NUMERICAL SIMULATION OF CHEMICAL WEAPON DETONATIONS

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ABSTRACT

The Huntsville Engineering and Support Center, U.S. Army Corps of Engineers, is currently involved in the location, removal, and demilitarization of stockpiled and non-stockpiled chemical munitions. To support the development of safe, efficient, and cost-effective approaches for demilitarizing these weapons, numerical simulations of the detonation of 9 chemical weapons were performed with CTH, an Eulerian hydrocode developed by Sandia National Laboratories. Arena test results were available for 4 of these weapons and comparisons to the CTH predictions showed very good agreement for both blast pressures and fragment velocities. However, as with all currently available numerical codes, fragment size distributions could not be predicted since it is beyond the state-of-the-art. The modeling of one weapon (the 4.7" artillery shell) and the results of the analysis are discussed in this paper. In addition, brief descriptions of the modeling results for the other 8 weapons are given, the development of two new Equation of State models for chemical weapons is discussed, and a brief summary of the lessons learned in performing hydrocode simulation of chemical weapon detonation is provided.

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INTRODUCTION

The Huntsville Engineering and Support Center, U.S. Army Corps of Engineers, is currently involved in the location, removal, and demilitarization of stockpiled and non-stockpiled chemical munitions. To develop safe, efficient, and cost-effective approaches for demilitarizing these weapons, the behavior of the munition after deliberate or accidental detonation must be known. Typically, this information has been generated through expensive and time-intensive arena tests, using rounds filled with chemical agent simulants. However, the state-of-the-art in computer modeling has reached a level where numerical simulations can be performed quickly and with a high degree of confidence and accuracy.

To determine the blast pressures and fragment loadings generated by chemical weapons, Southwest Research Institute (SwRI) personnel performed hydrocode simulations of the detonation of a number of these weapons, using CTH, an advanced, Eulerian finite difference code, which was selected after a critical review of existing codes. A total of nine chemical weapons, from different eras and with varied physical properties, were modeled with CTH. For four of these weapons, arena test results are available and comparisons to the CTH predictions show very good agreement for both blast pressures and fragment velocities. However, as with all numerical codes, fragment size distributions could not be predicted since it is currently beyond the state-of-the-art in failure modeling to predict the stochastic nature of fragmentation.

Finally, to examine the effects of the mechanical properties of the chemical agent on the detonation phenomena, two new Equation of State (EOS) models were developed, the first for VX, a persistent nerve agent, and the second for CG, a non-persistent choking agent. The effects of the EOSs upon the predicted blast loads and fragment velocities are briefly discussed.

CTH Hydrocode

After a review of the state-of-the-art in the numerical simulation of large deformation, short-duration problems, CTH was chosen to model chemical weapon detonations. CTH is an Eulerian finite difference code developed at Sandia, and currently used at approximately 500 sites. CTH uses a second order advection scheme and a highly sophisticated interface tracker.

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 ANEOS, an analytical EOS model. While both the EOS tables and ANEOS are computationally more expensive than simple analytic EOS models (Mie-Gruneisen, JWL, ideal gas, etc), their sophistication improves the accuracy of calculations and their range of applicability is much larger than the analytic models. EOSs for air and water (including phase transformations) are available in tabular form. Strength models in CTH 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.

WEAPON MODELING

CTH has been used to model a total of 9 different munitions, consisting of two weapon "classes": Projectiles and Thin-Walled Weapons. The Projectiles which were modeled include:

- 75-mm Shell (WWI era)
- 4.7-inch Shell (WWI era)
- 8-inch Shell (WWII)

The Thin-Walled Weapons include:

- 4.2-in Mortar (WWII)
- 4-in Stokes Mortar (WWI)
- 30-lb M1 Bomb (WWI)
- 100-lb M47 Bomb (WWII)
- M23 Landmine (Post-WWII)
- M55 Rocket (Post-WWII)

Due to space limitations, only one of these weapons, the 4.7-in shell, will be discussed in detail here. A cursory report for the other 8 weapons is given later in this paper and the reader is directed to Stevens '95, '96a, and '96b for full descriptions of the modeling of the other weapons. The 4.7-in shell is chosen for this paper because pressure gage data is available and because the shell does not completely fracture, making the analysis somewhat more challenging than for the other chemical weapons.

CTH MODELING OF THE 4.7-in SHELL

The 4.7-in Enamel Lined MK V artillery shell is a World War I vintage weapon, which was configured to deliver HS, CG, NC, PS, and other chemical agents. Figure 1 presents a dimensioned drawing of the weapon and Table 1 lists some of the physical properties.

Table 1. Physical Properties of the 4.7-in Shell (from Vargas et al. '94 and USA CMDA '94)

Projectile Length, excluding fuse	16.23"
Projectile Diameter	4.7"
Projectile Total Weight, Including Agent	41.7 to 43.8 lbs
Agent Weight	4.3 to 6.4 lbs
Burster Type	TNT
Burster Weight	0.27 lbs
Burster Length	6"

As part of the development of a chemical agent confinement structure for use by the Huntsville Corps of Engineers, SwRI performed arena tests on two full-size replica models of the 4.7-in shell (Vargas et al. '94). Two types of chemical agent simulants were used: sulfur hexafluoride and ethylene glycol. In the numerical analysis discussed later, the ethylene glycol-filled shell was chosen for modeling because it behaves in a somewhat similar manner to water. Fragments were recovered in celotex bundles that provided a recovery zone of approximately 120 degrees and break screens were used to determine velocities. Of the two pressure gages, only Gage 2, located at 48 inches away and at 45 degrees to the long axis from the rear of the munition, provided meaningful data. In both tests, the nose of the munition was severely fragmented but the cylindrical section of the body stayed intact.

CTH Model

The goal of the simulation was to show that CTH can predict the phenomena measured during the detonation of a chemical weapon. For the 4.7-in shell, this data consisted of fragment velocities and sizes, and one overpressure history at Gage 2. To calculate the blast pressure at 48 inches away, the model domain must be much larger than the size of the shell. However, to accurately represent the early portion of the detonation, when the casing fragments, the mesh must be highly refined on and near the shell. This requirement for small finite difference cells near the shell, coupled with the large size of the domain, results in a small time step and a very large number of cells. To overcome this, the user can "rezone" a problem, by suspending the analysis, modifying it, and then restarting it. Thus, in the early time of the detonation, the model can be run with a very fine mesh at the weapon and a coarse mesh elsewhere. Later, in the "rezone", the mesh can be coarsened near the weapon's original position and refined elsewhere.

Figure 2 presents a closeup of the CTH model of the 4.7-in shell; Figure 3 shows the entire problem domain. The initial mesh used 200 x 480 cells; the first rezone was performed at 700 µs and the mesh was reduced to 150 x 360 cells; the second and final rezone at 1500 µs decreased the mesh size to 100 x 240. The analysis was run to 5.1 ms by which time the blast wave has passed the pressure gages.

Material Modeling

Since the quality of the numerical simulation is a strong function of the constitutive models that are used, good EOS and strength models were needed for a successful analysis. For the 4.7-in shell, four materials were modeled: Steel, Chemical Agent, C4, and Air.

