



Hydrocode simulations of air and water shocks for facility vulnerability assessments

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Abstract

Hydrocodes are widely used in the study of explosive systems but their use in routine facility vulnerability assessments has been limited due to the computational resources typically required. These requirements are due to the fact that the majority of hydrocodes have been developed primarily for the simulation of weapon-scale phenomena. It is not practical to use these same numerical frameworks on the large domains found in facility vulnerability studies. Here, a hydrocode formulated specifically for facility vulnerability assessments is reviewed. Techniques used to accurately represent the explosive source while maintaining computational efficiency are described. Submodels for addressing other issues found in typical terrorist attack scenarios are presented. In terrorist attack scenarios, loads produced by shocks play an important role in vulnerability. Due to the difference in the material properties of water and air and interface phenomena, there exists significant contrast in wave propagation phenomena in these two medium. These physical variations also require special attention be paid to the mathematical and numerical models used in the hydrocodes. Simulations for a variety of air and water shock scenarios are presented to validate the computational models used in the hydrocode and highlight the phenomenological issues.

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1. Introduction

The vulnerability of facilities to shocks produced by explosives is a key element in assessments for various safety and anti-terrorism applications. Hydrocodes are widely used in the study of explosive systems and shocks in the vicinity of a charge or weapon. But their

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use in routine facility vulnerability assessments has been limited due to the computational resources typically required. These requirements are due to the fact that the majority of hydrocodes have been developed primarily for the simulation of weapon-scale phenomena. It is not practical to use these same numerical frameworks on the large domains found in facility vulnerability studies.

One issue associated with hydrocodes developed for weapon-scale analysis that prevent their use in large-scale scenarios is the required grid resolution. Typically a fine resolution is required because of the details used to represent the detonation process and its coupling with the fluid dynamics aspects. Standard approaches require numerous mesh cells within the explosive body itself. If a model is used that dictates fine meshing, then there are two options used: (1) adaptive meshing, or (2) remapping solutions into new meshes at various points in the simulation.

The approach reviewed here offers an alternative by how the detonation process is modeled. This relaxes the mesh requirements in the vicinity of the explosive. From an application standpoint, this is viable because in vulnerability assessments, typically damage “within the crater” is known to far exceed acceptable limits and the focus is on damage “outside the crater”. By not employing remapping, time is saved by reducing the need for a user to reinitiate a simulation. By not employing adaptive meshing, computational time can be saved, particularly when complex geometries are involved. The following information is to highlight the utility of this approach and a tool based on this approach in vulnerability assessments.

In terrorist attack scenarios, loads produced by shocks play an important role. Differences in material properties affect these wave propagation phenomena. An example of material property influences is the difference in the strength of shocks produced by the same charge size in air versus water. These physical variations also require special attention be paid to the mathematical and numerical models used in the hydrocodes.

Here, a hydrocode formulated specifically for facility vulnerability assessments is reviewed. Techniques used to accurately represent the explosive source while maintaining computational efficiency are described. Simulations for air and water shock scenarios are presented to validate the computational models used in the hydrocode and highlight the phenomenological issues. Attention is paid to the maximum pressure and total impulse predicted at various locations away from an explosive charge.

2. Computational model

The hydrocode discussed here is used for explosion scenarios involving condensed phase high-explosives (HE). It is titled the Computational Explosion and Blast Assessment Model (CEBAM) and is based on an earlier version developed for vapor cloud explosions (VCEs). The fundamentals of the code as used for VCEs are described in [1], while [2,3] show comparisons of CEBAM predictions with large scale explosion data. Clutter et al. [4] reviews use of the code in facility scale accident investigations which include many of the same tasks as found in vulnerability assessments. Here, the equations solved within the code are reviewed as well as the numerical techniques employed. The equations of state for the various materials involved are also presented.

2.1. Governing equations

The governing equations solved by the model are the Euler equations and includes a conservation equations for mass, which in differential form is:

$$\frac{\partial}{\partial t}(\rho) + \frac{\partial}{\partial x_j}(\rho u_j) = 0 \quad (1)$$

where ρ is density and u_j the velocity component in the x_j direction. The local density is dependent on the amount of each material present and a mass fraction formulation is used. The corresponding momentum equation is:

$$\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_j}(\rho u_i u_j) + \frac{\partial P}{\partial x_i} = 0 \quad (2)$$

where P is pressure and the energy equation is:

$$\frac{\partial}{\partial t}(\rho E) + \frac{\partial}{\partial x_j}(\rho u_j H) = 0 \quad (3)$$

where E represents the total energy and H the total enthalpy. The total enthalpy is defined as $H = E + P/\rho$ with the total energy being a sum of kinetic and internal energy through $E = e + |u|^2/2$. Along with this set of equations, an appropriate material conservation equation of the general form:

$$\frac{\partial}{\partial t}(\rho \alpha_n) + \frac{\partial}{\partial x_j}(\rho \alpha_n u_j) = \omega_n \quad (4)$$

is solved for each material involved. For the current problems of interest, the materials that can be involved include air, explosive, detonation products and water. The parameter α_n represents the local mass fraction of material n and will range between 0 and 1. The term ω_n represents a production source term for the material. Here, only the detonation products will need this term defined.

