AN OVERVIEW OF NUMERICAL SIMULATION OF CHEMICAL WEAPON EXPLOSIONS USING HYDROCODES

by

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ABSTRACT

The U.S. Army Engineering and Support Center, Huntsville, U.S. Army Corps of Engineers, is the Army's Mandatory Center of Expertise for the remediation of ordnance and explosive (OE) waste sites. The Center is also the design agency for the Army's Chemical Stockpile Disposal Program. To develop safe and efficient methods for removal of ordnance, the blast and fragment hazards caused by an explosion must be known. Typically, this information has been developed via expensive and time-consuming arena tests. However, the schedule for an OE remediation project often precludes performing an arena test. Additionally, many chemical weapons already recovered, or that we expect to find, are pre-World War II munitions. No arena test data exists for most of these weapons.

The Huntsville Center is investigating the use of hydrocode programs for use in predicting blast pressures and fragmentation from chemical weapons. Hydrocodes are used extensively in modeling explosions, high-velocity impacts, and other phenomena. It is believed that, if correctly used, hydrocodes can provide a fast and cost-effective alternative to arena testing, especially for the complex geometries of chemical weapons. The goal of this effort is to validate hydrocodes for prediction of chemical weapon's blast and fragment effects, and to develop guidelines for performing this type of analysis.

This paper presents an overview of the Center's investigation into hydrocode modeling of chemical weapons. A general overview of the capabilities of hydrocodes, and a description of available hydrocode programs is presented. Our efforts to model chemical weapons and chemical agents with two hydrocode programs are discussed. A brief comparison of hydrocode results to arena test data is provided. Some guidelines for hydrocode modeling are presented. A more detailed report on specific hydrocode model results will be presented in a second paper immediately following this presentation.

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Introduction

The Huntsville Engineering and Support Center, US Army Corps of Engineers, is the Army's design and construction agency for the Chemical Stockpile Disposal Program. The Center is home of the Corps' Technical Center of Expertise for Explosive Safety. Also, the Center is the Corps' Mandatory Center of Expertise and Design Center for Ordnance and Explosives. In this role, the Center defines Army and DOD policy for the remediation of sites contaminated with unexploded ordnance. Huntsville Center is also the central manager for the cleanup of more than 2,000 OEW-contaminated sites. These include active military bases under the Installation Restoration Program, formerly-used defense sites (FUDS) under the Defense Environmental Restoration Program, and sites slated for closure by the Base Realignment and Closure process. A large number of sites are contaminated with chemical warfare material.

In order to execute these missions, it is necessary to maintain and expand a capability to predict the effects of chemical weapons explosions. Especially for the OE remediation program, the ability to predict these effects is critical to providing safety in the event of an accidental explosion. Some level of protection must be afforded to personnel actively involved in recovering unexploded ordnance. Also, the general public must be protected from both personal injury and property damage. In order to provide adequate engineering safety controls, we must be able to predict the blast and fragmentation effects of these weapons, as well as the chemical agent effects.

The ability to predict chemical agent effects is well established. However, prediction of the conventional explosion effects of chemical weapons is not as straightforward a process. Conventional methods of predicting blast and fragment effects are not directly applicable to chemical munitions. There are a number of widely used techniques for predicting these effect from non-chemical weapons. In DOD, perhaps the most widely used are those methods found in TM 5-1300/NAVFAC P-397/AFM 88-2 (Department of the Army 1990). This and other references provide equations that permit the calculation of relatively conservative blast pressures and fragment weights and velocities. However, the presence of a chemical agent filler in a munition causes effects that can be quite different from those predicted by these equations. The agent will usually absorb some of the energy of the explosion, resulting in a reduction of the effective charge weight. This means the blast pressures from the explosion can be much less than those from the same weight of explosive alone. Also, fragment velocities can be only a small fraction of those produced by a conventional munition. Fragments are generally larger; chemical munitions can often burst open much like a pressure vessel, with a small number of larger fragments, instead of the large number of small, penetrating fragments from a conventional munition. Test data exists for some chemical weapons. However, much of this data is classified and not readily available. For many of the pre-World War II chemical weapons, no such data is available. It is possible to perform arena tests to develop data on effective charge weights for predicting blast pressures, and to determine fragment size and velocity distributions. Clearly, these must almost always be performed with simulated munitions, containing an agent simulant, since the detonation of the actual munitions will release the chemical agent. Such arena test programs are both time-consuming and expensive. Costs for testing for one munition can be $25,000 or more, and can take from weeks to months the perform.