Steel — The steel model consists of the Mie-Gruneisen (MG) equation of state, coupled with a plasticity model and a failure criteria to define rupture. The MG EOS employs a linear relationship between shock velocity and particle velocity and the Gruneisen parameter is inversely proportional to the density. To incorporate the effects of strain hardening, strain rate, and temperature on strength, the Johnson-Cook plasticity model was used (Johnson and Cook '83). Johnson-Cook material properties for 1006 steel were used for the shell casing, the burster, and the weld material; the constants are also given in Stevens '96b. Lastly, based on the results of the parametric study reported in Stevens '95, the principal stress criteria was used to define fracture. The constants for the MG EOS, the Johnson-Cook plasticity model, and principal stress criterion are given in Stevens '96a.

Chemical Agent — EOS models and material constants could not be found for chemical agents, which is not surprising given the obvious difficulty in testing such materials. Since the phase transition from liquid to vapor could absorb a significant amount of energy, a multiphase EOS model for water was used. Unfortunately, water is not as volatile as most chemical agents and, therefore, too much energy could be dissipated in the phase transformation. As another part of this project, the lack of EOS models for chemical agents was addressed through the development of two analytical EOSs, for CG and VX. Due to space limitations, this work is only briefly described later and the reader is directed to Stevens and Littlefield '96 for a full discussion.

One significant benefit of CTH is the availability of tabulated EOS data, referred to as the "Sesame" library. These tables are generated analytically with EOS programs or empirically with laboratory data or with a combination of these approaches. The tables cover a wide range of temperature and pressure and include the phenomena of melting, vaporization, sublimation, etc. The Sesame table for water was used as the EOS for the chemical agent.

C4— To model high explosives, the Jones-Wilkins-Lee Equation of State (JWL EOS) was used. In this model, the pressure and internal energy are a function of the volume and energy, as described in Kerley '91a and in Dobratz and Crawford '85. The material constants for C4 are found in Stevens '96a.

Air — While an ideal gas law approach would probably be satisfactory, the Sesame tabular data was used, primarily for its convenience but also for its completeness, i.e., the Sesame table can more accurately cover a much wider range of pressures and temperatures.

RESULTS AND COMPARISONS TO EXPERIMENTAL DATA

Figures 4 through 8 present the deformed shape and pressure distributions in the 4.7-in shell at selected times from the start of detonation up to 1.5 ms. Figures 4 and 5 show the "mushrooming" of the nose of the shell and rupture of the steel in the nose. It is interesting to note that the explosive has compressed and trapped the majority of the agent in the cylindrical body of the shell and very little agent has been dispersed. Figures 6 and 7 present a more distant view of the detonation at a later time; the explosive by-products have spread well outside the shell and the cylindrical body of the shell is still intact. Figure 8, at 5.1 ms, shows that the majority of the agent has finally been ejected from the body, and, also, that the cylindrical section of the shell is still intact.

Figure 9 presents the CTH-calculated velocities and the fragment velocities reported by Vargas et al. '94, as a function of angle around the periphery of the shell; 0 degrees is at the nose of the shell, 90 degrees is orthogonal to the long axis of the munition and 180 degrees is at the tail. The error bar on the experimental data represents one standard deviation above and below the mean (which is marked with the "X"); the actual scatter in fragment velocities is much larger than one standard deviation, with velocities as high as 1700 ft/s (518 m/s) and as low as 300 ft/s (91 m/s). This plot shows a good agreement between calculated and measured velocities, with most of the CTH data falling within one standard deviation of the experimental values. The data points with the lower velocities represent the larger fragments, including the cylindrical body, which stayed intact. There is one very high CTH value of approximately 800 m/s near 0 degrees (at the nose); this tracer was placed on the screw-on cap of the burster, close to the explosive.

The measured and calculated pressure and impulse histories at Gage 2 are shown in Figures 10 and 11, respectively. The calculated pressure pulse arrives a little earlier than the measured curve and its peak is smaller than measured. The delay in time of arrival could be experimental or, else, CTH overpredicted the shock velocity in air. The pressure spike in the CTH trace is not as sharp or as large as measured and it appears that CTH has "smeared" or diffused the pulse. However, considering the large variability typically seen when measuring blast histories from cased weapons, this comparison looks very good.

The impulse history in Figure 11 looks particularly good; the shape and peak values agree quite well, with the only large discrepancy being the time of arrival. The measured peak value was 8.99 kg/(m-s) (1.30 psi-ms) and the calculated value was 7.72 kg/(m-s) (1.12 psi-ms), for a difference of 14%, which, in the field of shock physics and explosives modeling, is considered quite small.

RESULTS FOR OTHER WEAPONS

Experimentally determined fragment velocity and size distribution data are available for 3 of the remaining 8 weapons: the 8-in Shell, the M23 Landmine, and the M55 Rocket (see Powell '83). Peak pressure data is only available for the 8-in Shell and the M55 Rocket. Overall, the CTH models did a very good job replicating the fragment velocities for these three weapons. For the M55 rocket, very good agreement was seen for the measured and calculated peak pressures at 4 of the 6 blast pressure gages. There was a factor of 3 difference at the remaining 2 gages, which isn't surprising given the variable nature of peak pressure readings (specific impulse is a more accurate measurement of the energy from an explosion; unfortunately, pressure histories were not reported in Powell '83). For the 8-in shell, the CTH values were consistently one tenth of the measured values, leading to speculation that the data were not properly recorded or reported; unfortunately, this could not be determined conclusively, despite attempts to do so.

EOS MODELING FOR CHEMICAL WEAPONS

Not surprisingly, models and material constants for chemical agents do not exist and, for expediency, an EOS for Water is often used to represent the agent. However, given the large amount of energy that can be absorbed during the change of state from fluid to gas, it is possible that the use of the Water EOS may not adequately represent chemical agent behavior, leading to potentially large errors in the CTH predictions. Therefore, as discussed in detail in Stevens and Littlefield '96, EOS models for chemical agent were developed, using ANEOS (ANalytical Equation Of State), which is a program created by Sandia National Laboratories to develop EOSs for materials for which only partial mechanical and chemical data are available. ANEOS is constructed from the underlying physical and thermo dynamical laws and has been successfully applied to numerous materials. ANEOS is integrated into CTH and can be directly applied; alternatively, another code, such as PANDA (Kerley '91b), can be coupled with ANEOS to produce the Sesame tabular form of EOS that is also used within CTH. The second approach is much faster computationally.

Of the more than 30 types of chemical agents that currently exist in stockpiled and non-stockpiled form, two agents, representing the extremes in physical behavior, were chosen for ANEOS modeling: 1) CG (or phosgene), a "non-persistent", highly volatile, choking agent; and 2) VX, a "persistent", non-volatile, nerve agent. Only limited data is available for these materials and ANEOS was used to fill a large portion of the tabular EOSs, as described in Stevens and Littlefield '96.

With these EOSs now available for the chemical agent modeling, two previously modeled chemical weapons were re-examined: 1) the 4.7-in Enamel Lined MK V artillery shell, and 2) the 8-in Shell, which can be configured for both VX and GB (a non-persistent, highly volatile nerve agent). The results of the "re-modeling" of the 4.7-in shell with the CG and VX EOSs was directly compared to the arena test data for the two rounds filled with the different simulants (ethylene glycol and sulfur hexafluoride. The comparisons of data from the CTH models of both weapons shows that the EOS chosen for the chemical agent can have a significant effect upon the predicted results.