The material equations are coupled to the energy equation through the definition of the internal energy which is related to the individual material enthalpies (h_i) through:

$$e = \sum_{i=1}^{NS} \alpha_i h_i - \frac{P}{\rho} \quad (5)$$

where

$$h_i = h_{f,i}^0 + \int_{T_r}^T C_{p,i} dT \quad (6)$$

It should be noted that this is one area where CEBAM differs from many of the other hydrocodes used for HE simulations. In those codes, a source term is explicitly included in the energy equation and parameters are used in this term based on the explosive involved. Here, the material enthalpy approach is taken for various reasons. First, CEBAM has the ability to model gas phase detonations and deflagrations as well as the HE detonations discussed here. Using the enthalpy approach produces a single modeling framework

useful for all scenarios. Also, this approach allows for the coupling of multiple explosion sources such as an event where an HE charge is used to initiate a gas phase detonation.

In addition to this set of equations, the equation of state for each material involved is included in the code along with the representation of the material source term. These are described next.

2.2. Equations of state

The amount of each material present at a given location not only sets the density but also sets the local pressure through their individual equations of state (EOS). For the gas phase materials, a Becker–Kistiakowsky–Wilson (BKW) equation of state of the form:

$$P = \frac{\rho R_u T}{M_w} [\phi(T)] = \frac{\rho R_u T}{M_w} [1 + x e^{\beta x}] \quad (7)$$

is used. This EOS was chosen because of its behavior near atmospheric conditions. Because of its functional form, at the lower pressures, the BKW EOS collapses to the ideal gas form. The parameters used in the BKW EOS for air and detonation products are taken from [6].

As mentioned, a primary focus of the hydrocode developed here is for efficient large-scale system simulation. Therefore, every aspect of the model has been investigated to see if numerical approaches can be taken to enhance efficiency. One simplification in the BKW EOS has been made with this in mind. Because of the enthalpy formulation used here and to facilitate the simulation of multiple explosion sources, temperature must be explicitly calculated during the simulation. If the functional dependence of ϕ in Eq. (7) on temperature is higher than order 1, then an iterative process must be used to extract temperature from the conserved variables. This can be computationally expensive since this process would have to be performed at each computational cell and at every time step. By introducing a linearized representation of the exponential term in the BKW EOS, the need to iterate is eliminated. This has been done in CEBAM and the accuracy of this substitution has been evaluated based on simulation results such as that presented here.

For the scenarios with water, the Tait equation of state is used which is in the form

$$P = B \left[\left(\frac{\rho}{\rho_0} \right)^\gamma - 1 \right] + A \quad (8)$$

with the constant used being taken from [7]. As can be seen in the functional form, the internal energy is not included in the Tait equation and is, therefore, applicable only to the liquid phase of the water. It has been used successfully in previous computational studies of underwater explosions such as that conducted in [8] as well as other underwater shock studies such as those of Hsieh [9]. Hsieh [9] also demonstrates that the Tait equation performs well even at very strong shock conditions when compared to more complex EOS options. It is used here because of its simplicity.

The fact that the Tait EOS is applicable only to the liquid phase of the water is not restrictive since the primary interest in the modeling performed here is the shock transmitted

through the water and not in other aspects such as the growth of the gas bubble produced by the detonation products. Such gas bubble production and cavitation would be key if the explosion occurred in close vicinity of the structure of interest. Here, the focus is on distances outside this regime.

2.3. Explosive source term

The final aspect of the computational model is the numerical representation of the explosive source term. The HE detonation model used is a prescription type model as described in [13], which is the most common class of model used in hydrocodes. In short, a prescription model pre-maps the computational cells that lay within the explosive to determine the time at which the detonation front will arrive at their particular location. This is simply done by knowing the detonation velocity and the ignition point. When the detonation front does arrive at a given cell, the reaction process is modeled through the explosive source term by the release of an amount of energy based on the explosive involved. Frequently, the time over which this energy is released is set not by physical parameters but the stability requirements of the code.

The current model does differ from the standard prescription model due to the use of the enthalpy formulation. Building on the previous models in CEBAM for VCEs described in [1], the detonation process is modeled as a one-step reaction process with the rate of reaction being inversely proportional to the detonation velocity.

In reality the detonation front is a closely coupled pairing of a shock and reaction front. As demonstrated in [13], the variation of properties across the two fronts can be explicitly modeled if a kinetics based detonation model is used. Across the two fronts the dependent variables change based on the shock jump conditions and the reaction process. The prescription type models do not explicitly resolve the two fronts but releases the correct amount of energy to produce the post reaction zone, or CJ, conditions.

