An efficient numerical method for the onset of blast waves generated by spherical detonation

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Abstract: Blast wave, generated by a high detonating spherical charge, is modeled using the Euler equations. The problem is split into two parts. The first part makes use of the isotropy to solve the problem in spherical radial coordinate. Overpressure distribution is presented and compared to both existing experimental and numerical data with very good agreement. The data transfer technique from the one-dimensional stencil onto the three-dimensional mesh is presented and its effectiveness, accuracy and efficiency are demonstrated. The second part consists on a three-dimensional computation fed with the isotropic remapped data. To show the feasibility of the 1D-3D combined method, the simulation is performed on a sample three-dimensional configuration and its results are presented.

Key–Words: Blast wave, Remapping techniques, Cartesian methods

1 Introduction

The increasing proportion of covered ways and tunnels in urban and suburban areas, together with the denser rail and road traffic, represent a stronger risk of severe accidents due to hazardous materials. As confinement is an aggravation factor of explosion effects, special safety measures have to be met in crowded underground structures and analysis tools are needed to simulate critical scenarios. This requires a better knowledge of blast waves in confined areas.

Conceptually, the main characteristic for any explosion is the rapid release of a huge quantity of energy from a compact volume in a very short time, typically of the order of the microsecond, which provokes a local pressure increase [1]. A supersonic wave is subsequently generated and propagates away from the detonation origin.

High explosive detonation and the generated blast waves have been extensively studied both theoretically and experimentally since several decades [1][2]. One of the commonly used methods for its simplicity and its accuracy to simulate the traveling blast wave is the shock tube model. However, it does not enable to simulate the detonation itself. Hence, the solution process must start with the onset of the blast wave, assuming that the explosive charge has been transformed at constant volume into hot gases at the so-called Chapman-Jouguet pressure. This detonation model is called the balloon analogue [1]. This one-dimensional approach has proven to be valid as long as the blast wave is freely propagating. In this case, it represents a good alternative to full three-dimensional approaches.

The present work combines the two approaches in an efficient way. Starting after the detonation, the one-dimensional model is used as far as applicable. The simulation then proceeds with a three-dimensional Euler method, with initial conditions provided by a novel remapping technique.

In this paper, the one-dimensional approach is applied to well admitted and documented test cases and compared to experimental and numerical data [3][4][5]. It is shown that the results are in very good agreement with the experimental data, with sig-
nificantly shorter computing time. After discussing the remapping technique, the feasibility of the 1D-3D combined method is illustrated on a sample three-dimensional test case.

2 The spherical problem

2.1 Physical and numerical model

The detonation preceding the blast wave is modeled by the balloon analogue [6]. Flow conditions for statically pressurised gases are specified within a balloon occupying the volume of the explosive charge. The pressure is set to the detonation pressure, or the so-called Chapman-Jouguet pressure, and the internal energy to the energy of the charge. The data for TNT are given in Table 1. The fictitious balloon membrane plays the role of the diaphragm in a shock tube. Its burst produces a blast wave traveling outwards and a rarefaction wave traveling inwards.

In the isotropic part of the blast wave propagation, the spherical Euler equations reduce to their radial component:

\[
\frac{\partial U}{\partial t} + \frac{1}{r^2} \frac{\partial (r^2 F)}{\partial r} = S, \quad (r, t) \in [0, L] \times [0, T]\] (1)

where

\[
U = (\rho, \rho u_r, \rho E)^t \] (2)

\[
F = (\rho u_r, \rho u_r^2, [\rho E + p] u_r)^t \] (3)

and

\[
S = (0, -\partial p/\partial r, S_h)^t \] (4)

\(r\) and \(t\) are the radial distance and the time, and \(T\) is the duration of the isotropic part. \(\rho\) and \(p\) stand for the density and the pressure, respectively, while \(u_r\) is the radial velocity. \(E\), the total specific internal energy, is given by: \(E = e + \frac{1}{2}u_r^2\), where \(e\) is the specific internal energy. \(S_h\) is an energy source term.

The computational domain \([0, L]\) is divided into two sub-domains: the balloon of radius \(R_c\) and the encompassing sphere of radius \(L\), where flow isotropy is satisfied, as depicted in Figure (1). The Euler equation (1) is complemented by an equation of state. For detonation products at extremely high enthalpy, the ideal gas assumption is not applicable, and the Johns-Wilkins-Lee (JWL) equation of state [7] is used instead:

\[
p = A \left(1 - \frac{\omega \rho}{R_1 \rho_c}\right) e^{-R_1 \rho_c/\rho} + B \left(1 - \frac{\omega \rho}{R_2 \rho_c}\right) e^{-R_2 \rho_c/\rho} + \omega \rho e \] (5)

\(A, B, R_1, R_2\) and \(\omega\) are adjustable constants for a given explosive and \(\rho_c\) is its density (see Table 1 for TNT-like explosive).

