Generalized interpolation material point approach to high melting explosive with cavities under shock

X F Pan, Aiguo Xu, Guangcai Zhang and Jianshi Zhu

Laboratory of Computational Physics, Institute of Applied Physics and Computational Mathematics,
PO Box 8009-26, Beijing 100088, People’s Republic of China
E-mail: Xu_Aiguo@iapcm.ac.cn

1 Author to whom any correspondence should be addressed.

Abstract
Criterion for contacting is critically important for the generalized interpolation material point method. We present an improved criterion by adding a switching function. With this method the dynamical response of high melting explosive with cavities under shock is investigated. The physical model used in this work is an elastic-to-plastic and thermal-dynamical model with Mie–Grüneisen equation of state. We address mainly the influence of various parameters, including the impacting velocity $v$, cavity size $R$, etc, on the dynamical and thermodynamical behaviour of the material. For the colliding of two bodies with a cavity in each, a secondary impacting is observed. Correspondingly, the separation distance $D$ of the two bodies has a maximum value $D_{\text{max}}$ in between the initial and second impacts. When the initial impacting velocity $v$ is not large enough, the cavity collapses in a nearly symmetric fashion, the maximum separation distance $D_{\text{max}}$ increases with $v$. When the initial shock wave is strong enough to collapse the cavity asymmetrically along the shock direction, the variation of $D_{\text{max}}$ with $v$ does not show monotonic behaviour. Our numerical results clearly indicate that the existence of cavities in explosives helps the creation of ‘hot spots’.

1. Introduction

Cavitation phenomena are ubiquitous in nature, ranging from solid and liquid to plasma. Cavity creation and collapse play a very important role in a large number of industrial processes, such as erosion of materials, ignition of explosives, comminution of kidney stones, etc [1–3]. The cavitation phenomena may occur on a mesoscopic scale, but generally have a profound influence on the response on the macroscopic scale. As for explosives, cavity collapse may result in jetting phenomena and consequently lead to a much higher temperature increase of the ‘hot spots’. Therefore, it has the potential to start local reactions leading to partial decomposition or run to full detonation [2]. On the one hand, cavitation acts as a means of increasing the sensitivity of explosives for ignition, but on the other hand, it represents a potential safety problem for handling such materials.

The interest in both considerations inspired theoretical, experimental and numerical work aimed at studying the influence of cavities on explosives [2, 4–14].

During the collapse procedure explosive material under consideration is highly distorted and the boundaries should be tracked, which proposes a very high requirement on the numerical methods. In the early studies, conventional Eulerian and/or Lagrangian schemes were used [5–9]. When conventional Lagrangian methods are used, the mesh distortion associated with large deformations reduces the accuracy and will probably terminate the computations; ultimately, a re-meshing treatment is required, which is not a straightforward task and generally inefficient. It is known that the conventional Eulerian code is not convenient to track the boundaries. To continue, several mixed methods have been proposed to combine the merits of the two methods and overcome their drawbacks. Among them, the arbitrary Lagrange–Euler (ALE) method [15] is a typical one. Several
researchers have used the ALE method to study the collapse of cavities in explosive materials [16]. The particle-in-cell (PIC) is a second typical mixed method [17]. It has also contributed to the research on inhomogeneous plastic-bonded explosives [18]. Additionally, a number of ‘meshless methods’ have been developed. To overcome the difficulty due to the distortion of mesh, the meshless method uses a series of discretized Lagrangian points to construct the shape function. Some meshless methods, such as smooth particle hydrodynamics (SPH) [19–21], dual particle dynamics (DPD) [22], etc, have been applied in the research on cavity collapse in explosive materials [22–24]. It should be mentioned that microscopic molecular dynamics (MD) has also brought some new understanding of the physics and chemistry involved [12–14]. Yet, even with the most powerful computers in use nowadays, the MD simulation is still far from reaching the practical spatial and temporal scales of real experiments [25].

The physical models used in previous numerical studies are mainly fluidic ones. Such models ignore many important characteristics of solids, such as plastic strain, hardening and effects relevant to the deformation history. In this study we revisit the material point method (MPM) [26], recently developed in the field of computational solid physics, by presenting a new contact criterion and then use it to study the dynamical response of high melting explosive (HMX) with cavities under shock.