In typical hydrocodes, the explosive is discretized with numerous computational cells. Therefore, the release of the energy produces an associated change in other properties such as density and pressure. As these models have been developed for weapon scale analysis, the fine discretization of the explosive is not restrictive and in fact is needed. However, for the current problems of interest, facility scale vulnerability assessments, such fine discretization in the explosive source is not needed and can be restrictive. The goal of the model developed here has been an appropriate representation of the explosive source that provides accurate shock propagation predictions away from the source. To promote efficiency, an approach that allows the source to be represented as either a portion of a computational cell or a small set of cells has been taken.

After reviewing the mathematical aspects of the prescription class of detonation models, the conclusion was that a technique that explicitly defined the change in location specific volume in addition to the defined energy release due to the detonation would work. This is accomplished by introducing an appropriate term in the source term vector of the governing equations. The accuracy of this approach can be determined by reviewing simulation results presented later.

There is some stipulations that do apply to this representation of the explosive source term. For instance, if the grid resolution used is such that the size of the charge is smaller than

a single cell, the actual shape of the charge cannot be discerned and the source is essentially a spherical charge. Shape effects, such as the scenario where a gas transportation truck is packed with explosives, can be modeled by using a refined grid. However, the necessary refinement is not nearly what is needed for typical hydrocodes. The issue of simulating a wide variety of charge shapes with the model is currently being investigated and will be presented in future documents.

2.4. Numerical formulation

The governing equations described above are solved using an Eulerian, Finite-Volume formulation. The code is a fully three-dimensional model so the vector of conserved variables is:

$$Q = [\rho, \rho u, \rho p v, \rho w, \rho E, \rho \alpha_{\text{air}}, \rho \alpha_{\text{HE}}, \rho \alpha_{\text{prod}}, \rho \alpha_{\text{H}_2\text{O}}]^T \quad (9)$$

where HE denotes the high explosive, prod the detonation products, and H₂O the water. The system of equations, when solved using the Eulerian, finite-volume formulation, takes the general form:

$$\frac{d}{dt}(QV) + \sum_{i=1}^3 R_i = \Omega \quad (10)$$

where Ω represents the local source term vector and R_i the spatial discretized flux terms in the i direction. This term is defined as:

$$R_i = (F\Gamma)_{i+1/2} - (F\Gamma)_{i-1/2} \quad (11)$$

with $F_{i\pm 1/2}$ denoting the fluxes at the two cell faces in the i direction and Γ the projected cell face area in the same direction.

The next aspect of the computational model is the definition of the flux terms at the cell interfaces. In previous work with CEBAM where only gas phase material was present, a Steger–Warming flux vector splitting scheme, as described in [10,11] was used. Simulations using this scheme in CEBAM have been documented in [1–3]. This also has proven accurate for the HE scenarios in air presented here.

For the simulations of explosions in water, presented here, the U-split version of the advective upstream splitting method (AUSM) as described in [12] is used. This scheme was selected based on the successful use of this scheme in earlier studies such as that in [8]. As it represents a new algorithm integrated into CEBAM, its formulation is reviewed here.

Using the AUSM scheme, the flux at the interface $i + 1/2$ will be:

$$F_{i+1/2} = \frac{1}{2}[u_{i+1/2}(Q_L + Q_R) - |u_{i+1/2}|(Q_L - Q_R)] + \widehat{P}_{i+1/2} \quad (12)$$

where Q_L and Q_R represent the state of the dependent variables on the left and right sides of the interface. The fluid velocity at the interface is given by:

$$u_{i+1/2} = u_L^+ + u_R^- \quad (13)$$

where

$$u_{\pm} = \begin{cases} \pm \frac{1}{4c}(u \pm c)^2, & |u| \leq c \\ \frac{1}{2}(u \pm |c|), & \text{otherwise} \end{cases} \quad (14)$$

with c being the speed of sound. The parameter $\widehat{P}_{i+1/2}$ represents the pressure flux vector at the interface and is defined as:

$$\widehat{P}_{i+1/2} = [0, \delta_{i1} P_{i+1/2}, \delta_{i2} P_{i+1/2}, \delta_{i3} P_{i+1/2}, 0, 0, 0, 0] \quad (15)$$

with the pressure at the interface being:

$$P_{i+1/2} = P_L^+ + P_R^- \quad (16)$$

with the pressure contributions from each side being:

$$P^{\pm} = P u^{\pm} = \begin{cases} \frac{1}{c} \left(\pm 2 - \frac{u}{c} \right), & |u| \leq c \\ \frac{1}{u}, & \text{otherwise} \end{cases} \quad (17)$$

The parameter δ_{ij} is equal to 1 when i equals j and 0 when they are different.

