initial stage of reaction to 11.0 \( \mu \)s at which combustion of the acceptor was almost completed. As the explosion proceeds, the pressure of the product gas changes the shape of the Brass con-vexly, but it does not affect the progress of the explosion. Moreover, the arrival time of the detonation wave front of the donor to reach the PMMA after initiation is about 5.0 \( \mu \)s, and the mean velocity is about 7600 m/s. Transmission and reflection due to the inter-action between detonation wave and PMMA occur at 7.0 \( \mu \)s and 9.0 \( \mu \)s, respectively. The first reflection and transmission are observed when the detonation wave front of the donor reaches the upper interface of the PMMA. The reflected wave propagates backwards, and then the transmitted wave enters the PMMA. At this time, the energy loss is converted into a pressure drop. Pressure attenuation occurs through the non-reactive material, and the maximum pressure of the shock wave is continuously reduced. A second reflection and transmission occurs when the shock wave impacts the bottom side of the PMMA. Finally, the transmitted wave into the acceptor causes ignition. PMMA and Brass are deformed as pressure is applied. Various superposition and refraction occur by the waves that pass through different media.

At the PMMA gap thickness of 11 mm, the detonation of 97.5% RDX was initiated by the pressure transfer, but at 12 mm, negative reaction is observed because the shock impact is lower than the critical initiating pressure reaching the acceptor. It was confirmed that the difference in pressure delivered by the gap thickness makes the ignition response different. The attenuating profile of the shock wave passing through PMMA is shown in Fig. 9. The final attenuating pressure at the points corresponding to the gap thickness of 11 mm and 12 mm were calculated to be 1.15 GPa and 0.918 GPa respectively. Table 6 compares the critical initiating pressure and 50% gap thickness derived from the gap test of [21] and [22]. The critical initiating pressure of 97.5% RDX was obtained at about 1 GPa between 11 mm and 12 mm gap thickness of SSGT, which is consistent with previously reported values. This is the threshold for the minimum pressure required to induce impact ignition of energetic materials. The critical initiating pressure of 97.5% RDX derived from the SSGT test and computational analysis can be assured to 1 GPa.

### 3.4. Closed chamber test

The test was used to further validate the response of a pyrotechnic device consisting of a donor charge, bulkhead, acceptor charge, and pyrotechnic propellant connected with a 10 cc sealed vessel for purging high pressure gases. The train configuration consisted of a donor charge of HNS+HMX, a bulkhead of STS, an acceptor charge of RDX, and the pyrotechnic propellant BKNO3. In the donor charge, HNS is a primer to a detonating HMX for generating a booster pressure. The ensuing pressure is progressively attenuated through the bulkhead. The bulkhead length is a critical parameter for initiating the acceptor charge and subsequently ig-
Fig. 8. Shown reaction progress for donor (top) and acceptor (bottom), pressure and density for PMMA (middle) and Brass (both sides). (a) 11 mm Gap and (b) 12 mm Gap at times $t = 2.0, 3.5, 9.0, 10.0, \text{and} \; 11.0\mu s$.

Table 6

SSGT results for 97.5% RDX

<table>
<thead>
<tr>
<th></th>
<th>Threshold pressure (GPa)</th>
<th>50% gap thickness (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>LSGT (1966) [21]</td>
<td>0.92</td>
<td>-</td>
</tr>
<tr>
<td>SSGT (2007) [22]</td>
<td>1.05</td>
<td>-</td>
</tr>
<tr>
<td>Present SSGT - experiment</td>
<td>-</td>
<td>11.51–11.56</td>
</tr>
<tr>
<td>Present SSGT - simulation</td>
<td>0.918–1.15 (1.026)</td>
<td>11.0–12.0 (11.5)</td>
</tr>
</tbody>
</table>

Fig. 9. Time trace of attenuating pressure along the PMMA thickness in the SSGT simulation.