The MPM is a descendant of the PIC extended to solid mechanics [27–31]. Compared with the above-mentioned methods, the MPM provides a robust and efficient treatment of large deformation issues and a convenient framework for modelling contact between large numbers of contacting bodies. In MPM, each body is discretized by a collection of Lagrangian material points carrying all the information required to advance the solution; the Eulerian background computational mesh is used to solve the governing equations and the mesh solution is then used to update the information on the material points. Specifically, at each time step, the MPM calculations consist of two parts: a Lagrangian part and a convective one. Firstly, the computational mesh deforms with the body, and is used to determine the strain increment and the stresses carried by the particles. Then, the new position of the computational mesh is chosen (particularly, it may be the previous one); and the velocity field is mapped from the material points to the mesh nodes. This method has been applied to handle engineering problems with large strain [32, 33] and/or dynamical energy release rate [34], fracture in heterogeneous material [35], dynamics failure [36, 37], hypervelocity impact [38], thin membranes [39], granular materials [18, 40–42], etc. The generalized interpolation material point (GIMP) method uses a variational form and a Petrov–Galerkin discretization scheme to overcome the numerical noise of previous MPM [26].

We study not only the collapse of cavities but also the deformation and dynamical response of cavities before collapsing under shock. These are important for better understanding the ignition of explosives. The elastic-to-plastic and thermal-dynamics model with the Mie–Grüneissen equation of state obeying the Rankine–Hugoniot curve is used to simulate the mechanical and thermal behaviour of the material. The model used here is more suitable for simulating the dynamical response of the solid material under shock than previous ones.

This paper is organized as follows. In section 2 we briefly describe the generalized interpolation material point method where the contact algorithm is improved. In section 3 the new scheme is validated by several benchmark tests and is then used to study cavitated high melting explosives. Section 4 concludes the paper.

2. Approach

2.1. The generalized interpolation material point method

For continuum bodies, the conservation equation for mass is

$$\frac{d\rho}{dt} + \rho \nabla \cdot v = 0, \quad (1)$$

where $\rho$ is the mass density and $v$ is the velocity.

In GIMP and MPM, the continuum bodies are discretized with $N_p$ material particles. Each material particle carries the information of position, velocity, temperature, mass, density, Cauchy stress, strain tensor and all other internal state variables necessary for the constitutive model. Since the mass of each material particle is equal and fixed, equation (1) is automatically satisfied. At each time step, the mass and velocities of the material particles are mapped onto the background computational mesh (grid). The mapped nodal velocity $v_j$ is obtained through the following equation,

$$\sum_j m_{ij} v_j = \sum_p m_p v_p N_i(x_p), \quad (2)$$

where $m_{ij}$, $v_p$ and $x_p$ are the mass, velocity and position of particle $p$, respectively. $N_i$ is the shape function, $i$ and $j$ indices of node.

In the early version of MPM, the grid shape function $N_i$ is not smoothed in the construction of the weighting function, which causes numerical noise as the material points cross computational grid boundaries. Bardenhagen et al [26] presented a family of methods named the GIMP methods in which the interpolation functions are in $C^1$ (as opposed to MPM, which are in $C^0$). In this paper the following smoothed shape function in $C^1$ is used, $N_i = \Phi(r_x) \Phi(r_y)$, where $r_x = |x_p - x_i|/L, r_y = |y_p - y_i|/L, L$ is the length of the cell, and $\Phi(r)$ is given as follows:

$$\Phi(r) = \begin{cases} \frac{7 - 16r^2}{16} & r \leq 0.25, \\ \frac{1 - r}{(5 - 4r)^2} & 0.25 < r \leq 0.75, \\ \frac{(5 - 4r)^2}{16} & 0.75 < r \leq 1.25, \\ 0 & r > 1.25. \end{cases} \quad (3)$$