LESSONS LEARNED

The information and experience developed during the CTH modeling of chemical weapon detonation was gathered and presented in Stevens '96c. It is recommended that this information be reviewed prior to developing CTH or other hydrocode models for chemical weapons. A brief summary of the lessons learned include:

- *Training*— A formal short course is highly recommended for new and experienced users, since CTH and similar codes are always evolving.

- *Meshing* — To minimize mesh effects, keep the aspect ratios under 1.5 and keep the change in cell size, from cell to cell, below 5%.

- *Meshing* — To represent a flexural response in a thin walled structural element, use at least 6 cells through the thickness.

- *Rezoning*— Use rezoning to allow the model domain to expand or to refine the mesh for later times when gross motion is more important.

- *EOS Modeling* — When possible, use existing EOSs and material constants. Ignore the temptation to "tweak" constants to improve results.

- *EOS Modeling* — If using CTH, use the Sesame tables where possible; in general, Sesame tables are more comprehensive, covering a greater regime of pressures and temperatures and they require no material constants.

- *Strength Modeling* — If possible, use Johnson-Cook, due to its large database of material constants and the numerical modeling community's general confidence in its results.

- *Failure Modeling* — For chemical weapon modeling in which significant fragmentation occurs, the failure criteria is not critical; for other situations with smaller or more controlled damage, failure modeling can be critical and parametric studies should be performed to choose the best approach and material constants.

- *Predicting Fragment Velocities* — Use a very fine mesh near and on the weapon, for the early part of the analysis. Specify a liberal number of tracers on the metallic parts. Execute the analysis until the velocity histories of the fragments/tracers reach a near constant value.

CONCLUSIONS

The CTH model of the 4.7-in shell was able to predict both fragment velocities and blast pressure history quite well; it should be emphasized that this analysis was performed using published and easily-found material models and material constants and no adjustments were made to improve correlations. The strong correlation that has been shown for the experimentally determined weapons effects data and the numerical predictions serves to validate CTH as an effective software package for modeling the detonation of chemical weapons.

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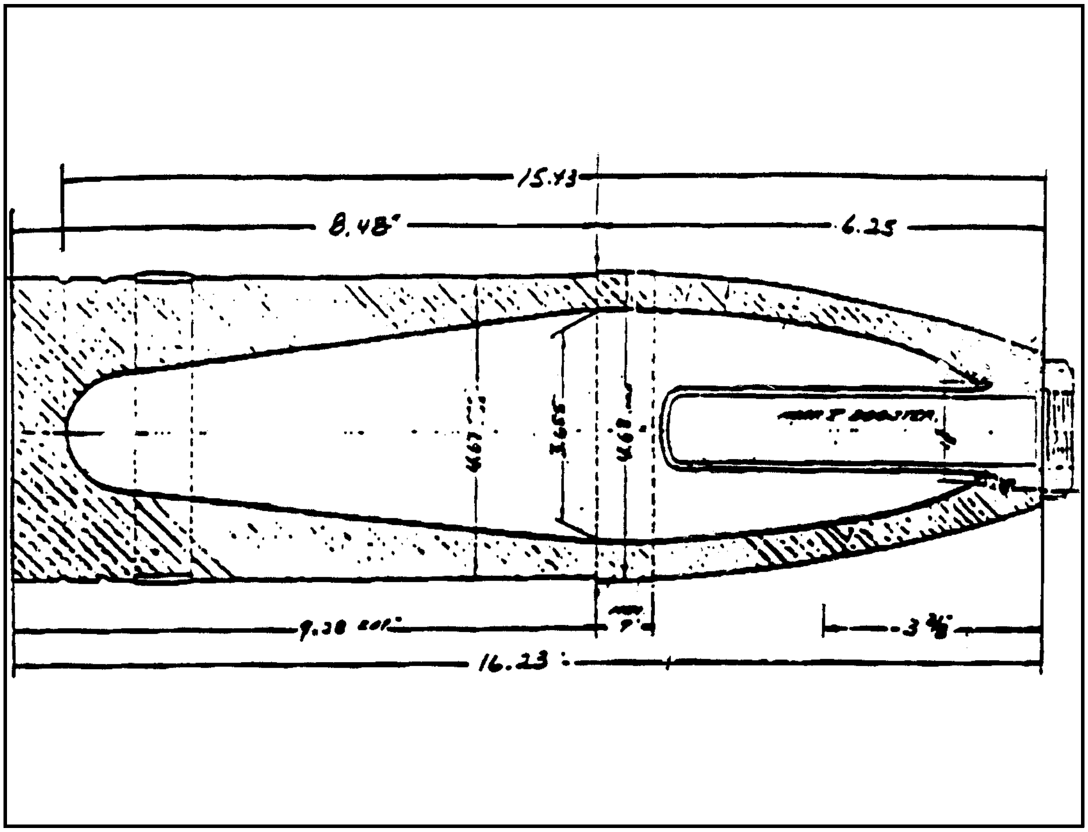