Second order spatial accuracy is achieved by correct definition of the left and right state variables, Q_L and Q_R , using a variable extrapolation. Second order accuracy in time is achieved using a predictor-corrector method. Both approaches are detailed in [10,11].

3. Comparison with experimental data

The hydrocode described here is for use in predicting the shock loads on facility components produced from HE charges in air and water. Therefore, there are two primary characteristics of the code that must be evaluated regarding accuracy. The first is the ability to correctly capture the propagation of shock, compression and expansion waves. An excellent test scenario for this aspect is the shock tube configuration. Results using CEBAM for such configurations are presented here.

The second key aspect is the representation of the explosive source. As the interest here is the shock loading on structural components away from the charge, of primary interest is the modeling of the energy addition process. It is this that sets the pressure field away from the charge. Therefore, an appropriate evaluation of this aspect of the code is to compare predictions of the pressure and impulse field for explosive charges. This is done here for both air and water mediums.

3.1. Shock tube data

Countless shock-tube scenarios have been simulated with CEBAM with good agreement. Clutter et al. [5] provides documentation regarding this aspect of the code. Therefore, here only a few examples are shown. Predicted time histories for the configuration shown in

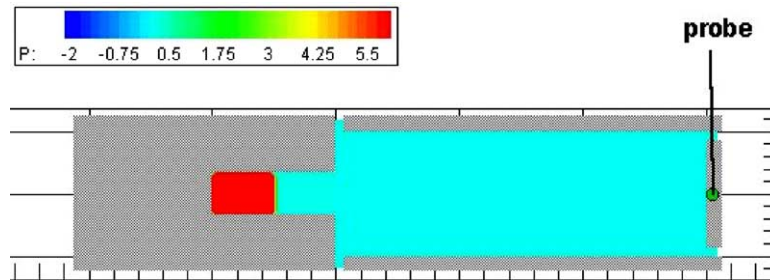


Fig. 1. One shock tube configuration used for CEBAM validation.

Fig. 1, at the probe location denoted in the figure, are compared to test measurements at this location. The overall length of this test device was on the order of 6 ft. The energy source was pressurized air.

The pressure loading on a structural element can come from the initial shock as shown in Fig. 2. However, loadings can be generated by secondary compression waves as shown in Fig. 3. The pressure time history is also highly dependent on expansion waves generated in the domain. The wide variety of high and low pressure regions are evident in Figs. 2 and 3. Fig. 4 shows the entire time history for the probe.

CEBAM has been evaluated against multiple shock tube data sets such as that shown in Fig. 5 taken from a vented tube described in [5]. This device also used high pressure air as the energy source. CEBAM has proven accurate in the capturing of all types of shock, compression, and expansion waves. Data such as the examples presented in this section can be used to validate the ability of codes to correctly model the fluid dynamic process. This is the first aspect of validation mentioned above. The next is the explosion source component which is addressed next.

3.2. Air blast data

Here, the sub-model used to represent the detonation of explosive material, detailed earlier, is demonstrated. The model allows for the definition of the chemical properties of the actual explosive involved. However, even today, typically in vulnerability assessments, TNT is assumed. Even if a different explosive is known to be the primary threat, a TNT equivalence is usually established. This is due in part to the historical use of TNT in analytical and handbook assessment methods.

The actual chemical properties of the explosive affects how the energy is released during the detonation process. Given the predominate use of TNT in vulnerability assessments, that is the explosive first integrated into the CEBAM code. A scenario of a spherical charge located in an un-obstructed environment is simulated. The consolidated data found in [14] for TNT is used as a benchmark for comparison. Fig. 6 shows the CEBAM predictions for a TNT charge and good agreement for both pressure and impulse is found. Fig. 7 shows time histories recorded away from the charge using numerical pressure probes. The characteristics and trends, such as the scaled distance at which no negative phase is present, are consistent with experimental data.