See also figure 1. Equation (3) is a weighting function with support in adjacent cells and the next nearest neighbour cells. This specialization has the advantage that it develops a weighting function in $C^1$ with a minimal amount of additional complexity.
In equation (2), the consistent mass matrix, $m_{ij}$, is

$$m_{ij} = \sum_{p} m_{p} N_{i}(x_{p}) N_{j}(x_{p}).$$

In practice, we generally replace $m_{ij}$ with a lumped, diagonal mass matrix so that equation (2) becomes

$$m_{i} v_{i} = \sum_{p} m_{p} v_{p} N_{i}(x_{p}),$$

where lumped mass is

$$m_{i} = \sum_{p} m_{p} N_{i}(x_{p}).$$

The conservation equation for momentum reads,

$$\rho \frac{dv}{dt} = \nabla \cdot \sigma + \rho b,$$

where $\sigma$ is the stress tensor and $b$ is the body force. The weak form of equation (7) based on the standard procedure used in the FEM [28, 29] can be written

$$\int_{\Omega} \rho \varepsilon \frac{dv}{dt} \, d\Omega + \int_{\Gamma} \delta v \cdot (\sigma \cdot n - t) \, d\Gamma + \int_{\Omega} \rho \varepsilon \cdot b \, d\Omega = 0,$$

where $n$ and $t$ are the outward normal unit and traction vectors on the boundary.

Since the continuum bodies are described with the use of a finite set of material particles, the mass density can be written as

$$\rho(x) = \sum_{p=1}^{N_{p}} M_{p} \delta(x - x_{p}),$$

where $\delta$ is the Dirac delta function with dimensions of the inverse of volume. The substitution of equation (9) into equation (8) converts the integral into the sums of quantities evaluated at the material particles, namely,

$$m_{i} \frac{dv_{i}}{dt} = (f_{i})^{\text{int}} + (f_{i})^{\text{ext}},$$

where $m_{i}$ is the lumped mass and the internal force vector is given by

$$(f_{i})^{\text{int}} = - \sum_{p} M_{p} \sigma \cdot (\nabla N_{i}) / \rho_{p},$$

and the external force vector reads

$$(f_{i})^{\text{ext}} = \sum_{p=1}^{N_{p}} N_{i} b_{p} + f_{i}^{c},$$

where the vector $f_{i}^{c}$ is the contact force which is the external nodal force not including the body force and is illustrated in the following section.

An explicit time integrator is used to solve equation (10) for the nodal accelerations, with the time step satisfying the stability condition. The critical time step is the ratio of the smallest cell size to the wave speed. After the equations of motion are solved on the cell nodes, the new nodal values of acceleration are used to update the velocity of the material particles. The strain increment for each material particle is determined with the use of the gradient of the nodal basis function evaluated at the material particle position. The corresponding stress increment can be found from the constitutive model. The internal state variables can also be completely updated. The computational mesh may be discarded, and a new mesh is defined, if desired for the next time step. As a result, an effective computational mesh could be chosen for convenience [31].

2.2. Contact algorithm

The GIMP method provides a natural no-slip contact algorithm based on a common background mesh. But a natural contact algorithm has two drawbacks: firstly, premature contact occurs because the velocities of two bodies are mapped on the same nodes though the distance between the bodies may be still two or even more times the length of the cell, which may cause the numerical noise of stress; secondly, it is impossible to separate the contacting bodies. Bardenhagen et al [40] have proposed a contact algorithm to simulate the interactions of the grains of granular material, in which the contact between bodies is handled when the velocity field of the individual particles in contact differs from the single, centre-of-mass velocity field in the cell containing contacting particles. A multi-mesh mapping scheme is proposed by Hu and Chen [43]. In the multi-mesh mapping scheme, each material lies in an individual background mesh rather than in the common background one. The meshing process of spur gears is simulated by Hu and Chen with their contact algorithm. To avoid interpenetration and allow separation in the gear meshing process, the normal velocity of any particle at the contact surface is calculated as the contact force which is the external nodal force not including the body force and is illustrated in the following section.