Given these limitations on both predicting methods and testing, it was decided to investigate the use of hydrocode programs for modeling chemical weapons explosions. It is believed that the use of hydrocodes can provide good predictions of conventional blast effects. This paper summarizes some of the results of the efforts to model chemical weapons explosions using hydrocodes. Additional information, in more detail, is provided in a companion paper presented at this conference (Stevens 1996e).

Hydrocode Programs

A hydrocode is an advanced computer program (or usually a series of programs) designed to perform modeling of complex, dynamic, continuum mechanics problems. Hydrocodes were first written to aid in the development of nuclear weapons. The original codes did not feature adequate models of the strength of solid materials, and all materials were modeled as fluids. Thus, metals and other materials of normally significant strength were treated as fluids, with no viscosity, and the expression, "hydrodynamic computer code," later shortened to "hydrocode," was used to refer to these programs. The original development of hydrocode programs was performed mostly at Department of Energy laboratories, in support of the design of nuclear weapons. Over the years, the codes have been improved and modified for other military and non-military applications, and unrestricted versions of many codes can be obtained in the open marketplace.

Hydrocode programs use a discretized mesh, or grid, in two or three dimensions, to model the materials being evaluated. Either finite element or finite difference techniques are used, but most modern codes us finite difference modeling. Spatial discretization can be performed in an Eulerian, Lagrangian, of Arbitrary Eulerian Lagrangian (ALE) setting. In an Eulerian model, the mesh or grid remains fixed in space, and materials are permitted to move through the mesh. This approach is often best for problems involving fluid and gas flow. In a Lagrangian model, the mesh is attached to the material and moves with it as it deforms. In an ALE approach, the material is convected with respect to the mesh, which also moves, according to a user-specified scheme for remeshing or rezoning. This approach can span both fluids and solids. In all three cases, large deformations can be modeled, although the Eulerian and ALE approaches are best for large distortions. An Eulerian code can be used for the entire analysis of a conventional or chemical weapon detonation. A Lagrangian analysis would most accurately model the rupture of the casing, up to the time at which the casing breaks up (depending strongly on the quality of the constitutive model). However, due to large deformations in the explosive, agent, and air, a Lagrangian model will break down after rupture of the casing, because of the large distortions of the mesh. This part of the analysis is best handled by an Eulerian code. Finally, in principle, the ALE approach could handle the entire analysis. For modeling the complex nature of weapons explosions, the best results appear to be obtained through the use of an Eulerian framework combined with finite difference discretization.

Hydrocodes use equations of state (EOS) to model the hydrostatic response of materials and relate pressure, density, temperature, and internal energy of the materials. Constitutive strength models are used to represent the shear resistance and strength of the materials. Failure models are use to compute the response of the materials to stress and predict material rupture or yield. These models combine to form a series of coupled, non-linear, partial differential equations, for which no implicit solution exists. Solution of the problem is obtained by numerical integration over time. In this manner, the problem being modeled can be examined over a relatively long period of time, using very small time increments.

Many different hydrocodes currently exist, with their only common feature being the use of explicit time integration for temporal discretization. Unlike an implicit solution, explicit time integration does not require the formulation of a global stiffness matrix for each material in the model. Neither does it require the evaluation of equations of motion at the elemental or nodal level. This method is only conditionally stable, and a very small time step is typically required. However, for events that occur over very short periods of time, such as explosions or high-velocity impact, the small time step is not an inconvenience.

Tasks Performed in Hydrocode Evaluation

The following tasks were performed in the investigation of hydrocode modeling:

- A literature search was performed to identify examples of the use of hydrocodes in modeling chemical weapons effects.
- An extensive list of hydrocode programs was compiled, and a comparative evaluation of a subset of these codes was undertaken to determine which codes might be the most useful.
- A single hydrocode was selected for use in this effort.
- Using the selected hydrocode, a set of nine chemical munitions were modeled and analyzed. This analysis was performed to predict near-field blast pressures and impulses and fragment masses and velocities.
- Results of the hydrocode modeling of four munitions were compared to arena test data.
- The effects of varying equations of state for chemical agents was evaluated by developing and EOS for each of two chemical agents, and comparing their results.
- A set of "lessons learned" and recommendations for hydrocode modeling of chemical munitions was prepared.

This paper covers all but the last two items. These items, plus more detail on exact modeling techniques, are discussed our the companion paper, “Numerical Simulation of Chemical Weapon Detonations” in these proceedings.

Selection of a Hydrocode for Chemical Munitions Modeling

An important part of this effort was to identify existing hydrocode programs and, based on a comparative evaluation, select a single code for use. The hydrocodes identified are listed below. Information about the codes was obtained via available literature and through contacts with experts in this field. Comments are based on the experience of the authors or on discussion of each code with code developers. Definitions: FD = finite difference, FE = finite element, PD = public domain, C = commercially available, 2D = two-dimensional, 3D = three-dimensional.