Figure 1. 4.7-in Enamel Lined MK V Munition

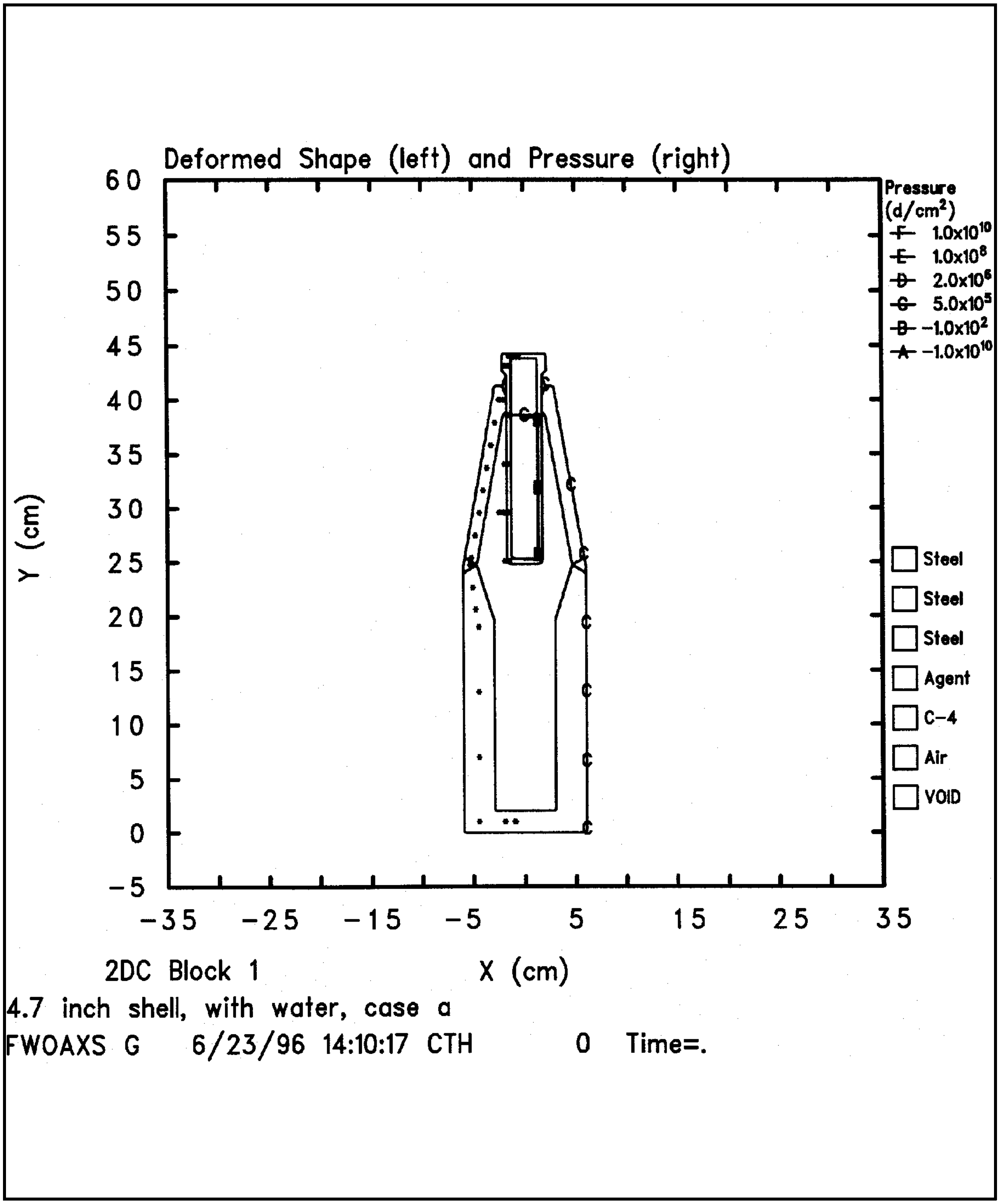

Figure 2. CTH Model of the 4.7-in Shell, Closeup

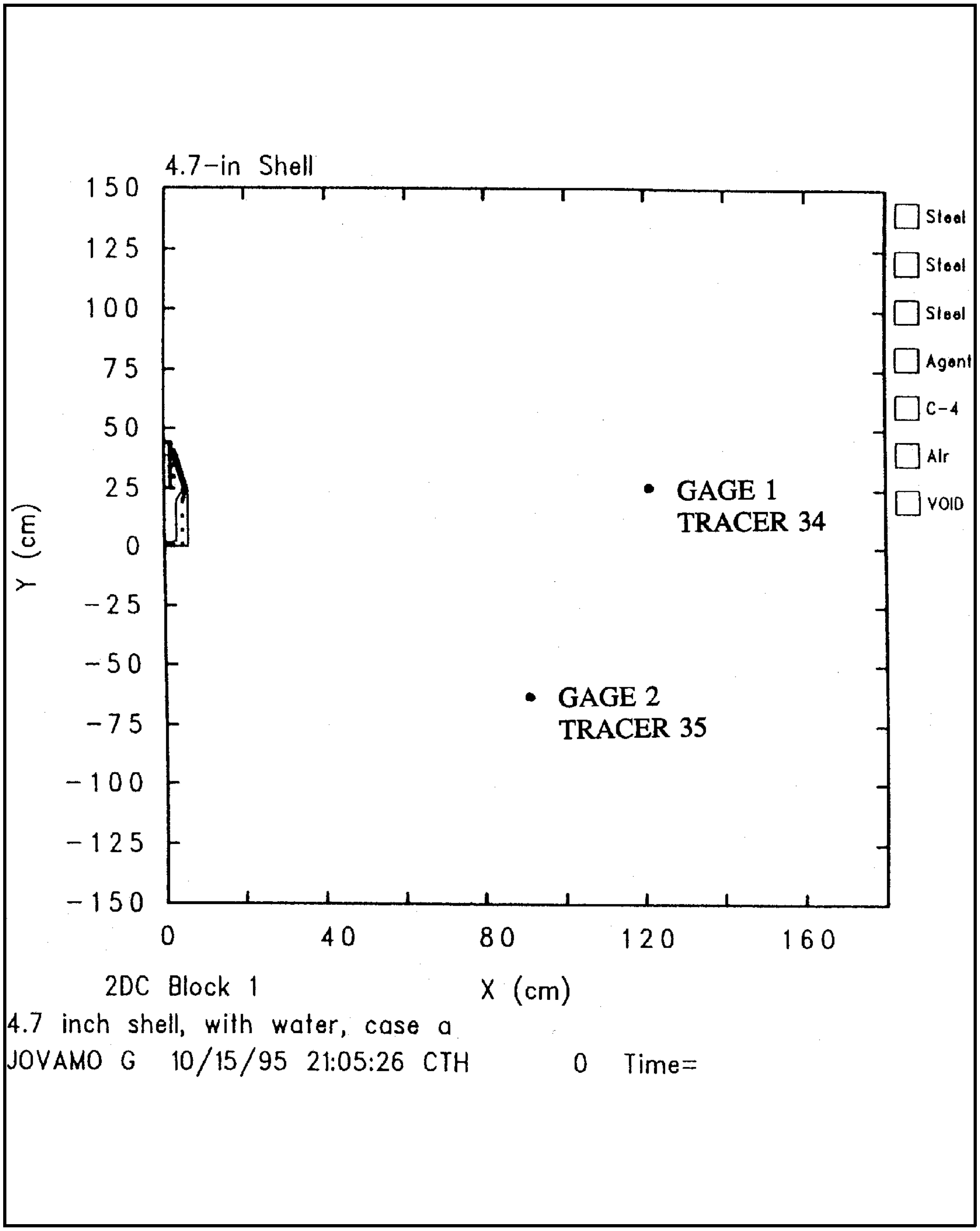

Figure 3. CTH Model of the 4.7-in Shell, Entire Domain and Location of the Pressure Gages