In this paper, whether two bodies contact or not is judged according to their distance. In the improved contact algorithm, if the velocities of bodies $p$ and $q$ are mapped on the same node $i$ (seen in figure 2), the distance between bodies $p$ and $q$ is calculated. We denote the distance between bodies $p$ and $q$ as $\mathcal{R}_{pq}^{\text{int}}$, which can be calculated as

$$\mathcal{R}_{pq}^{\text{int}} = n_{pq} \cdot r_{p} - n_{pq} \cdot r_{q},$$

where the vector $f_{i}^{c}$ is the contact force which is the external nodal force not including the body force and is illustrated in the following section.
where \( \mathbf{n}^{pq} \) is the normal direction of the contacting interface pointing from bodies \( p \) to \( q \). \( \mathbf{r}_i^p \) and \( \mathbf{r}_i^q \) are the vectors pointing to node \( i \) from bodies \( p \) and \( q \), respectively. \( \mathbf{n}^{pq} \cdot \mathbf{r}_i^p \) and \( \mathbf{n}^{pq} \cdot \mathbf{r}_i^q \) can be chosen as

\[
\mathbf{n}^{pq} \cdot \mathbf{r}_i^p = \max (\mathbf{n}^{pq} \cdot \mathbf{r}_i^p, m = 1, 2, \ldots, N_p)
\]
and particle \( p \) is in body \( p \), (14)

\[
\mathbf{n}^{pq} \cdot \mathbf{r}_i^q = \min (\mathbf{n}^{pq} \cdot \mathbf{r}_i^q, m = 1, 2, \ldots, N_q)
\]
and particle \( q \) is in body \( q \), (15)

where \( \mathbf{r}_i^p \) and \( \mathbf{r}_i^q \) are the vectors pointing to node \( i \) from particles \( p \) and \( q \), respectively. \( N_p \) and \( N_q \) are the numbers of particles belonging to bodies \( p \) and \( q \), respectively.

The criterion of contact can be written as

\[
\mathbf{n}^{pq} \cdot \mathbf{r}_i^p \leq \frac{L}{2},
\]

where \( L \) is the length of the cell. If equation (16) is satisfied, the velocities of \( p \) and \( q \) are adjusted to new values so that the normal components of them are equal, then the strain and stress of all the particles are updated. Hence, equation (16) plays the role of a switch function. Once bodies \( p \) and \( q \) contact, they move together along the normal until they separate, so the acceleration along the normal of body \( p \) is equal to that of \( q \) during the course of the contact. That is,

\[
\mathbf{a}_i^p \cdot \mathbf{n}^{pq} = \mathbf{a}_i^q \cdot \mathbf{n}^{pq},
\]

where \( \mathbf{a}_i^p \) and \( \mathbf{a}_i^q \) are the accelerations of bodies \( p \) and \( q \) at node \( i \), respectively. They can be obtained from the Newtonian second law. Also the normal contact force \( f_{i}^{norm} \) can be derived. Note that the normal contact force must be nonnegative. So, once \( f_{i}^{norm} \) is negative, bodies \( p \) and \( q \) are not in contact in the next time step.

The contact algorithm has been finished up to now without friction. In the case with friction the Coulomb friction is applied to calculate the tangential contact force.

2.3. Constitutive model and the equation of state

In this paper, the material is modelled using von Mises plasticity with linear hardening [3]. A plastic model dictates a linear elastic response until a yield criterion is reached. The von Mises yield criterion is \( 3J_2\rightarrow Y^2 = 0 \), where \( Y \) is the plastic yield stress, \( J_2 \) is the second invariant of \( \mathbf{\sigma} \), \( J_2 = \frac{1}{2} : \mathbf{\sigma}, \mathbf{\sigma} \) is the deviatoric stress tensor, \( \mathbf{\sigma} = \mathbf{\sigma} - \text{Tr}[\mathbf{\sigma}]/3 \).

The linear hardening means that \( Y \) increases linearly with the second invariant of the plastic strain tensor. If \( 3J_2 > Y^2 \), the increment of equivalent plastic strain \( \mathbf{\varepsilon} \) can be calculated as \( \mathbf{\varepsilon} = (\sqrt{3J_2 - Y})/(3G + E_{\text{tan}}) \), where \( G \) and \( E_{\text{tan}} \) are the shear and hardening modulus, respectively. The increment of the plastic energy can be calculated as \( dW_{p} = \mathbf{\varepsilon} \cdot \mathbf{\sigma} \cdot Y \). It is totally translated into internal energy.

