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CSQ Calculations of H_2 Detonations in the Zion and Sequoyah Nuclear Plants

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Sandia Corporation
for the
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EXECUTIVE SUMMARY

The nuclear reactor safety community has long been aware of the possibility that large amounts of free hydrogen might be generated during some accident sequences. However, the probability of large hydrogen releases was generally believed to be extremely low. The presence of hydrogen in containment buildings was thus regarded as an insignificant safety issue. Events of the fairly recent past have caused that perception to change.

Sandia National Laboratories is engaged in an extensive program, sponsored by USNRC, involving many safety-related aspects of hydrogen mixtures in reactor containment buildings [1]. The questions addressed in the program include the generation, transport, and removal of hydrogen, as well as combustion of hydrogen mixtures. This report deals with a very limited aspect of Sandia's hydrogen program: the estimation of detonation-caused loads on containment structures. The response of the containment buildings to the loads is not carefully examined here and would require further study.

In the event of a loss-of-coolant accident, a water-cooled nuclear reactor may release significant amounts of free hydrogen to its immediate environment - the containment building. If oxygen is present, detonation or combustion with a transition to detonation conceivably could take place. The integrity of the containment might then be threatened by detonation waves, detonation-induced shock waves, or missiles, depending on details of the plant design and the progress of events. Of obvious interest, therefore, is the magnitude and nature of loads caused by detonations in hydrogen:air mixtures, and the potential such detonations have for creating missiles from equipment or structural features. Also of interest is the possibility of analyzing the influence of flow obstructions on flame acceleration and deflagration-to-detonation transitions. The objective of the work described here was to obtain at least partial answers to these questions, and to provide some information on the severity of the threat posed by hydrogen detonations.

A well-established computer program, CSQ, which solves continuum mechanics problems for two-dimensional motion, was used to analyze detonations of a hydrogen:dry air mixture in a large, dry containment building (Zion) and in subcompartments of an ice condenser containment (Sequoyah). The program solves finite difference analogs for the differential equations describing the balance of mass, momentum, and energy, together with equations of state for the materials involved. CSQ incorporates accurate thermodynamics, has been used for a wide range of problems, and has compared well with experimental data.

For the calculations described here, CSQ was modified to include a model which forces detonations to occur whenever a threshold pressure is exceeded, by converting unburned to burned material at a constant rate. Both the threshold pressure and conversion rate are input values for a given problem.

The numerical smoothing inherent in CSQ, due both to finite mesh size and an artificial viscous pressure, result in peak detonation pressures somewhat below the theoretical Chapman-Jouguet values. In addition, a well-behaved calculation usually requires that a detonation wave build up to a steady wave over some distance, so that boundaries in a given problem might be encountered before peak calculated pressures are observed. For some problems, this effect of lowering predicted boundary loads may be counterbalanced by an assumption of axial symmetry, but to an unknown degree.

The Zion calculation consisted of a model for the structure, empty except for the detonable mixture, with detonation initiated at the center of the floor. In this calculation, as in most of those described in this report, the peak boundary loads were produced by wave interactions subsequent to the arrival of the detonation wave, rather than the detonation wave itself.

In two calculations for a lower subcompartment of Sequoyah, with different ignition geometries, the models again contained only the detonable mixture. As was the case in the Zion calculation, wave interactions in the detonation products produced high pressures of short duration on the problem boundaries.

For the upper compartment of Sequoyah, calculations were carried out for both axially symmetric and Cartesian (plan view) representations. We do not expect this structure would survive an isochoric adiabatic combustion of a globally distributed hydrogen:air mixture - even one which is too lean to detonate. Therefore, only detonations of localized mixtures were considered in this sequence of calculations. The detonable mixture was confined to a region in, or near, the ice condenser upper plenum, and the remainder of the compartment filled with dry air. Various detonation locations and degrees of confinement of the mixture were specified. For the axially symmetric problems, and the Cartesian problems where applicable, compression waves in the air interacted to produce the highest boundary loads. In one of the problems in Cartesian coordinates with the detonation products free to expand into the compartment, an unrealistic result was produced by the sensitivity of the detonation criterion. The results of all the other calculations described in this report appeared to be physically reasonable. No definite conclusions could be drawn as to the relative effects of the assumption of axial symmetry, and of the tendency of the numerical method to underpredict detonation pressures. A modification of a simple impulsive failure criterion was applied for the Sequoyah upper compartment calculations, and was exceeded in every case; the potential for containment damage implied by this result depends on the amount of conservatism embodied in the criterion.

It was observed in these calculations that direct detonation loading of containment structures may be less threatening than the results of compression wave interactions subsequent to, or away from, the detonation waves themselves. The detonation criterion used in the calculation could be improved with a better approximation of the reaction processes involved, but only one of the calculations would be expected to yield very different results.

It should be emphasized that the objective of this work was to evaluate the nature and strength of loads that could be produced by detonations. Whether the loads calculated could actually result in containment failure should be the subject of other studies.

I. INTRODUCTION

This report presents results from eleven calculations concerning the detonation of a dry hydrogen:air mixture in various models of nuclear reactor containment structures. One calculation treats a large, dry containment (Zion); the remaining analyses consider separate portions of an ice condenser containment (Sequoyah). The calculations were carried out with a well-tested, two-dimensional continuum mechanics code, using a simplified model that forces detonation to occur. All problem boundaries were treated as rigid - that is, no attempt was made to characterize the response of the structures to the loads imposed on them.