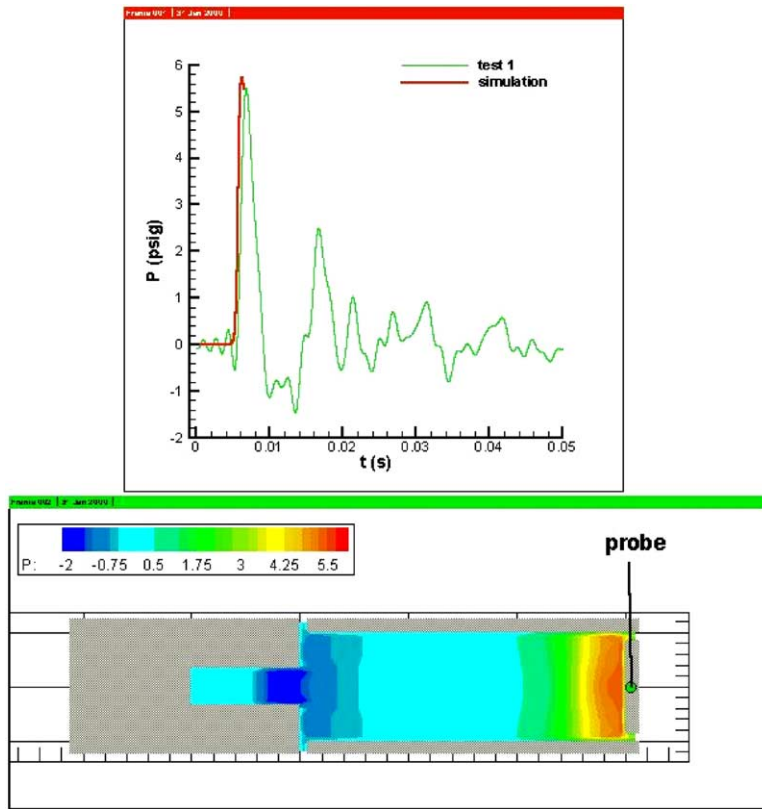


Fig. 2. Example results showing predicted pressure field and reflection of initial shock.

The predicted impulse data does show a slight over prediction close into the explosive. This is being investigated but is most likely due to the representation of the explosive charge as only a fraction of a computational cell. Since the purpose of CEBAM, as formulated and presented here, is for facility vulnerability assessments and not close-in processes such as spalling, this is viewed as acceptable.

For the simulation presented here, the initial conditions and grid spacing were such that the explosive charge occupied only a fraction of one computational cell. Therefore, no region of high density mesh cells was needed. CEBAM simulations have been performed for various charge sizes and all scale favorably to the experimental data. Also, CEBAM has compared favorably to other HE test data sets. However, this information is of a sensitive nature and cannot be shared in an open format.

3.3. Water blast data

The malicious use of explosive laden watercraft is a highly probable event. Therefore, the ability of CEBAM to predict the shock loads from such an event is assessed. As discusses

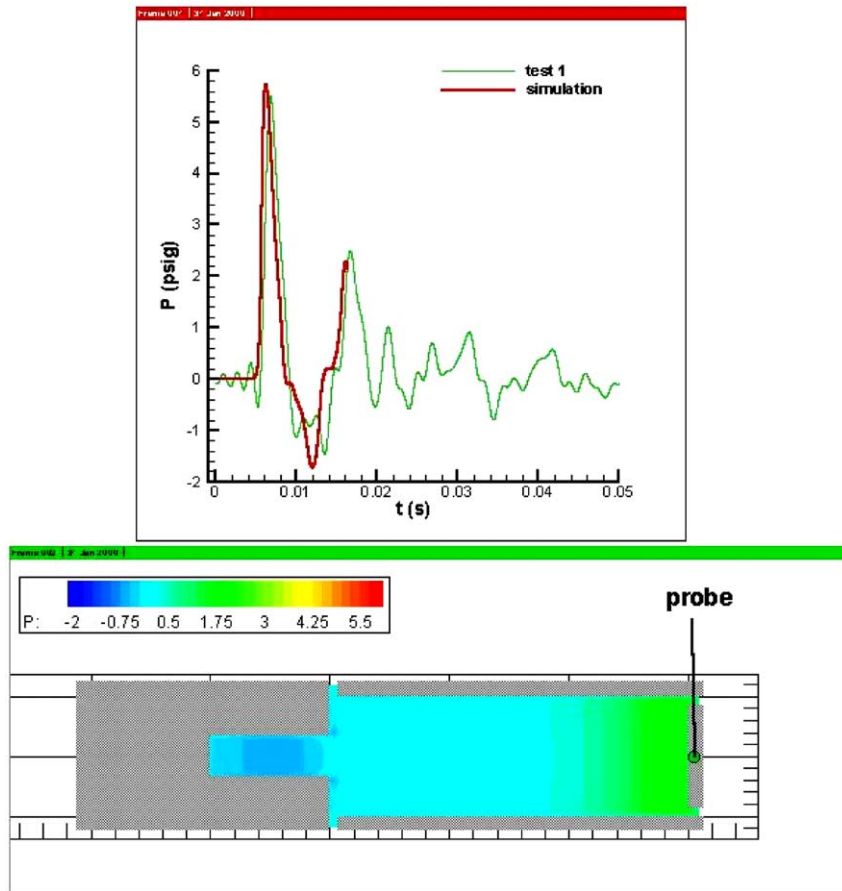


Fig. 3. Example results showing predicted pressure field and reflection of secondary shock.

in [15], depending on the location of the structures concerned, the threat scenario will be an explosive charge either on the surface of the water or submerged. Here, the case of a submerged charge is simulated. As in the case of the air shocks discussed earlier, of primary interest is the prediction of loads some distance from the charge.

For the test case presented here, the explosive charge was placed in essentially an infinite domain of water. This was to mimic the free water scenario used in testing and theoretical work. In the case of underwater explosions in a body of water, a variety of waves can be produced due to the free surface and the water-body bottom. For a further discussion of these various issues see [15]. In the free water scenario, it is only the direct wave that is produced.