The pressure \( P \) is calculated by using the Mie–Grüneisen state of equation, which can be written as

\[
P - P_H = \frac{\gamma(V)}{V} [E - E_H(V_H)].
\]

This description is consistent with the Rankine–Hugoniot curve. In equation (18), \( P_H, V_H \) and \( E_H \) are pressure, specific volume and energy on the Rankine–Hugoniot curve, respectively. The relation between \( P_H \) and \( V_H \) can be estimated by experiment and can be written as

\[
P_H = \begin{cases} 
\rho_0 S_0 \left( 1 - \frac{V_H}{V_0} \right), & V_H \leq V_0, \\
\rho_0 u_c^2 \left( \frac{V_H}{V_0} - 1 \right), & V_H > V_0,
\end{cases}
\]

where \( \rho_0 \) is the density, \( \lambda \) is the parameter in the linear ratio, \( U_i = \rho_0 + \lambda U_p, U_i \) and \( U_p \) are shock velocity and velocity of the particle, respectively. In this paper, the coefficient of Grüneissen \( \gamma(V_H) \) is taken as a constant and the transformation of specific internal energy \( E \) is taken as the plastic energy. Both the shock compression and the plastic work cause the increase of temperature. The increase in temperature from shock compression can be calculated as

\[
\frac{dT_H}{dV_H} = \frac{c_v^2}{c_v \left[ (\lambda - 1) V_0 - \lambda V_H \right]^2} - \frac{\gamma(V)}{V} T_H,
\]

where \( c_v \) is the specific heat. Equation (20) can be derived from thermal equation and the Mie–Grüneissen state of equation [45]. The increase in temperature from plastic work can be calculated as

\[
\frac{dT_p}{c_v} = \frac{dW_p}{c_v}.
\]

Both equations (20) and (21) can be written in the form of increments. In this work the thermal dissipation is not taken into account. Such a treatment is reasonable for cases where the propagation speed of shock is much faster than that of the thermal dissipation.

The material constants are chosen to model the energetic crystal high melting explosive. The elastic modulo is 11.87 GPa, the Poisson ratio is 0.25, the density is \( 1.9 \times 10^{-3} \text{ g mm}^{-3} \), the initial yield strength is 100 MPa, the hardening modulo is 0 MPa, the heat capacity is 1250 J kg\(^{-1}\) K\(^{-1}\)). The coefficient of Grüneissen is taken as 1.1, \( \lambda = 2.6 \) and the sound speed \( c_0 = 2740 \text{ m s}^{-1} \) [1].
3. Results

In this paper we focus on the two-dimensional case. The shock wave to the material target is loaded via the impacting by a second material block with symmetric configuration and opposite velocity. The initial shock is along the vertical direction. We apply periodic boundary conditions to the simulated system in the horizontal direction. As the first step, we set a single cavity in the HMX block. Such a simulation model also corresponds to a very wide system with a row of cavities parallel to the impacting plane. We study various cases with different cavity radii and with different strengths of shock. The influence of an existing cavity on the contact of bodies is investigated and a secondary impacting is observed. In the cases of strong shock, the influence of cavity size and the impact speed on the ‘hot-spot’ is systematically investigated.

3.1. Validation of the improved contact algorithm

The newly proposed contact algorithm is validated by simulating the impacting of two identical solid bodies with opposite velocities in the vertical direction. The initial speed of each body is set to be 300 m s\(^{-1}\). Initially, the distance between the two bodies is set as 4 mm. The width and height of the blocks are set at 40 mm and 50 mm, respectively. Figure 3 shows the pressure along the vertical direction calculated by different contact algorithms, where the impacting interface is at \(y = 0\). From the numerical results we can see that both the GIMP with Bardenhagen’s contact algorithm and the MPM without contact algorithm give an unreasonable and too high pressure in the vicinity of the impact interface.

![Figure 3. Pressure distribution along the vertical direction at time \(t = 0.014\) ms. The impacting interface is at \(y = 0\). Previous contact algorithms present an unreasonable and too high pressure in the vicinity of the impact interface.](image)

3.2. Dynamical response to weak shock

Due to the ability to withstand the deformation of shear and tension, cavities in the solid material will not collapse when the shock is very weak. Figure 4 shows a series of snapshots for a case with an initial impact speed of 150 m s\(^{-1}\). The size of the blocks is the same as in section 3.1 and the radius of each cavity is 10 mm. The global procedure can be described as follows:

(a) The two bodies contact and a shock wave is loaded to each. The shock waves in the two bodies move forward to the two cavities. The pressure of shock is about 900 MPa (see figure 4(a)).