Downstream of the blast wave, the ideal gas law applies and reads in caloric form, with \(\gamma\) as the ratio of specific heats:

\[
p = (\gamma - 1)\rho e \] (6)

Boundary conditions are a full reflection condition at the explosive charge center and a non-reflective condition at the outer boundary. Initially, the pressure is set to the Chapman-Jouguet pressure inside the balloon and to the ambient pressure in the outer domain. The numerical scheme used to solve equation (1) is the so-called \(S_0^\alpha\) scheme [8]. The time step of this second order explicit scheme is limited by the CFL condition:

\[
\Delta t \leq CFL \times \min\left(\frac{\Delta x}{|u_r| + c}\right) \] (7)

where \(c\) is the local speed of sound and \(CFL = 0.8\). This value was found to be appropriate for all calculations. In addition, the Flux-Corrected Transport algorithm [9] has been used to prevent numerical oscillations associated with strong gradients.

2.2 Application

The test case is the detonation of an 18.5 \(g\) TNT explosive charge. In the early stage, the very high speed of sound due to prevailing hot gases leads to very small allowable time steps, of the order of \(10^{-11}\) s. The pressure and the temperature decay in time and the time step consequently increases up to about \(10^{-9}\) s. Figure (2) presents the peak overpressure vs the reduced distance \(Z = r/\rho_c^{1/3}\). The calculation with JWL equation of state is in very good agreement with the experimental data of Mills [3] and Henrych [4] as well as with numerical results from Brode [5]. The systematic underestimation of the numerical results

![Figure 1: Sub-domains involved in the isotropic computational domain.](image-url)
## 3 The three-dimensional problem

### 3.1 Physical and numerical model

When isotropy is no longer applicable, blast wave propagation must be carried on by a full three-dimensional approach. The flow is modeled by the three-dimensional Euler equations. The numerical solution method is a Cartesian unstructured finite-volume cell-centered scheme. For space discretization and time integration, the explicit upwind scheme coupled with a second-order intermediate time stepping method are used [12].

The flow is initially at rest over the three-dimensional domain except inside the sphere of radius $L$ and centered at the explosive charge where the flow is disturbed by the blast wave calculated by the one-dimensional method. The one-dimensional data have thus to be mapped onto the three-dimensional mesh. This is done thanks to the 1D-3D remapping technique described in the following.

### 3.2 Data remapping techniques

For remapping data from a one-dimensional mesh onto a three-dimensional much coarser mesh, an appropriate technique has to be developed that must be robust, accurate and weakly mesh sensitive. Some algorithms are tested and among them two are presented here. The first technique consists on integrating the time variations of the quantity to remap over a duration corresponding to the time step used in the three-dimensional simulation. The second technique proceeds by taking the chord mean value of this quantity at a given time. To simplify reasoning, it is supposed to remap the pressure $p$ from one-dimensional stencil onto three-dimensional one, other physical quantities are dealt with in the very same fashion.

At the volume cell $i$, the time integral of $p_{i}^{3D}$ over a time step $\Delta t^{3D}$ reads:

$$ p_{i}^{3D} = p_{i}^{*}(t_{0}) + \int_{t_{0}}^{t_{0}+\Delta t^{3D}} \left( \frac{\partial p_{i}^{1D}}{\partial t} \right)^{*} dt \quad (8) $$

where $p_{i}^{*}$ and $(\partial p_{i}^{1D}/\partial t)^{*}$ are linear interpolations, from one-dimensional stencil, of the pressure and its time derivative, respectively, at the center of the three-dimensional cell $i$.

For the chord mean value technique, the cell pressure $p_{i}^{3D}$ is given by the formula:

$$ p_{i}^{3D} = \frac{\int_{r_{M}}^{r_{N}} p_{i}^{1D}(r) \, dr}{r_{N} - r_{M}} \quad (9) $$

where $M$ and $N$ are the intersection points between the surface of the cell $i$ and the line that joins the center of this cell to the center of the explosive charge.