The gas-generating propellant. It is important to verify that the explosive train operates properly as a well-controlled and reliable Through Bulkhead Initiator (TBI), a common pyrotechnic device. As the sympathetic pressure to be transferred to an acceptor charge depends on the thickness of the bulkhead, an accurate analysis is required for prediction of the shock-to-detonation transition process of a composite system arranged in a train configuration. In order to quantify the detonation response of high explosives by a shock impact in such a system, we set out to clarify the relationship between ignition sensitivity and threshold pressures.

Fig. 10 shows the pyrotechnic initiator-chamber assembly on the left and the computational domain on the right. The donor-gap-acceptor train configuration is utilized to ignite the propellant (BKNO₃) for uniform gas generation into a chamber. A pressure sensor measured the central wall pressure fluctuation during the event. The sensor utilized in the current study was of the model #102B of PCB piezotronics which was connected to ICP model 484b signal conditioner and a DAQ system. The test was repeated by increasing the bulkhead thickness in 0.1 mm increment, in order to find the optimal operating condition. The test was carried out from 10 to 16 sets at one point where the Go/No-go reactions were observed alternately.

Table 7 summarizes the results of the closed chamber explosion test according to bulkhead thickness. Go/No-go was judged based on pressure measurement where a Go condition indicated an increase in pressure while No-go conditions indicated no increase in pressure. The test was repeated three times until 3.7 mm bulkhead thickness showing the Go reaction and more samples were used to ensure the reliability of the result between 3.8 mm and 4.0 mm which showed Go and No-go tendency. A total of 16 trials were performed at 3.8 mm and only 3 trials were No-go. At 3.9 mm
out of 10 were No-go. While, no-go reaction was observed in all samples from 4.0 mm.

Fig. 11 shows the chamber pressure history over time at bulkhead thickness of 3.8 mm and 4.0 mm. In the case of the Go reaction, a pressure increase due to the combustion gas injection was observed. The maximum pressure in the 10 cc chamber was increased to about 5 to 6 MPa. In case of No-go, oscillation due to ignition is observed while maintaining the initial pressure. Therefore, it can be seen that there is an operating critical point of the pyrotechnic device between the bulkhead thickness of 3.8 mm and 4.0 mm.

In order to observe the initial reaction of the assembly, the sampling rate was measured for precision up to 2000 µs with 20 GHz as shown in Fig. 12. Raw data and the low-pass filtered pressure measurement are also shown. The pressure perturbation is clearly observed downstream when the cut-off frequencies \( \omega_n = 300 \text{ KHz} \) and \( \omega_n = 100 \text{ KHz} \) are applied. The filtered data was derived by the Eq. (64) where \( \tau \) is the inverse of the cut-off frequency \( \omega_n \) as a filtering time constant, \( s \) and \( K \) are respectively a Laplace transform variable and a gain in the passband.

\[
\text{Output} = \frac{Y}{X} = \frac{K}{\tau s + 1} \tag{64}
\]

From the results, it can be seen that the combustion gas of BKNO3 flows into the dump chamber when the pressure rises at about 100 µs from the start of the explosion. After 500 µs, one can observe a swirling flow which seems to be due to the propagation of oscillating reacting waves in the closed chamber. The FFT results obtained by converting the pressure signal with time into the frequency domain are shown in Fig. 13. The observed frequency was about \( \omega_* = 8.3 \text{ KHz} \). This particular frequency is due to the time characteristics of the oscillating flow bouncing inside the chamber.

Fig. 14 shows the calculation results on Go/No-go reactions in the explosive train configuration with two bulkhead thicknesses (3.8 mm and 4.0 mm). This reflects the observation of positive and negative responses at around 3.9 mm in the closed chamber test. The sequential reaction of the explosives to donor (HNS+HMX) / bulkhead (STS) / acceptor (RDX) occurs by the shock wave propagation. When a high-pressured wave front reaches the acceptor, the chemical reaction is initiated and the thermal energy generated by the reaction supports the propagation of detonation wave. The peak pressure of shock wave is gradually decreased when it passes through the non-reactive STS bulkhead, because the compression consumes energy. The Go reaction can be observed if the shock wave with the minimum pressure to ignite the acceptor is reached.
Fig. 13. Power spectral densities of closed chamber test data.