(b) The shocks arrive at the cavities, then rarefactive waves are reflected back to the material in between the two cavities. The cavities begin to shrink in a nearly isotropic fashion (see in figure 4(b)).

(c) The rarefactive waves reach the surface of contacting, and then the two bodies begin to separate (see figure 4(c)). Note that if there is no cavity inside, the two bodies will not separate so early.

(d) The two bodies continue to separate until the distance between the two bodies reaches the maximal value (see in figure 4(d)); then the two bodies begin to move closer again because the particles, being above the upper cavity and below the lower cavity, are still moving towards the contacting surface, which draws the separating bodies back.

(e) The approaching two bodies collide again. They stay together until the rarefactive waves reflected from the lowermost and the uppermost free surfaces arrive at
the contacting surface. Then, they separate again (see figure 4(e)).

(f) After (e), the two bodies separate. This is the final separation. The terminal configuration of cavities is still approximately circular. From the whole procedure, we can see that, due to the existence of cavities, the two bodies get a secondary impact.

In order to comprehend more clearly the phenomena of the secondary impact, we alter the impacting speed (in the limit of no collapse) and the size of the cavity. Figure 5 shows the effects of the initial impacting speed on the maximum separation distance between the two bodies after the first impact. In figure 5, \( D \) represents half the distance between the two impacting surfaces. It varies with time \( t \). The initial impacting speed is set as 100 m s\(^{-1}\), 150 m s\(^{-1}\) and 200 m s\(^{-1}\), respectively. In all cases the phenomena of the secondary impact are observed. The maximum value of \( D \) is denoted by \( D_{\text{max}} \). The larger the initial impacting speed, the larger the value of \( D_{\text{max}} \).

Figure 6 shows the effects of cavity size on the separation distance between the two impacting bodies. Here \( D \) and \( D_{\text{max}} \) have the same meanings as in figure 5. The initial radius of each cavity is set as 6 mm, 8 mm and 10 mm, respectively. It can be seen that the larger the radius of the cavity, the larger the value of \( D_{\text{max}} \). That is to say, the larger the cavities, the easier to observe the phenomenon of the secondary impact. Naturally, if the radius of the cavity diminishes to zero, the secondary impact disappears.

3.3. Dynamical response to strong shock

If the shock is strong, asymmetric collapse of the cavity will occur. When the radius of cavity is set to be 6 mm, 8 mm and 10 mm, respectively, the corresponding minimum impact speed \( v \) for the cavity to collapse asymmetrically is 120 m s\(^{-1}\), 150 m s\(^{-1}\) and 200 m s\(^{-1}\), respectively. That is to say, the smaller the radius of the cavity, the easier for the cavity to collapse asymmetrically. This is because larger curvature is easier to accumulate particles. The course of the collapse of the upper cavity can be described as follows: when the shock reaches the cavity, the upstream side of the cavity will reflect a rarefactive wave which propagates downwards: see figure 7(a). This causes the pressure in the region close to the upstream side of the cavity to be lower than around. Then, the neighbouring particles accumulate towards the lower side of the cavity, which will accelerate the upward speed of particles there. There are two factors that influence the deformation of the cavity. One is the accumulation of the particles at the lower side of the cavity, the other is the resistance of the solid material to shear. The competition of the two factors determines how the cavity deforms. Obviously, as the impact speed increases, the resulting shock becomes stronger, and the influence of the accumulation of the particles becomes stronger. If the strength of the material close to the lower side of the cavity cannot withstand the accumulation of particles, the upward speed of...
Figure 8. The maximum relative velocity versus the initial impacting speed. The radius of cavity is set at 6 mm, 8 mm and 10 mm, respectively.

Figure 9. The maximum relative velocity versus the radius of cavity. The impact speed is set at 500 m s\(^{-1}\).

Figure 10. The separation distance versus time \(t\) for different impacting speeds with strong shock. Here \(D\) has the same meaning as in figure 5.