ARTOO/TOODY, 2D Lagrangian FD code, developed by Hermann et al., Sandia National Laboratories (PD). This code is not currently being maintained or improved. It used mostly for benchmark tests at Sandia, and is generally considered to be a “developer’s” code.

AUTODYN, a 2D and 3D, combined Eulerian/Lagrangian FD code developed by Birnbaum and Cowler, Century Dynamics (C). Capable of fluid/structure interaction for "conventional" problems; however, it cannot handle the creation of many new interfaces during weapon breakup. Can utilize a number of different numerical techniques to optimize the analysis.

CALE, an Arbitrary Lagrangian Eulerian (ALE) code developed by Lawrence Livermore National Laboratory (LLNL); PD. Still in the developmental/debugging stage. Does not have a fracture model and is, therefore, not able to predict fragmentation phenomena

CTH, an Eulerian Finite Difference (FD) hydrocode from Sandia (PD). Has been used at approximately 500 sites throughout the U.S. Uses a second order advection scheme and a highly sophisticated interface tracker. CTH also has a fragment mover for examining the motion of debris that are smaller than a computational cell.

DEFEL, a 2D Lagrangian FE code, developed by Flis, Miller, and Clark at Dyna East Corporation (C). Have sold a few copies of the code but don't really support users or continued development. Similar to EPIC-2.

DYNA, a 3D Lagrangian FE code, developed at LLNL by J. Hallquist (PD). A robust and mature code with large base of users. However, large deformations of fluids and gases are not easily modeled.

DYSMAS, a 3D coupled Eulerian/Lagrangian, FD/FE code, developed by IndustrieanlagenBetriebsgesellschaft, Germany (C).

DYTRAN, a 3D Lagrangian FE code based on DYNA3D, developed by Hallquist, marketed by McNeal-Schwindler Corporation (C). Essentially the same as DYNA3D.

EPIC, a Lagrangian FE hydrocode, developed by G. Johnson at Alliant TechSystems, (PD). Similar in capabilities to DYNA and PRONTO, but primarily developed for warhead interactions.

HELP/METRIC, 2D and 3D Eulerian FD code, developed by Walsh et al., S-Cubed, (C). Code is not readily available; S-Cubed is now using other people's codes.

HEMP, 2D FD Lagrangian code, developed by M. Wilkins at LLNL. The "grandfather" of multidimensional Lagrangian codes; has been successfully applied to warhead modeling but is no longer supported.

HULL, 3D coupled Eulerian/Lagrangian FD code, developed by Matuska et al., Orlando Technologies, Inc., (C). Advanced code with Eulerian, Lagrangian and ALE; however, not capable of modeling numerous new fracture surfaces during weapon breakup.

K3, 3D Eulerian FD code, developed by May et al., Kaman Sciences (C). Stopped using it 5 to 10 years ago; essentially a 3D version of CSQIII.

PEPSI, Lagrangian FE code, developed by Hunkler and Paulus, Deutsch-Franzosisches Forschunginstitut, France, (C).

PISCES, 3D coupled Eulerian/Lagrangian FD/FE code, developed by Physics International Company (C). Code was sold to McNeal-Schwindler Corporation, who no longer markets it in the U.S.; it is available in Europe.

PRONTO, a Lagrangian FE code, developed by Flanagan and Taylor at Sandia (PD). A robust and mature code with large experience base, but not suitable for gas and fluid modeling.

SOIL, 3D Eulerian FD code, developed by W. Johnson, Computer Code Consultants, Inc. (C). The predecessor to many of today's Eulerian FD codes; no longer in active use or development.

STEALTH, 3D Lagrangian FD code, developed by Hofmann, Science Applications International Corporation (C). Written for the Electric Power Research Institute, who have since archived it.

As mentioned previously, a Lagrangian code is not capable of modeling the large motions of the agent, HE byproducts, and air, during the detonation process. This eliminated a number of the hydrocodes, including ARTOO/TOODY, DEFEL, DYNA, DYTRAN, EPIC, PEPSI, PRONTO, and STEALTH. Other codes were removed for various reasons: CALE, still in development; DYSMAS, violates requirement to "buy American"; HELP/METRIC not available to outside users; K3, no longer used or supported; PISCES, no longer available; SOIL, no longer used or supported. The three remaining candidates were AUTODYN, HULL, and CTH. All three codes have excellent capabilities and showed promise in modeling chemical weapons, although each has its own, unique advantages and disadvantages. Based partially on capabilities, and partially on program availability, CTH was selected for use in this effort.