Fig. 14. Timed images of calculated pressure contour at 3.8 mm (left), and 4.0 mm (right) bulkhead thicknesses of the explosive train configuration. Precisely tracked energetic and inert boundaries are shown in solid lines.

Fig. 15. Calculated shock pressure trajectory in donor / bulkhead / acceptor of the explosive train configuration.

Fig. 16. Shock impedance matching of STS and RDX.

Otherwise, a No-go reaction appears. The arrival time of the wave front of HNS to HMX was 0.35 μs, and the total burning time of HNS is 0.6 μs. The reaching time of the wave front of HMX to STS was 0.7 μs, and the total burning time of HMX is 0.8 μs. The pressure wave passing through the STS then reaches the acceptor RDX at 1.7 μs. At this time, a Go (3.8 mm) reaction was obtained when sufficient pressure was applied to acceptor, and a No-go (4.0 mm) reaction was observed. This result is attributed to the pressure attenuation occurring more as the bulkhead thickness increases. The pressure profile along the centerline of the explosive train configuration is shown in Fig. 15. The ZND pressure of the donor is about 45 GPa, and the pressure gradually decreases as it passes through the STS bulkhead. The acceptor is initiated at around 1 GPa. Therefore, the energy loss caused by the shock wave passing through the STS and the critical initiating pressure of the high explosive are two important factors for determining the reliable operation of the pyrotechnic train.

When an acoustic wave traveling in one medium encounters the boundary of a second medium, reflected and transmitted waves are generated. The shock impedance is a measure of
the amount by which the motion induced by a pressure applied to a surface is impeded. Reflection and transmission of a wave normally incident on the interface between materials with different impedance characteristics. In a linearized homentropic planar wave, the characteristic shock impedance is defined as the multiplication of density and sound speed in the material. As the wave is propagating from material 1 to material 2, the reflection and transmission is found as shown in Eqs. (65) and (66) [23].

\[
T = \frac{p_1}{p_i} = \frac{2\rho_2 c_2}{\rho_2 c_2 + \rho_1 c_1} = \frac{Z_2 + Z_3}{Z_2 + Z_1}
\]

(65)

\[
R = \frac{p_T}{p_i} = \frac{\rho_2 c_2 - \rho_1 c_1}{\rho_2 c_2 + \rho_1 c_1} = \frac{Z_2 - Z_1}{Z_2 + Z_1}
\]

(66)

The gap test can be, ideally, regarded as the sequence of two processes. Firstly, wave propagates from reacting energetic material (material 1) to a bulkhead material (material 2). Subsequently, the wave from bulkhead material (material 2) propagates to an unreacted energetic material (material 3). The resulting transmission from this sequence of two transmissions can be reduced by applying Eq. (65) twice. The resulting transmission is given by Eq. (67).

\[
T = T_{1 \rightarrow 2} \cdot T_{2 \rightarrow 3} = \frac{2\rho_2 c_2}{\rho_2 c_2 + \rho_1 c_1} \cdot \frac{2\rho_3 c_3}{\rho_3 c_3 + \rho_2 c_2}
\]

(67)

The shock speed relations are given by Eq. (68).

\[
u_{\text{shock}} = c_0 + s u_{\text{particle}}
\]

(68)
\(C_0\) and \(s\) are bulk sound speed and linear Hugoniot slope coefficient respectively. \(s\) is given by Eq. (69).

\[
s = \frac{du_{\text{shock}}}{du_{\text{particle}}} \tag{69}
\]