Also, the phenomenon of secondary impacting is observed in the cases with strong shock. Figure 10 shows the effects of the initial impacting speed \(v\) on the separation distance \(D\) between the two impacting bodies. The initial impacting speed \(v\) is set at 230 m s\(^{-1}\), 300 m s\(^{-1}\), 500 m s\(^{-1}\) and 700 m s\(^{-1}\), respectively. In contrast to the cases with weak shock, \(D_{\text{max}}\) does not increase monotonically with the initial impact speed. When the initial impact speed is not very large (lower than 300 m s\(^{-1}\)), \(D_{\text{max}}\) increases correspondingly; but when the impact speed is large (higher than 300 m s\(^{-1}\)), \(D_{\text{max}}\) decreases. The critical case with \(v = 300\text{ m s}^{-1}\) is referred to figure 7. A physical explanation based on the case with \(R = 10\text{ mm}\) is as below. When the impacting speed \(v\) is lower than 300 m s\(^{-1}\) (see figure 4), the cavities shrink but without jetting. The strength of the rarefactive wave increases with the initial impacting speed \(v\). When \(v\) is larger than 300 m s\(^{-1}\), the cavities collapse and cave in, which dissipates a considerable amount of kinetic energy. The amount of dissipated energy exceeds the increase in the total kinetic energy via increasing \(v\). Therefore, the strength of the rarefactive waves does not increase with \(v\) but decreases.

3.4. On ‘hot-spots’

The reactivity of porous energetic material depends greatly on the nature of the ‘hot-spots’ formed by shocks as they move through the material. As observed in the gas-gun experiments [44], coarse HMX produces ‘hot-spots’ that are large enough to persist for a long time whereas fine material seems to produce ‘hot-spots’ that are smaller in size and dissipate quickly. The threshold-to-initiation is the limit where exothermic chemical energy release is balanced by energy dissipated away from the ‘hot-spot’ reaction. In the work of Baer et al [1], the mesoscale processes of consolidation, deformation and reaction of shocked porous energetic materials are studied using shock physics analysis of impact on a collection of discrete HMX ‘crystals’. In our work, we focus on the ‘hot-spots’ produced in the shocked HMX material with cavities.
Figure 11. Snapshots for the impact of two blocks with a single cavity in each. Impact velocity \( v = 300 \text{ m s}^{-1} \). From blue to red (or from black to white in the greyscale printed issue), the colour in the figure shows the increase of local temperature. The unit of temperature is K. 

- (a) \( t = 0.004 \text{ ms} \), 
- (b) \( t = 0.006 \text{ ms} \), 
- (c) \( t = 0.014 \text{ ms} \), 
- (d) \( t = 0.020 \text{ ms} \), 
- (e) \( t = 0.025 \text{ ms} \), 
- (f) \( t = 0.030 \text{ ms} \). (Colour online.)

Figure 11 shows the global procedure of the production of the ‘hot-spots’. The impact speed is 300 m s\(^{-1}\), the initial sizes of the blocks are the same as those in section 3.1, and the initial radius of every cavity is 10 mm. The initial temperature of the simulated system is 300 K. In order to display it clearly, only the upper block is shown. The procedure can be described as follows:

(a) The two blocks collide and the shocks begin to propagate towards the cavities. The temperature in the shocked pure HMX is about 310 K (see figure 11(a)).

(b) The shocks reach the cavities, then rarefactive waves are reflected back from the upstream boundaries of the cavities, the temperatures in the regions which are first shocked and then rarefacted by the waves decrease a little (see figure 11(b)).

(c) The shocks continue to propagate. The sizes of the cavities reduce as time goes on, the vertical deformation is more serious than the horizontal one. In contrast to the last item, the temperatures in the regions neighbouring the upstream sides of the cavities increase. The reason is that the plastic work increases continuously (see figure 11(c)).

(d) A jet appears in each cavity, and the temperature of the jet material increases as time goes on (see figure 11(d)).

(e) The jet material impacts the downstream side of the cavity, which causes a distinct increase of temperature to about 520 K (see figure 11(e)).

(f) The cavities continue to collapse until they are crammed; a ‘hot-spot’ with a temperature of about 520 K is produced in each colliding region (see figure 11(f)).

Figure 12. The impact speed dependence of the temperature of the ‘hot spot’. The radii of cavities are set at 6 mm, 8 mm and 10 mm, respectively. The unit of temperature is K.

(d) A jet appears in each cavity, and the temperature of the jet material increases as time goes on (see figure 11(d)).