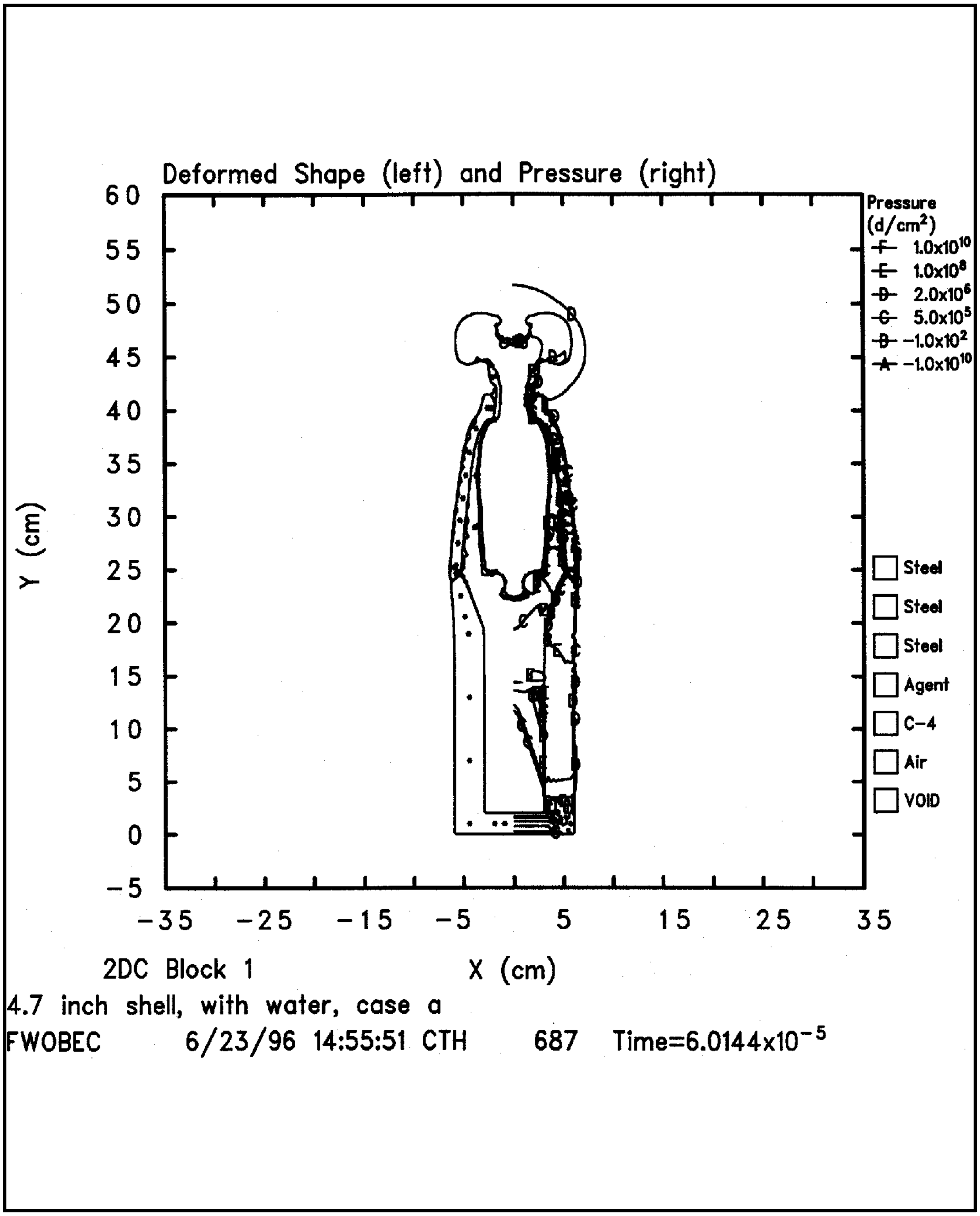

Figure 4. 4.7-in Shell, Deformed Shape and Pressure Contours, Time = 60 μs

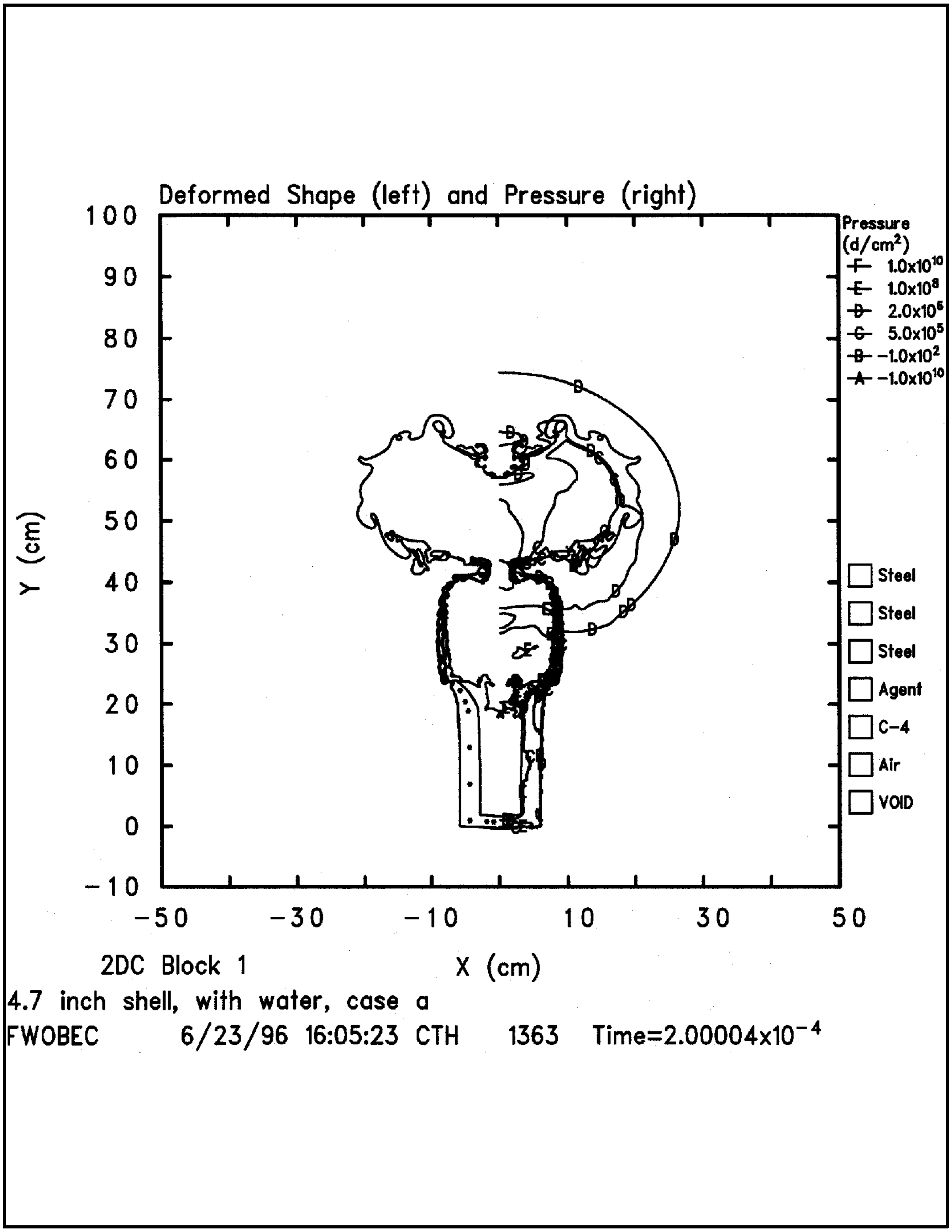

Figure 5. 4.7-in Shell, Deformed Shape and Pressure Contours, Time = 200 μs