To evaluate the predictions by CEBAM, test data from [7] is used. This test data compares well with the theoretical free water curve. Fig. 6 shows a comparison of both the predicted peak pressure and impulse from CEBAM for a TNT charge to this data. For these initial tests

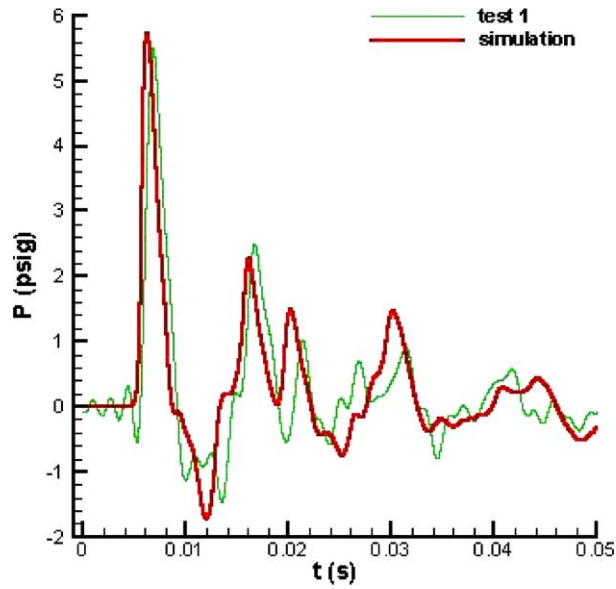


Fig. 4. Entire time history simulated for the tube of Fig. 1 compared to test data.

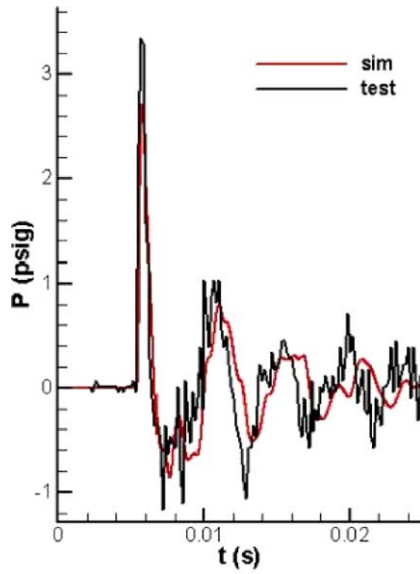


Fig. 5. CEBAM simulation results compared to test data taken from a second shock tube.

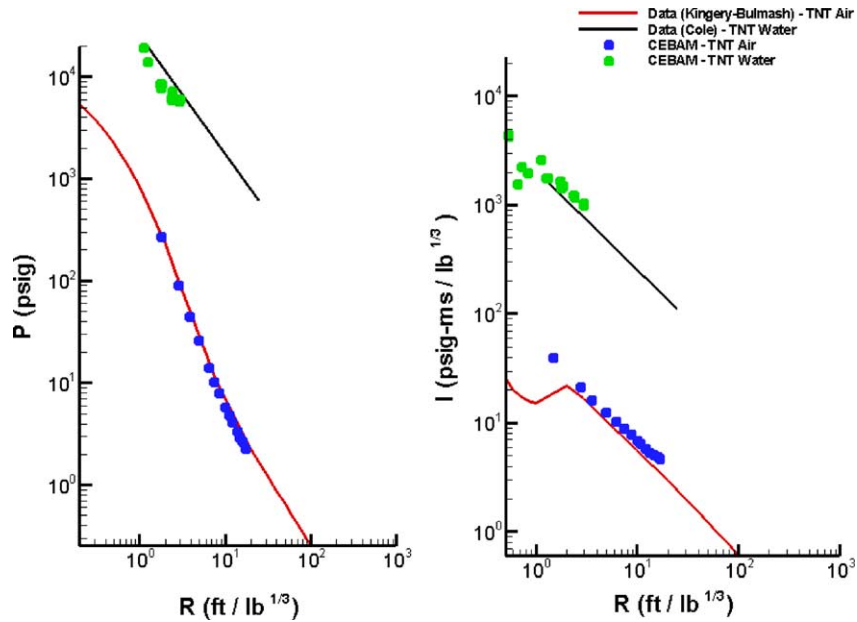


Fig. 6. Comparison of TNT test data and CEBAM predictions for a spherical charge.

only a limited water domain was simulated and good agreement is found. Time histories are not presented since such experimental data was not readily available in the open literature used for the current study. Additional comparisons are being conducted to further validate the water model.