(e) The jet material impacts the downstream side of the cavity, which causes a distinct increase of temperature to about 520 K (see figure 11(e)).

(f) The cavities continue to collapse until they are crammed; a ‘hot-spot’ with a temperature of about 520 K is produced in each colliding region (see figure 11(f)).

Figure 12 shows the temperatures of ‘hot-spots’ produced by different impact speeds for different sizes of cavities. It can be seen that the temperature increases nearly parabolically with the impacting speed \( v \) for a fixed size of cavity, which is consistent with the Hugoniot relation, \( P = \rho_0 (c_0 + \lambda u) \), where \( u = v/2 \) is the particle speed after shock. At the same time, plastic work also increases nearly parabolically with the impacting speed \( v \). Also, it can be found that the temperature of the ‘hot-spot’ produced in smaller cavities is higher than that in larger ones with the same impact speed. As analysed in section 3.3, the maximum relative speed produced by smaller cavities is larger than that by larger ones, which causes higher temperature, for the investigated cases.

4. Conclusion

The dynamical response of high melting explosive with cavities under shock is investigated by the generalized interpolation material point method where the criterion for contacting is improved. An elastic-to-plastic and thermal-dynamical model with the Mie–Grüneissen equation of state obeying the Rankine–Hugoniot curve is used to simulate the mechanical and thermal behaviour. The phenomenon of secondary impacting is observed for the case of colliding of two bodies with a single cavity in each. For weak shocks, the cavities shrink in a nearly symmetric way, and the phenomenon of secondary impacting becomes more distinct as the impact speed increases. But for strong shocks, the situation becomes complex because the asymmetric collapse of the cavity influences the reflection of shock. The course of collapse of...
the cavity is studied for various cavity sizes. For the checked cases, smaller cavities collapse more easily. Our numerical results show that the existence of cavities greatly helps the creation of ‘hot-spots’ with a much higher temperature, which is very important for igniting the explosive materials. The influence of various factors, including impact speed and size of cavity, on the temperature of ‘hot-spots’ is investigated. The temperature of ‘hot-spots’ increases nearly parabolically with the impact speed for a fixed cavity size. The smaller the cavity, the higher the temperature of ‘hot-spots’, for the cases investigated. If the cavity is too small, the effects of cavity collapse become very weak. Future work includes the incorporation of thermal diffusion, strain rate effects, etc into the simulations, and cases with cavities filled by gases.

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References

[1] Baer M R, Kipp M E and van Swol F 1998 Micromechanical modeling of heterogeneous energetic materials 11th Int. Detonation Symp. (Snowmass)
[2] Bourne N K 2002 Shock Waves 11 447
[3] Xu A, Pan X F, Zhang G and Zhu J 2007 J. Phys.: Condens. Matter 19 326212
[4] Bowden F P and Yoffe A D 1952 Initiation and Growth of Explosion in Liquids and Solids (Cambridge: Cambridge University Press)
[5] Kang J, Butler P B and Baer M R 1992 Combust. Flame 89 117
[6] Mader C L and Kershner J D 1985 The three-dimensional hydrodynamic hot spot model Proc. 8th Int. Symp. Detonation (Albuquerque, NM) pp 42–52
[7] Mader C L and Kershner J D 1989 The heterogeneous explosive reaction zone Proc. 9th Int. Symp. Detonation (Portland, OR) pp 693–700
[8] Mader C L 1979 Numerical Modelling of Detonations (Berkeley, CA: University of California Press)
[9] Cooper S R, Benson D J and Nesterenko V F 2000 Int. J. Plas. 16 525
[10] Bourne N K 1989 Cavity collapse in a heterogeneous commercial explosive Proc. 9th Symp. (Int.) Detonation (Office of the chief of Naval Research, Arlington, VA) pp 869–78
[11] Bourne N K and Field J E 1999 Proc. R. Soc. Lond. A 455 2421
[12] Maillot J-B 2003 MD simulations of hotspots, Session K1—Energetic Materials and Detonation VII
[13] Holian B L, Germann T C, Maillot J-B and White C T 2002 Phys. Rev. Lett. 89 285501
[14] Yang Q, Zhang G, Xu A, Zhao Y and Li Y 2007 Acta Phys. Sin. (in Chinese) (at press)