CTH is an Eulerian finite difference code developed at Sandia, and currently used at approximately 500 sites throughout the U.S. CTH uses a second order advection scheme and a highly sophisticated interface tracker. CTH also has a fragment mover for examining the motion of debris that are smaller than a computational cell. EOS models include Mie-Gruneisen, ideal gas, JWL, and modified JWL, as well as two particularly attractive options: tabulated EOSs for a large number of materials and an analytical EOS model, ANEOS. While both the EOS tables and ANEOS are computationally more expensive than simple analytic EOS models, their sophistication improves the accuracy of calculations and their range of applicability is much larger than the analytic models. Strength models include 5 plasticity models: von Mises with softening and density degradation, pressure dependent plasticity, Johnson-Cook, Zerilli-Armstrong, and the Steinberg-Guinan-Lund. Failure theories include Johnson-Cook fracture and pressure or stress dependent brittle fracture. The only apparent potential shortcoming to CTH is its inability to model the metal casing with a Lagrangian mesh. However, the second order interface tracker is very accurate was expected to predict the motion of the casing quite well.

Hydrocode Modeling

A total of nine different chemical weapons were modeled in this effort. These munitions were selected based on a number of factors. Chemical (and indeed, conventional) munitions can be generically divided into thin-walled and thick-walled munitions. It was desired to span both types. Chemical munitions have been available since World War I, and we wanted to examine typical weapons from all eras. Several of the weapons were selected because they are the principal weapons in the US chemical weapons stockpile, which is currently being demilitarized. Others were chosen because of the likelihood of discovering these weapons on formerly-used defense sites, especially World War I era sites. Also, several were included because arena test data, giving both overpressure and fragmentation data, are available for comparison with hydrocode analytical results. Those marked with an asterisk (*) are munitions for which unclassified arena test data are available. The weapons modeled in this effort included:

- Projectiles (or Thick-walled Munitions):
  - 75-mm Shell (World War I era)
  - 4.7-inch Shell (World War I era)*
  - 8-inch Shell (World War II era)*

- Thin-Walled Munitions:
    - 4.2-inch Mortar (World War II)
    - 4-inch Stoker Mortar (World War I)
    - 30-pound M1 Bomb (World War I)
    - 100-pound M47 Bomb (World War II)
    - M23 Land Mine (Post-World War II)*
    - M55 Rocket (Post-World War II)*

A typical hydrocode model of a chemical weapon is shown in Figure 1. This is a two-dimensional CTH model of the 75-mm artillery shell. The left side of the image is the material map, which shows the location of each material and will, at later time steps, illustrate the deformed shape of the round. The right side of the image is a map of pressures in the material. All of the CTH models for this effort were executed in two dimensions. Therefore, expanding pieces of material or fragments are actually expanding annuli, or rings. Figures 2 and 3 show the 75-mm shell at 40 and 100 microseconds, respectively, after detonation of the burster. At 100 microseconds, the outer shell immediately adjacent to the burster has ballooned out or "mushroomed", and is breaking up. Directionally, overpressure wave is expanding out from the front of the round, which is to be expected, since the weapon was modeled with no fuse or nose plug in place. Figure 4is an expanded view of the shell at 1100 microseconds (1.1 milliseconds). At this point, the overpressure wave around the munition has become more directionally uniform, and most of the agent has been driven out of the casing. Interestingly, the cylindrical portion of the shell, below the burster, has remained intact. At the end of the analysis, at 5.0 milliseconds, this part of the shell was still intact. Again, this is expected behavior, since most chemical rounds were designed to burst open to disperse the chemical agent, but not specifically to create fragments from the entire casing.

Comparison of Hydrocode Results to Test Data

The overpressure values computed using CTH showed reasonable agreement with overpressures measured in arena tests. In general, the computed peak pressures were only 15% lower than the measured pressures for the 4.7-inch round. Impulses were also in good agreement. For the M55 rocket, very good agreement was seen between the calculated and experimental peak pressures on most of the gages. For the 8-inch shell, the pressures computed by the hydrocode were one order of magnitude higher than the test data. An examination of the data leads the authors to believe that this difference is due to an error recording the test data. The reasons for this are as follows: The arena tests for the 8-inch shell, the M23 land mine and the M55 rocket were all performed as part of the same test program (Powell 1983). Pressure gages were located at identical locations for each munition. The M55 rocket contained 3 pounds of burster explosive and 10 pounds of chemical agent simulant. The 8-inch round contained 7.35 pounds of burster explosive and 14.5 pounds of agent simulant. The rocket had about half the amount of burster explosive for about the same amount of agent. Pressures from the rocket were measured at 8 to 22 psi, but pressures from the 8-inch round at the same distances were measured to be 0.94 to 2.35 psi. We believe that given the larger burster, and the similar amount of agent, that the actual pressures were significantly higher than measured.