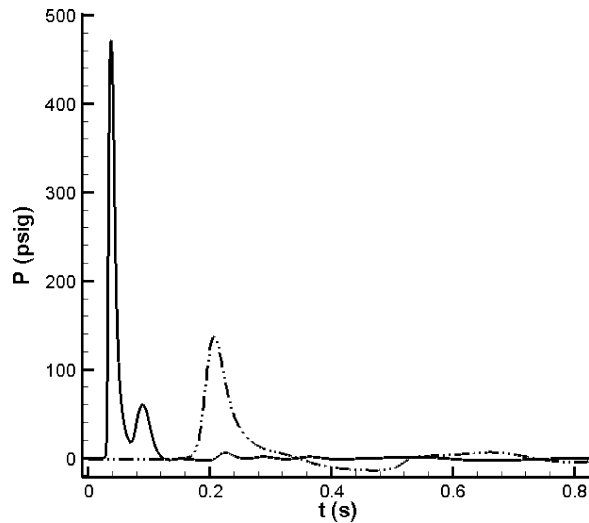


Fig. 7. Representative time histories at locations away from the charge as predicted by CEBAM.

4. Example explosion scenario calculations

Vulnerability assessments typically include evaluating the explosion process in a complex geometric configuration. CEBAM has been used for various geometric scenarios. These have ranged from a setting which encompasses only a few structures such as those depicted in Figs. 8 and 9, to larger domains such as urban settings as shown in Figs. 9 and 10. Also, more complex geometric configurations such as that seen in Fig. 11 can be involved.

As data for such scenarios are extremely limited, direct comparisons to model output is difficult. Therefore, model users and developers are restricted to validate the sub-models

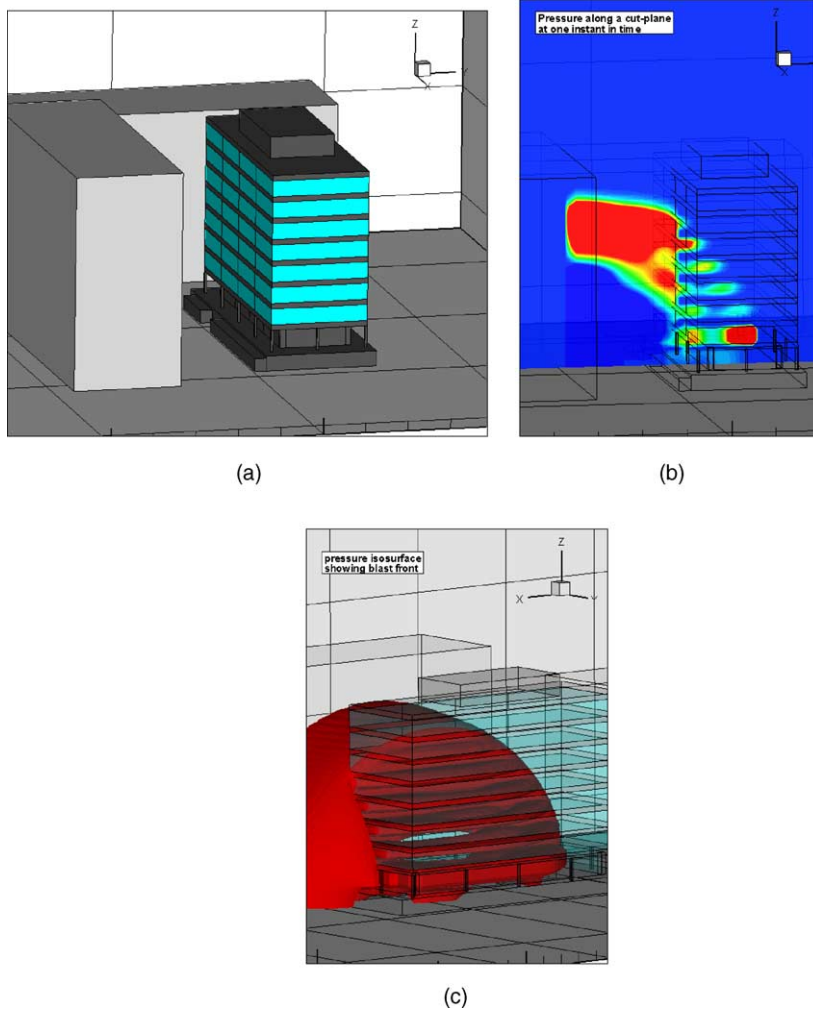


Fig. 8. (a) Single building scenario assessed in CEBAM. Images show: (b) the pressure contour along a plane through the middle of the building and (c) a pressure isosurface denoting the blast front.