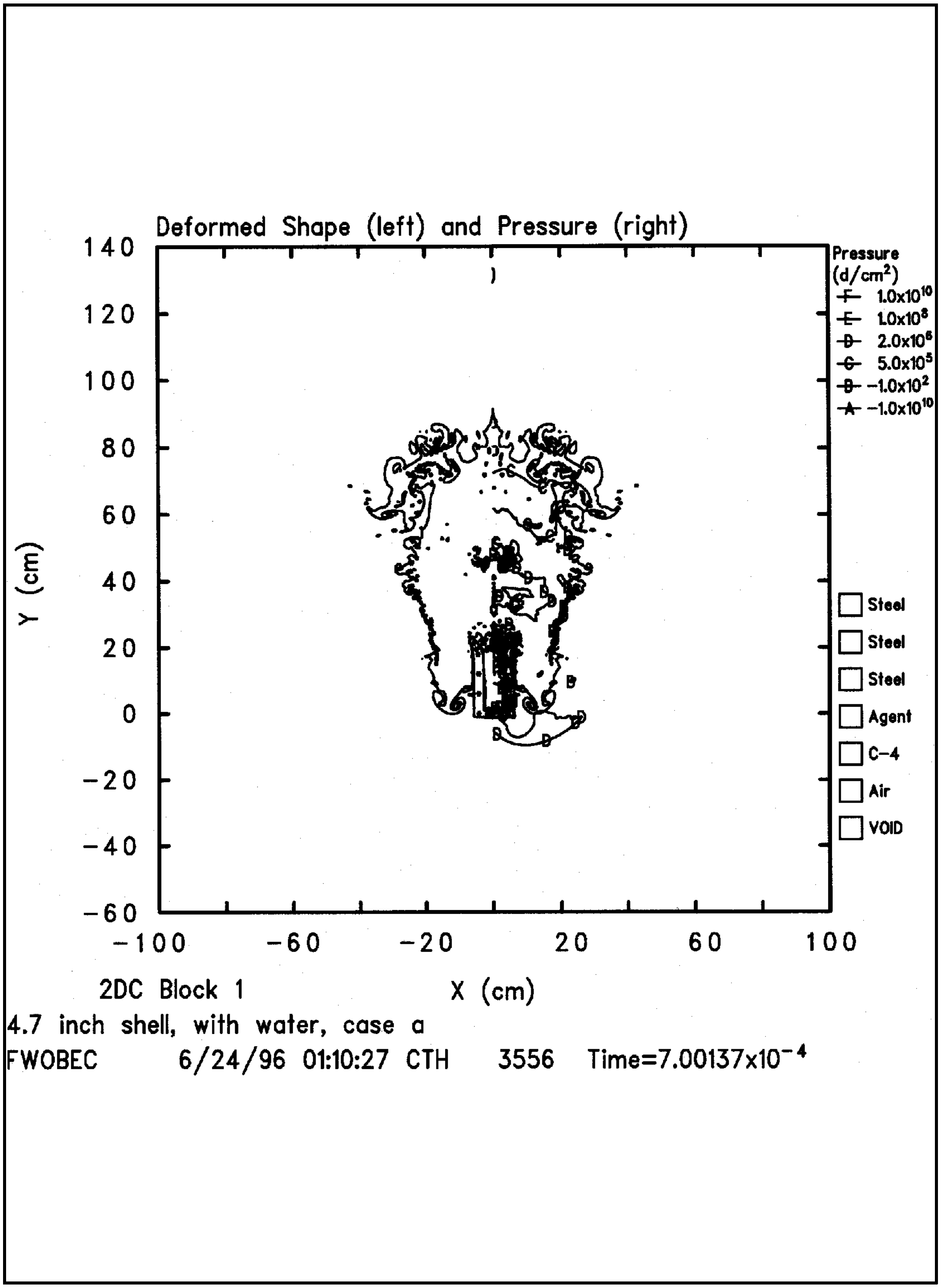

Figure 6. 4.7-in Shell, Deformed Shape and Pressure Contours, Time = 700 µs

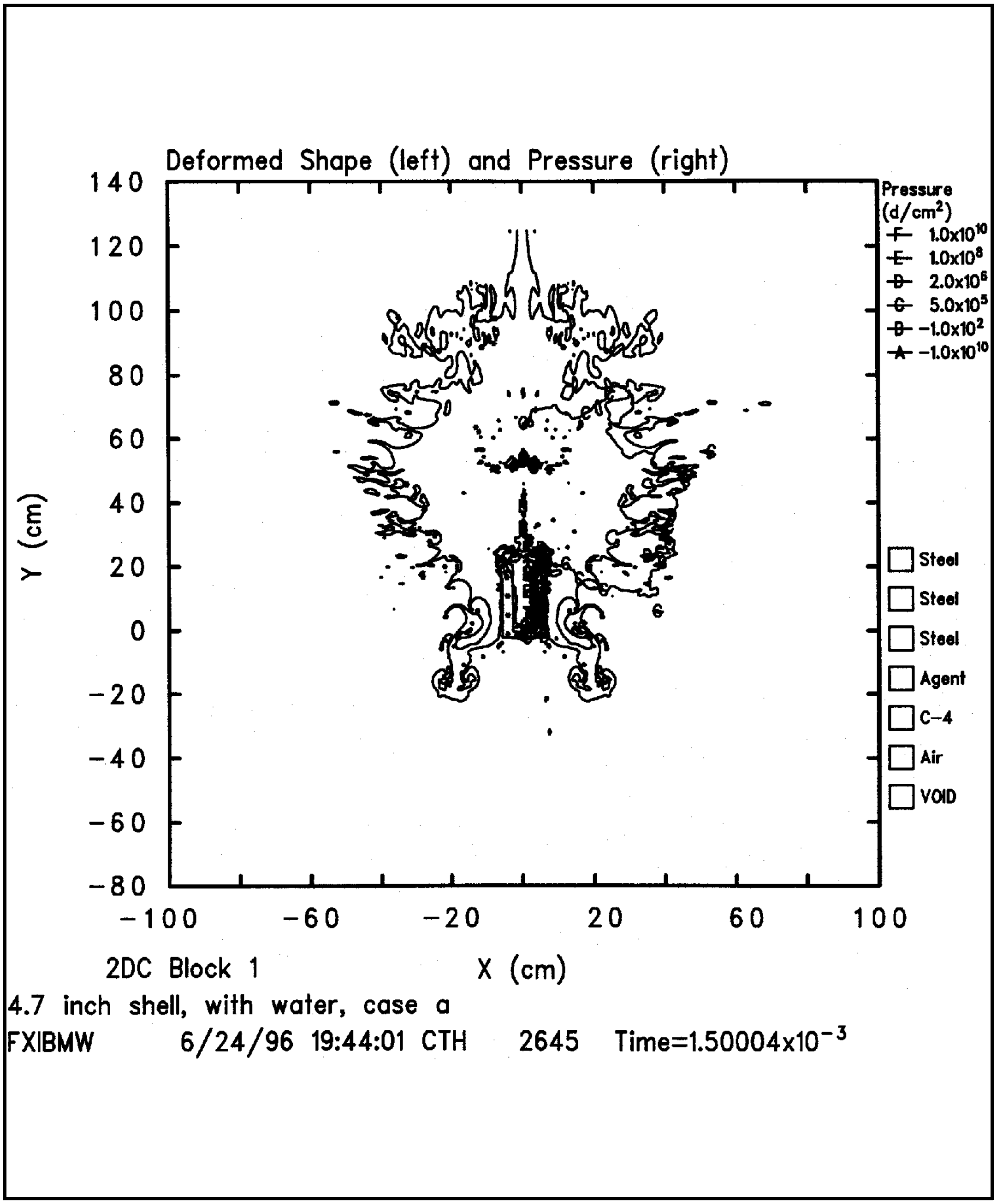

Figure 7. 4.7-in Shell, Deformed Shape and Pressure Contours, Time = 1500 μs