Overall, the hydrocode appears to predict pressures well. The peak of the overpressure pulse typically appears to arrive at a gage location a little earlier than the measured pulse, and the peak appears to be somewhat lower. The pressure pulse predicted by CTH does not appear to be as sharp or as large as the measured pulse, and it appears that CTH smears the pulse over time. Impulses agree quite well.

The CTH models did a good job of matching the fragment velocities of the various tested munitions. Most of the CTH velocity values fall within one standard deviation of the experimental velocity values. The hydrocode results appear to provide sufficiently accurate results to be able to predict both velocity and trajectory of fragments.

Limitation of Fragment Size Predictions

One serious limitation of hydrocodes lies in their inability to predict the size or mass of fragments. Fragmentation is a highly nonlinear and stochastic process that occurs over a very short time period. The underlying small-scale mechanisms are not clearly understood and have not been or can not be adequately investigated in the laboratory. Therefore, adequate theoretical or empirical models to predict fragment size distributions do not exist, despite 30 or more years of intense effort by some of the best scientists in the world. Thus, the prediction of fragment sizes for dynamically loaded materials is currently beyond the state-of-the-art in material modeling and all existing hydrocodes are incapable of adequately modeling it.

Results and Conclusions

Based on the results of our efforts, hydrocode programs appear to provide reasonable calculations of the overpressures produced by chemical weapons. With appropriate modeling, plus application of reasonable safety factors, hydrocode modeling can provide a reasonable alternative to arena testing to determine the blast loads from chemical weapons. Also, hydrocodes appear to do a good job of predicting fragment velocities. However, hydrocodes still cannot predict fragment size distributions. Additional development of modeling techniques, or alternative methods of fragment size predictions, are needed.

The CTH code was used exclusively for this effort. Future work will include replicating at least some of the chemical weapon models using the other two best-candidate codes, HULL and AUTODYN. The goals of this effort will be to determine if these two codes can provide similar results, to determine the differences in modeling techniques, and to more completely validate these results, techniques, and guidelines for hydrocodes in general rather than one specific code.

Additional detailed information on these efforts, as well as a report on the effects of variations in Equations of State and a discussion of general lessons learned, can be found in our conpanion paper, “Numerical Simulation of Chemical Weapon Detonations” in these proceedings.

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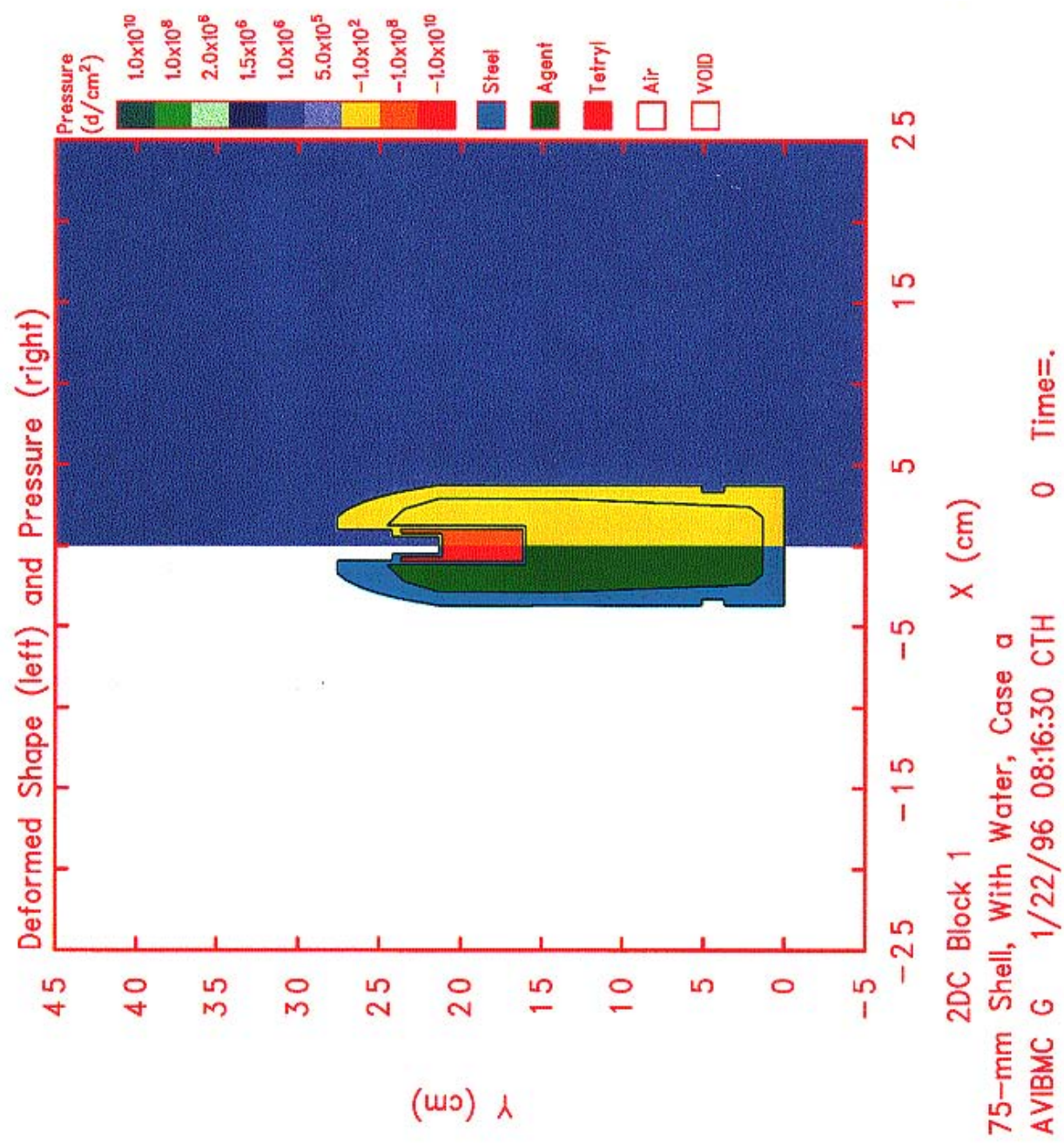