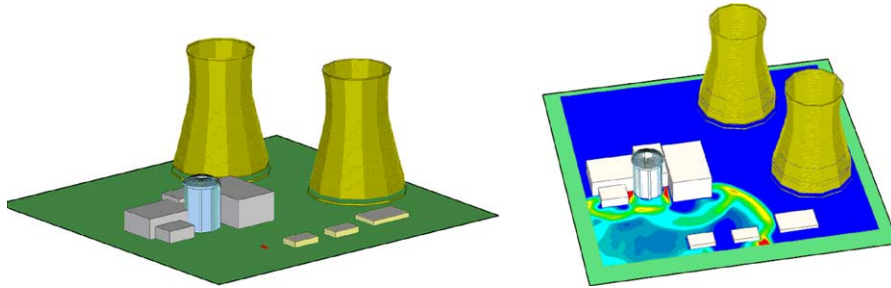


Fig. 9. CEBAM simulation results showing the pressure variation across the ground some time after detonation.

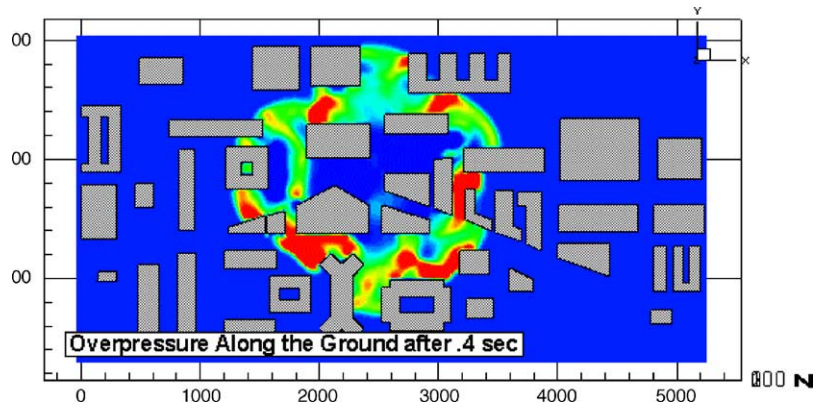


Fig. 10. CEBAM simulation for a car bomb scenario in an urban setting.

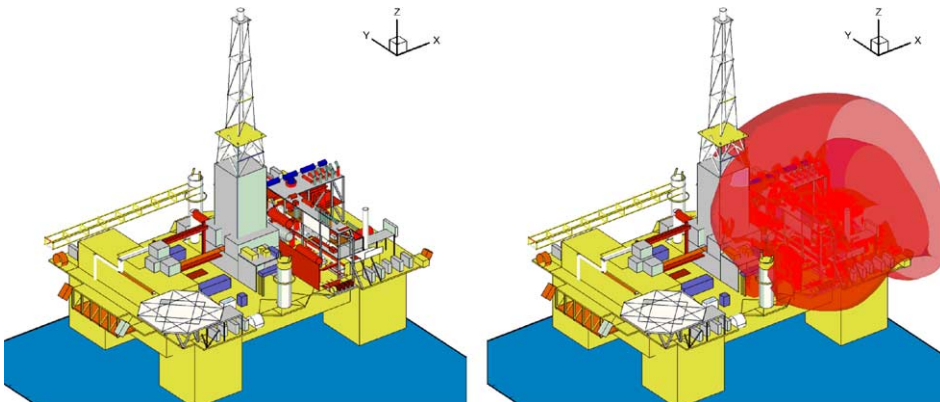


Fig. 11. Industrial facility vulnerability assessment using CEBAM.

of a tool that are known to affect the accuracy of the predictions made for more complex scenarios. Here, attention has been paid to two of the primary sub-models, the representation of the explosive source and the propagation of compression waves through air and water. Based on data such as that presented here, the approach used to represent the explosive source and detonation process produces the correct shock output. Also, as evident in the section on shock tube data, CEBAM accurately predicts the interaction of shock, compression, and expansion waves with objects. Detailed comparisons between CEBAM results and test data for gas explosions in complex geometries are represented in [1–3].

Currently in CEBAM, the structural response to blast loadings is handled using an empirically based model. The response modes of the majority of structures of interest in such assessments are such that this decoupled approach is adequate. The use of CEBAM in this approach is detailed in [4,15].

5. Summary and conclusions

The use of hydrocodes in facility vulnerability assessments has been very limited, primarily due to the computational requires of typical hydrocodes. Here, modeling techniques used to increase efficiency have been described. Using a tailored explosion source model, the charge can be represented within a single cell. This approach relaxes the grid refinement required when using typical hydrocodes.

The numerical model used in CEBAM to simulate explosions in both air and water have been detailed. The accuracy of the model to handle compression, shock, and expansion waves is evident by the shock tube comparisons. The accuracy of the explosion source model for charges in air and water is demonstrated as well. The use of the various equations of state for the multiple materials is proven to be both efficient and accurate.

Using a hydrocode formulated specifically for vulnerability assessments greatly increases efficiency and the types of scenarios that can be simulated as evident in the example geometries shown here. CEBAM has been used for multiple facility assessments where the blast loads on structures are of interest. In these assessments, many times the structures of interest are not in the immediate vicinity of the charge and the approach detailed here is appropriate. The use of CEBAM for extremely close-in scenarios such as breaching is currently under investigation.

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