### Table 1: TNT data.

<table>
<thead>
<tr>
<th>Specific energy, $E_c$</th>
<th>Density, $\rho_c$</th>
<th>Detonation speed, $U$</th>
<th>Detonation pressure, $P_{CJ}$</th>
<th>$A$</th>
<th>$B$</th>
<th>$R_1$</th>
<th>$R_2$</th>
<th>$\omega$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$kJ/kg$</td>
<td>$kg/m^3$</td>
<td>$km/s$</td>
<td>$GPa$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>4870</td>
<td>1580</td>
<td>8500</td>
<td>21</td>
<td>3.73</td>
<td>3.74</td>
<td>4.15</td>
<td>0.90</td>
<td>0.35</td>
</tr>
</tbody>
</table>

Figure 2: Distribution of the relative overpressure $\Delta p/p_0$ vs the reduced distance $Z = r/M_c^{1/3}$.
Figure (3) shows the distribution, after data remapping, of the overpressure on a cross-section of a cube. The three-dimensional mesh size in the Figure (3)-(c,d) is eight times finer than in the Figure (3)-(a,b). It can be shown that the time integral method (a,c) is not preserving the isotopic proprieties of the flow and is more mesh-sensitive than the chord mean value method (b,d).

Figure (4) presents the comparison between the overpressure given by the one-dimensional calculations and the one remapped by the two techniques onto the three-dimensional domain. Here too, it can be seen that the chord mean value method is more accurate than the time integral method in both cases of coarser and finer grids.

Since the chord mean value method is at the same time fast, isotropy conservative, accurate and low mesh-sensitive, it is chosen to perform the following 1D-3D data remapping.

3.3 Three-dimensional test results

The test case simulates the propagation of a blast wave inside a rigid and closed cube of 1m edge. A TNT spherical charge of 0.3kg is located at the center of the cube. The simulation is led over $5 \times 10^{-3}$ s. The procedure that performs the simulation is described bellow.

First, the solver lets the one-dimensional routine performing simulation over a time $T^{1D} = 2 \times 10^{-4}$ s. This time corresponds to a wave propagating up to 0.43m from the blast center. At this stage, the time step $\Delta t^{1D}$ is about $2.5 \times 10^{-11}$ s and increases with time, like aforementioned in section 2, until about $\Delta t^{1D} = 2 \times 10^{-9}$ s at the end of the one-dimensional simulation. The solver prepares then the data in order to be injected as initial conditions for the three-dimensional simulation through the remapping routine as previously described. Then, the three-dimensional calculation can be performed. Because the three-dimensional mesh size is approximately 150 times larger than the one-dimensional stencil, its time step $\Delta t^{3D}$ is much larger, of the order of $10^{-6}$ s, at the beginning of the three-dimensional simulation part. This time step is about three orders of magnitude higher compared to a fully three-dimensional simulation, which is about $3 \times 10^{-10}$ s. In other words, for the same mesh size, while the simulation time using the 1D-3D combined method takes about one hour CPU-time, it turns quite prohibitive using the fully three-dimensional approach since it would take considerably much more time. In this regard also, the 1D-3D combined method seems to be highly desirable and more efficient compared to an approach that handles three-dimensional simulation of the blast waves from the onset.

Figure (5) represents the evolution of the iso-Mach in a cross-section of the cube from 0.2ms to 1ms. Although the mesh is Cartesian, isotropy is nicely kept on until blast waves reach the solid walls where they are reflected and propagate back to the box center. When arrived to the center, a new spherical wave is formed by the superposition of the reflected waves from the box walls. This process will continue while, due to numerical dissipation, the energy of the waves decays. No significant flow disturbance is shown after 1ms, whose leads shortly the fluid into rest.

4 Conclusion

High detonating and exploding spherical charge is modeled. The generated blast wave is simulated in two parts. The first one is led, where the flow isotropy is fulfilled, by means of a spherical model. Both the ideal gas and John-Wilkins-Lee equations of state governing hot detonation products are examined. Strong shock traveling through the fluid flow is successfully captured by the numerical model. The ideal gas law leads to slightly overestimating the maximum peak of pressure while the JWLEquation of state gives, at lower numerical cost, high quality results compared to both experiments and well established numerical data. When the isotropy is no longer valid, the simulation proceeds with a three-dimensional method provided with initial condition by a remapping technique. Among the tested 1D-3D remapping techniques, the chord mean value method is found to satisfy best at the same time accuracy and low mesh-sensitivity. This technique is therefore used to supply with initial conditions the three-dimensional simulation part. The one-dimensional part, the remapping technique and the three-dimensional part constitute the 1D-3D combined simulation method. Through a three-dimensional test case, the method is demonstrated to be ready for blast wave simulations in complex three-dimensional geometries in order to validate the entire developed method.

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References:

Figure 3: Iso-pressure on the middle cross-section.


Figure 4: Pressure distribution.

Figure 5: Iso-Mach at different times.