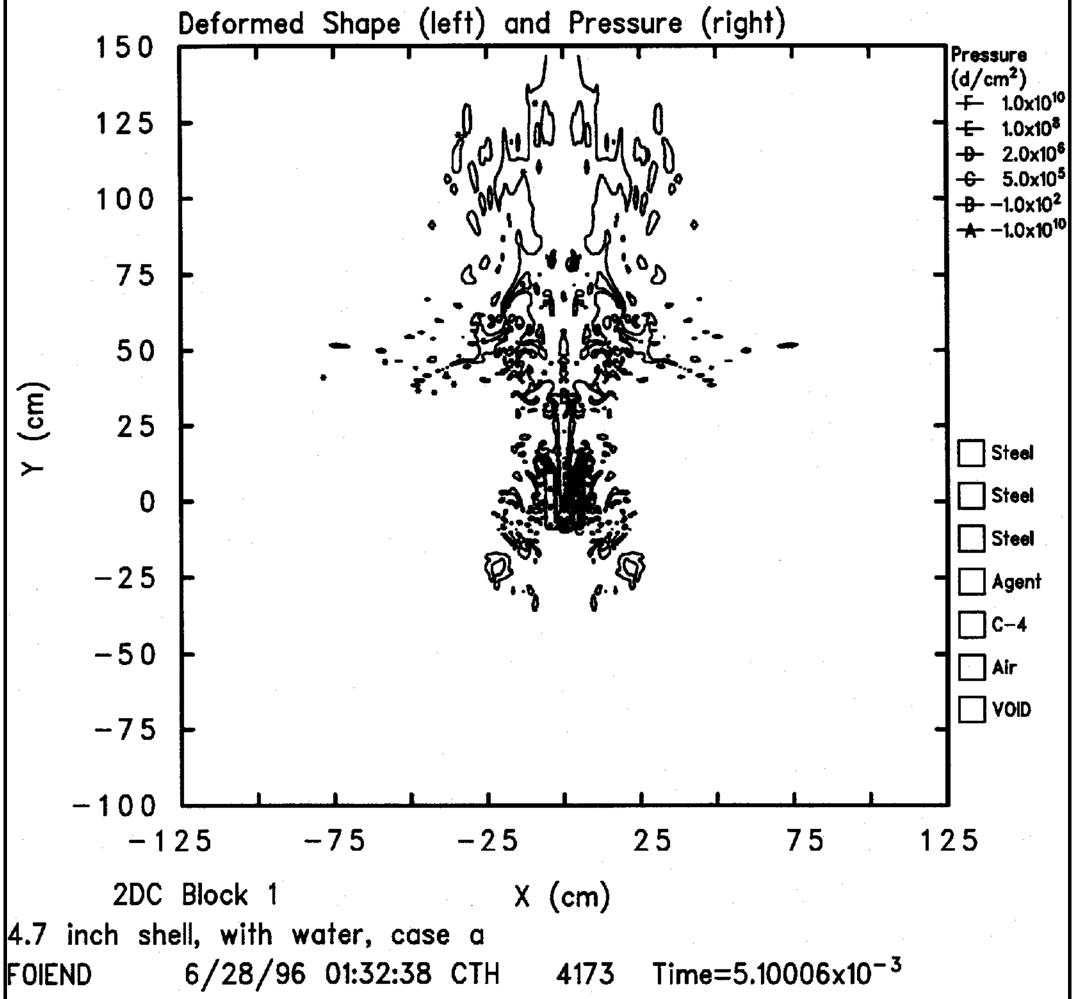

Figure 8. 4.7-in Shell, Deformed Shape and Pressure Contours, Time = 5100 μs

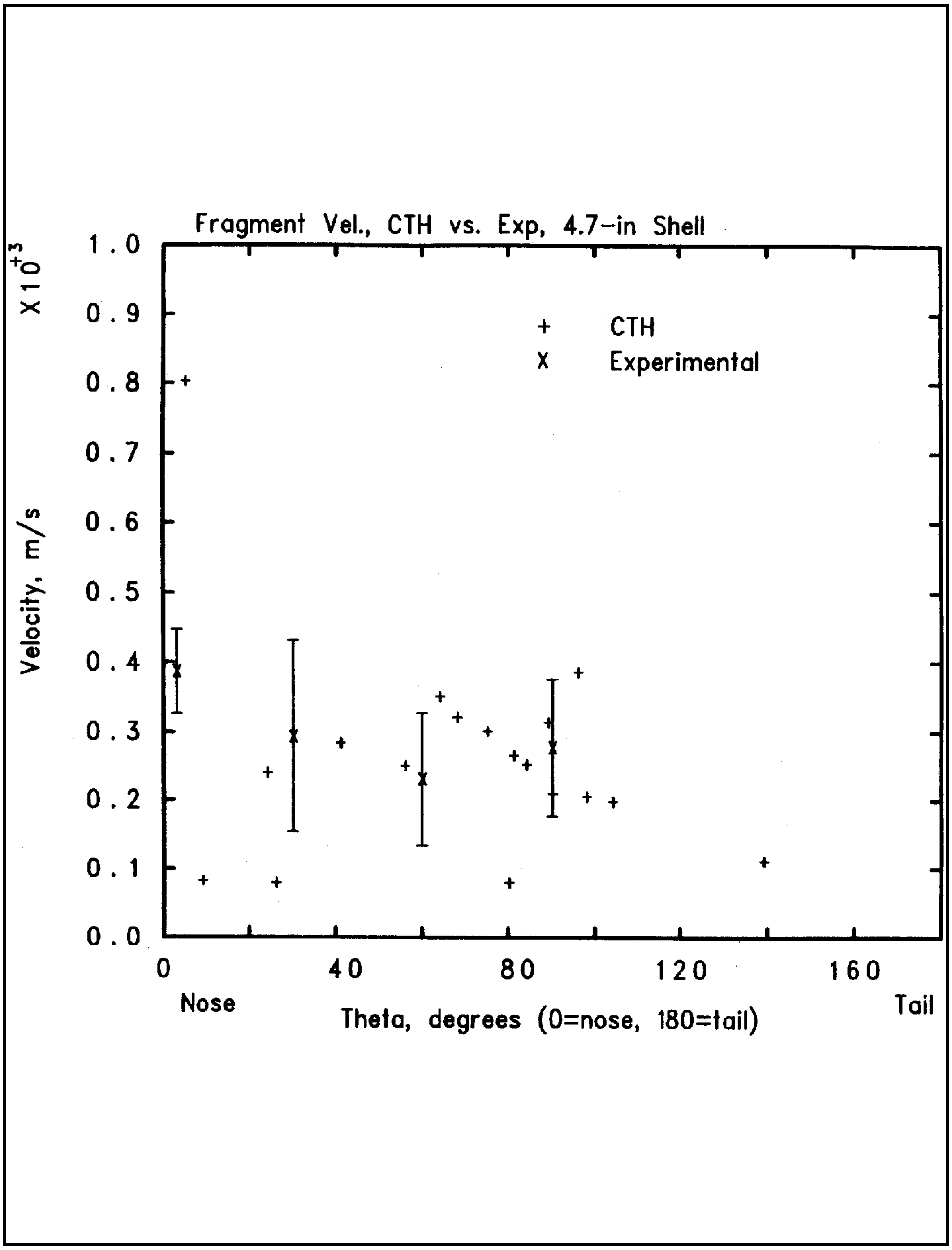

Figure 9. 4.7-in Shell, Comparison of Predicted and Measured Fragment Velocity Histories