Figure 1. CTH Model of 75-mm Shell, Time = 0 microseconds

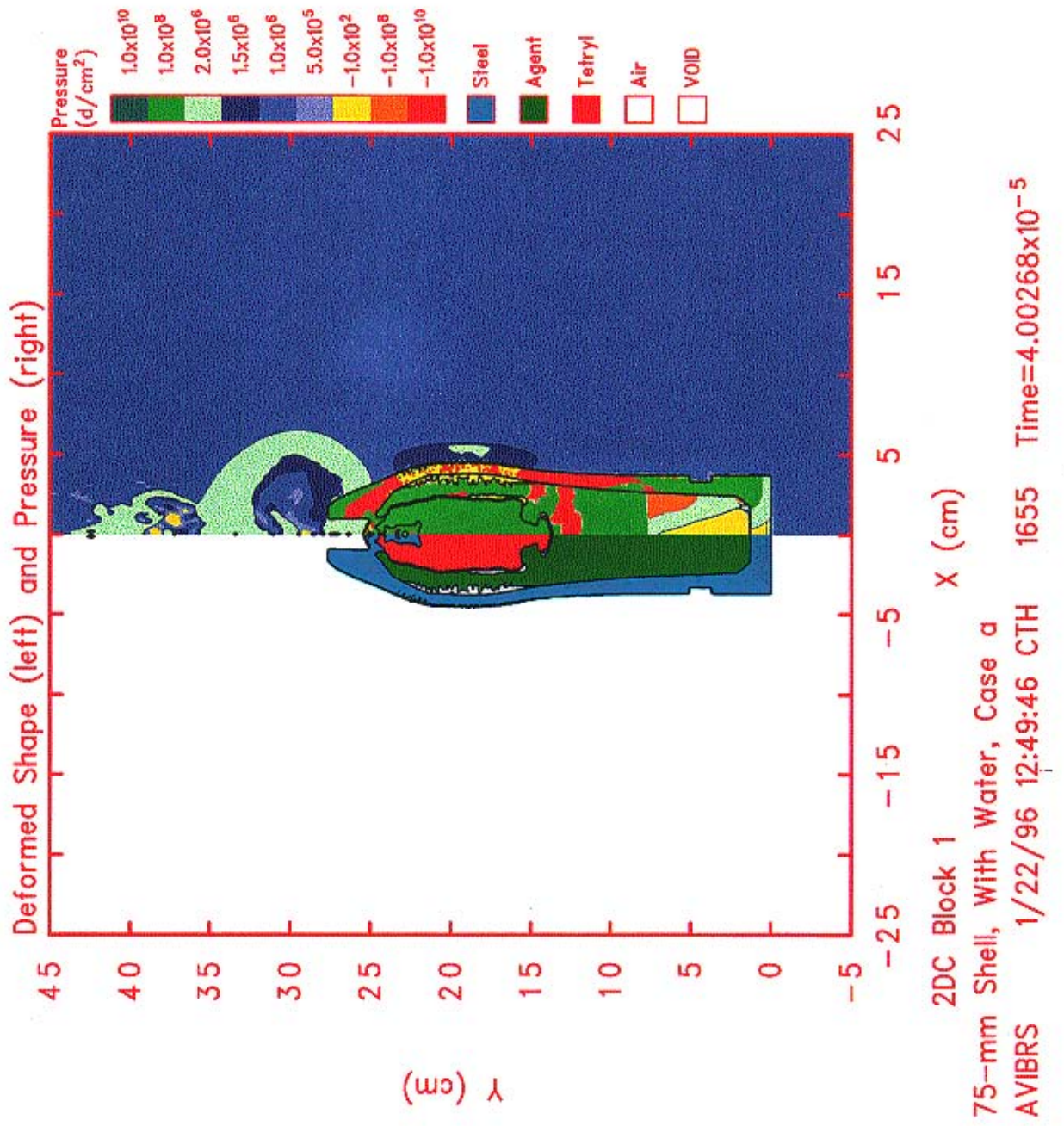

Figure 2. CTH Model