Here, the shock velocity is \(u_{\text{shock}}\) and the material particle velocity is \(u_{\text{particle}}\). The shock velocity and particle velocity were assumed to follow a linear relationship, and \(\rho \Gamma\) was assumed to be a constant. The impedance matching equation is given by Eq. (70).

\[
p = \rho_0 (C_0 + s_0 u_{\text{particle}}) u_{\text{particle}} \tag{70}
\]

Fig. 16 shows shock impedance matching of STS and RDX. The shock Hugoniot parameters of solid state of RDX explosive are \(C_0 = 2600\) m/s and \(s_0 = 1.86\). When the incident pressure of 1.0 GPa is applied to RDX acceptor, the transmitted pressure is about 0.2 GPa. Transmission coefficient being the ratio between incident pressure and transmitted pressure is calculated to be 0.2 while reflection coefficient is 0.8.

Fig. 17 shows that reactive flow motion generated by the pyrotechnic initiator composed of detonator (HNS+HMX) / bulkhead (STS) / acceptor (RDX) / pyrotechnic propellant (BKNO3), flowed into a 10 cc closed chamber. The bulkhead thickness is set to 3.8 mm. The explosive train consisting of detonator, bulkhead and acceptor completes its reaction in about 2.0 μs. Then, another 40 μs is consumed to fully deflagrate the propellant, BKNO3. The hot product gas fills the closed chamber in approximately 50 μs. In the figure, a shadowgraph is shown in the upper, and pressure is shown in the lower half of each timed image. The release pressure wave into the chamber starts to bounce off of the right-end wall, which is repeating at every 130 μs. This time characteristic is in a striking agreement with the dominant frequency measurement from Fig. 13 (\(\omega_c = 8.3\) KHz). More in-depth analysis is desired to reveal the effect of various types of wave superposition on the combustion field.

The predicted shape change of the inert-reactant boundaries after the test is quite intriguing. As the pressure is attenuated in the bulkhead as such the most of donor pressure is transmitted into the acceptor, causing a higher compression of the gap during successive acceptor initiation. Donor and acceptor expand in all directions due to the internal pressure buildup. A cross sectional view of an actual sample is shown at the rightmost bottom in Fig. 17. The transmitted shock pressure becomes increasingly high near the central axis of the donor and acceptor due to a highly reactive detonation front in the center. The resulting curvature of STS is therefore concave and it seems to have evolved into a very similar shape between the experiment and calculation. The dynamic shape change of the stainless casing for donor, acceptor, and propellant is also compared between actual photographic image and numerical result from the particle level set tracking. The donor and acceptor cavities are expanded in all directions due to detonation pressure buildup. The resulting cavity shape change is quite precisely predicted from the present simulation as depicted in Fig. 18.

Fig. 19 shows the comparison of the pressure fluctuation measured from experiment and calculation in the chamber. One can confirm that the periods of the longitudinal wave motion and the periods of the peaks in the chamber match quite well. This means the originality of the acoustic wave is the captured wave inside the chamber, which keeps on bumping into top and bottom sides of the chamber to generate the acoustic wave motion towards an interior domain.

4. Conclusion

A detailed discussion on the hydrodynamic modeling of a pyrotechnic device is presented. The numerical methodology for tracking multi-material boundary interactions as well as severely transient fluid-structure coupling between high explosive charges and metal bulkhead are described. The material modeling techniques for both reactive and inert materials are also explained in regards to their empirical and theoretical bases. The performance of a resulting energetic component system arranged in a train configuration is demonstrated via the pressure measurement of a high pressure burned gases of the BKNO3 propellant, inside a dump chamber. The developed method is shown to be reliable for reproducing the shock-to-detonation transition and material-to-material shock attenuation that govern the performance of the whole system. As the numerical modeling of the energetic component system involving detonation of high explosives, deflagration of propellant, and structural deformation of bulkhead is systematically and thoroughly discussed in this paper, one can implement the outlined contents into a shock physics code for a full scale hydrodynamic simulation of a similar system.

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References