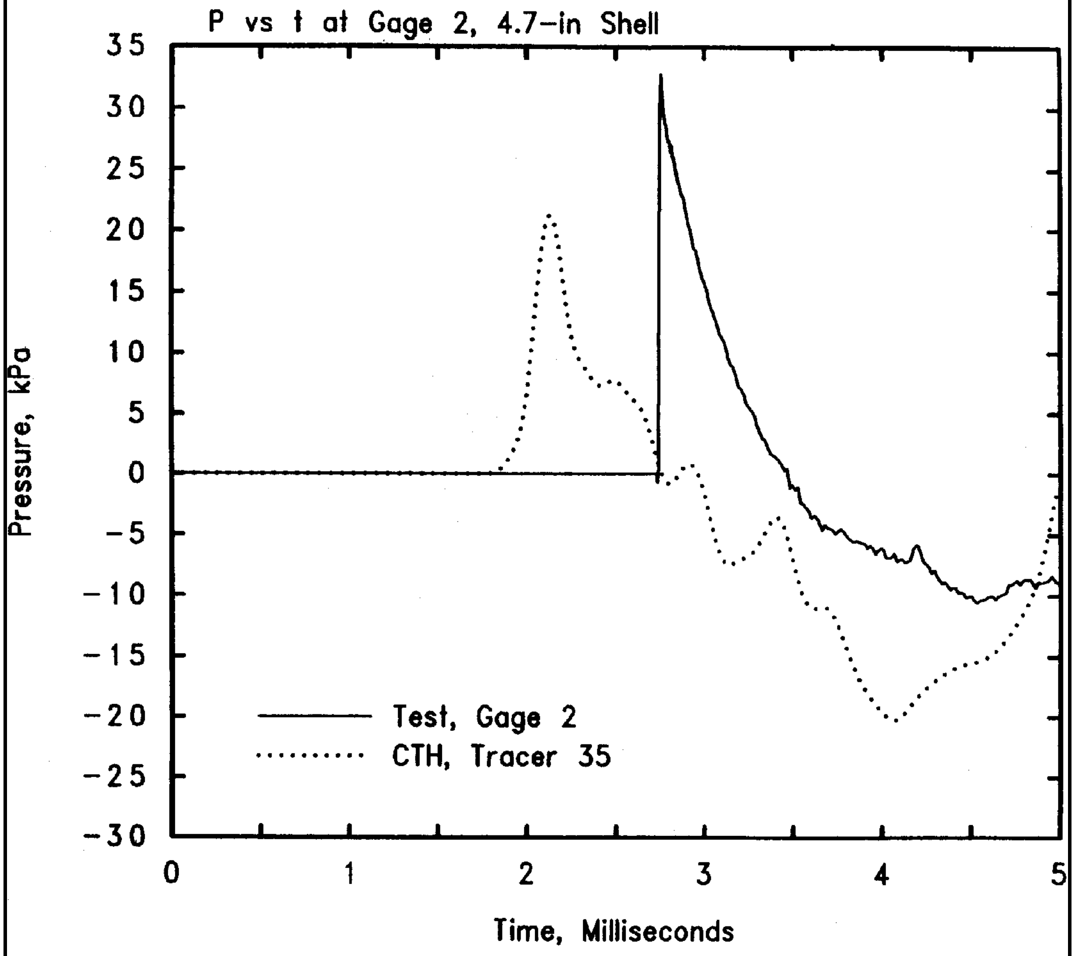

Figure 10. 4.7-in Shell, Predicted and Measured Pressure History at Gage 2

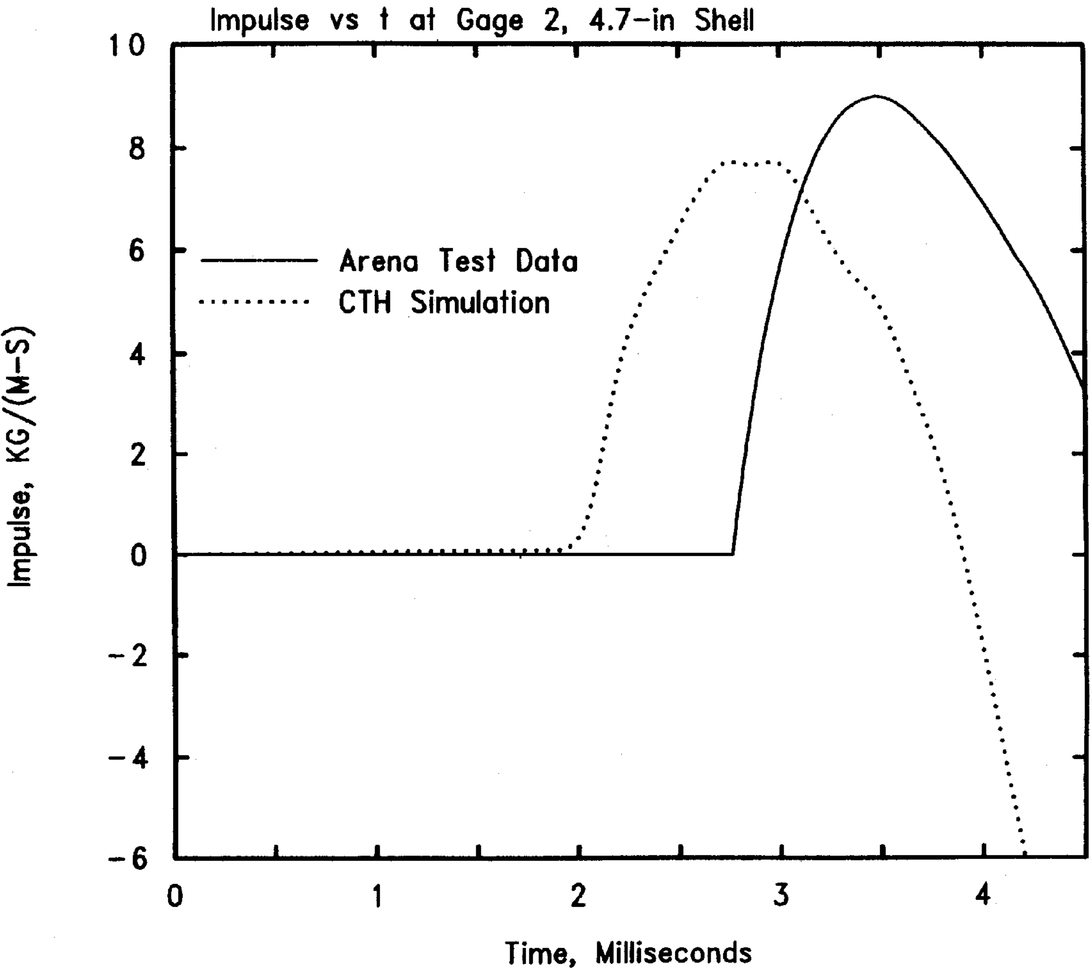

Figure 11. 4.7-in Shell, Predicted and Measured Impulse History at Gage 2