of 75-mm Shell, Time = 40 microseconds

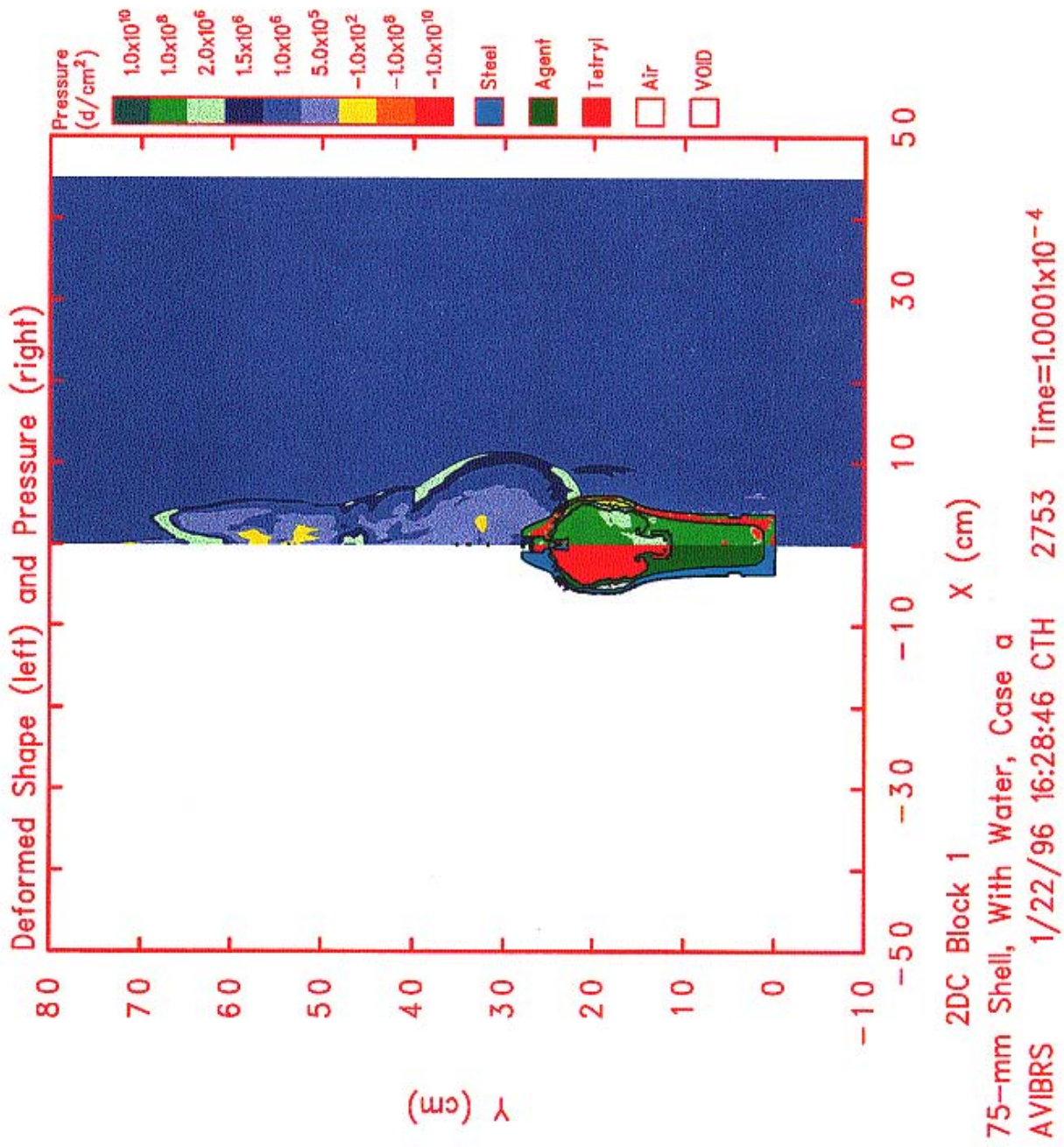

Figure 3. CTH Model of 75-mm Shell, Time = 100 microseconds

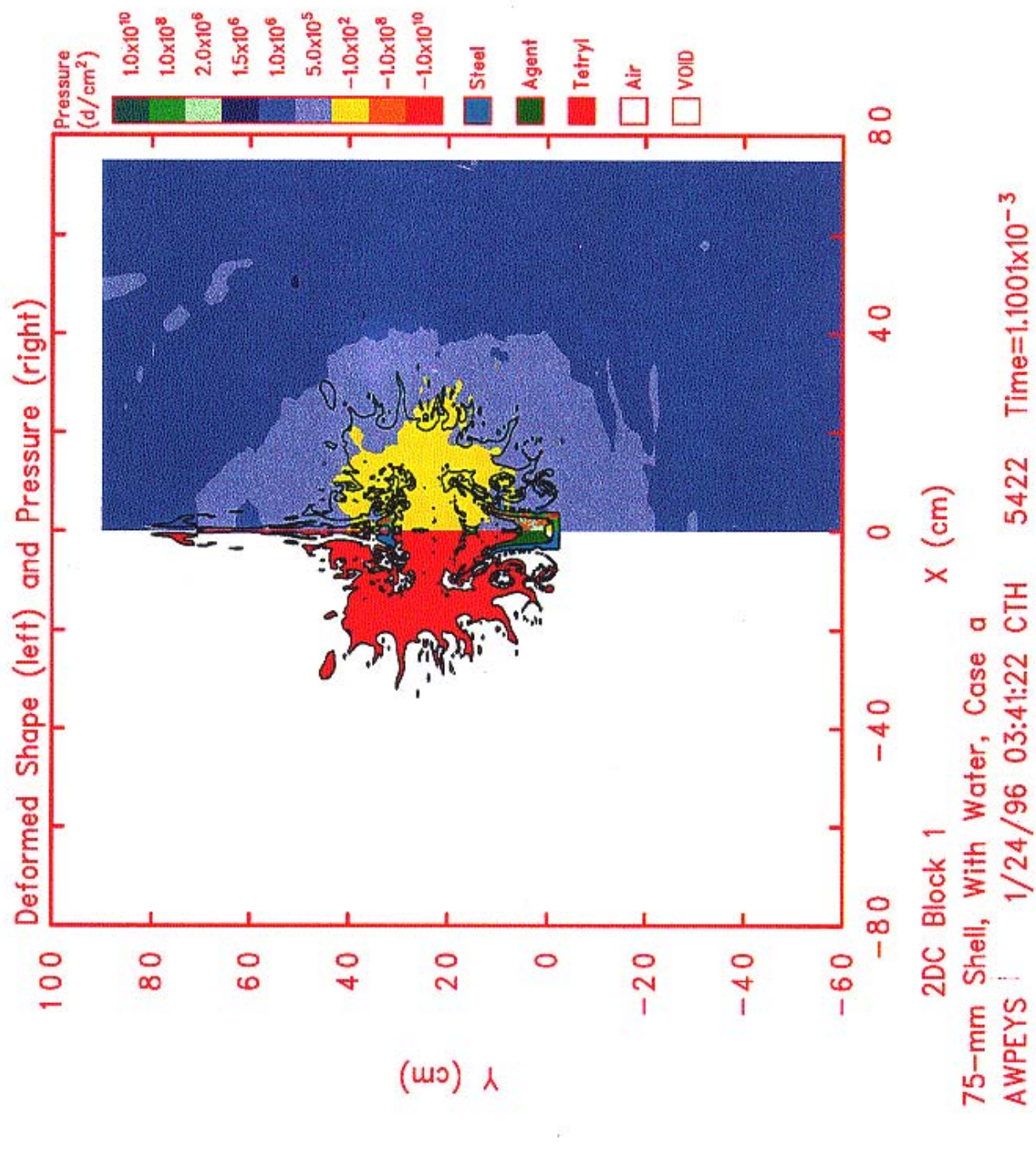

Figure 4. CTH Model of 75-mm Shell, Time = 1100 microseconds