The Zion containment was considered to be completely filled with the detonable mixture, was modelled without internal structures or reactor system components, and was assumed to be axially symmetric. A spherical detonation wave was initiated at the center of the floor, and the calculation was carried out past the time when all peak loads on the boundary should have occurred. As a consequence of the strong interactions of reflected shock waves at the axis of symmetry, local dynamic pressures far exceeded the estimated static rupture pressure, but only for very short periods (5 - 10 ms). Because of the complicated spatial and temporal variations in the boundary loads, a dynamic structural analysis would need to be performed before an accurate assessment of the threat posed to the integrity of containment could be made.

Two of the calculations for the Sequoyah plant involved a lower subcompartment - above the reactor vessel head and below the control rod drive missile shield. Axial symmetry was again assumed. For both a detonation initiated at a central point, and in a ring high on the outer boundary of the compartment, the loads calculated do not appear to directly threaten containment. The total impulse might be enough to propel the shield upward (assuming it remains in one piece), but not rapidly enough to contact the containment dome. A more detailed analysis would be required to consider the possibility of spalling fragments off the top of the missile shield.

The remaining eight calculations dealt with the upper compartment of the Sequoyah containment, which has a thin, mostly unsupported, steel liner and a relatively low estimated failure pressure (~ 0.4 MPa). A proposed system for safe disposal of hydrogen generated during a loss-of-coolant accident (LOCA) includes deliberate combustion in the ice condenser plants. Glow-plug igniters are distributed throughout the upper and lower compartments and in the plenum above the ice condensers.

Sandia has postulated that transition to detonation might conceivably occur in the ice condenser upper plenum (ICUP) under certain accident conditions. Therefore, eight calculations were performed to estimate the potential impulsive loads that could be generated by a detonation in the ICUP.

The detonable mixture was placed in the ICUP region, and in six of the calculations, the remainder of the compartment contained dry air. Of these six, three were axially symmetric representations of the elevation view of the compartment, and three were Cartesian coordinate representations of the plan view. The remaining two calculations were also plan views, with the upper plenum completely enclosed with rigid walls.

The peak pressures in the upper compartment calculations ranged from about 1.6 to 4.0 MPa, with the largest observed in two of the axially symmetric problems. As a preliminary attempt to assess the possible consequences of these loads, the local impulse was compared with an impulsive failure criterion, which was found to be exceeded by as much as a factor of five. The failure criterion has been called "very conservative" but no quantitative estimate of the safety margin has been made. Also, the criterion does not take account of spatial variations in loads, or of resonance effects resulting from repeated loading.

As mentioned earlier, the treatment of the hydrogen:air mixture forces detonation to occur, once it is initiated. The method is actually capable of describing combustion processes in much more detail, but more experimental information is required to refine the model. With a better model for treating the behavior of reacting hydrogen:air mixtures, the computational method used here could provide a reasonably accurate representation of the influence of flow fields on deflagrations, in addition to the boundary loads already available. However, a well-defined and economical assessment of the response of containment structures to detonation-caused loads would require dynamic structural analysis with some other model.

II. ANALYTICAL MODEL

The two-dimensional continuum mechanics code CSQ[2] is a well-established, widely used computer program which solves finite difference analogs of the differential equations for the balance of mass, momentum, and energy, together with equations of state for the materials in a particular problem. The code incorporates accurate thermodynamics. CSQ has been applied to a wide range of problems, and has produced results which compare well with experimental data. The code is thus an appropriate tool for estimating detonation-caused loads on containment structures.

During each timestep, CSQ solves finite difference analogs of the partial differential equations in Lagrangian form. A spatial rezoning to the original mesh is then performed, with appropriate rules for mixing of materials and averaging of thermodynamic properties - the resulting treatment is essentially Eulerian. Calculations may be carried out in either rectangular Cartesian or cylindrical coordinates. The numerical method embodied in CSQ includes a "pseudo-viscosity" to smooth discontinuities, so that the solutions to the partial differential equations match shock wave solutions near a steady wave which separates regions of constant properties[3]. The strength of the artificial viscous pressure relative to the "real" pressure in a material is an input variable; in practice, values which produce reasonably smooth approximations to shocks somewhat reduce the peak pressure in a Chapman-Jouguet (C-J) detonation wave, although the total momentum calculated is correct. The finite mesh size necessary for the calculation also has the effect of underestimating detonation pressure. The boundaries of the containment compartments were treated as perfectly smooth and rigid, and pressure and temperature histories were saved at selected boundary points. The elimination of structural materials permits the calculations to be carried out more economically than would otherwise be the case. The pressure histories may be used as boundary conditions in structural-response calculations.

The constitutive models used to describe the hydrogen:air:steam mixtures were derived from rules for mixtures of the constituents in thermodynamic equilibrium[4]. The models were used to construct tabular equations of state for use in the CSQ calculations. In addition, a modified form of the equation-of-state test program, CKEOS2[5], was used with the tables to compute and check C-J conditions, final states for isochoric, adiabatic burns, and isentropes from the C-J state to the original density.

In order to use the equation-of-state information to calculate detonations, it was necessary to modify CSQ. For each cell in the computational mesh, the pressure is compared to a threshold value. If the threshold is exceeded, the mass fraction of unburned gas (initially 1.0) is reduced at a fixed rate, and that of the burned gas (initially 0.0) is increased by the same amount. Both the threshold pressure and the conversion rate are input numbers.

The detonation treatment outlined above is a simplification of a method originally developed for describing the response of solid high explosives[6]. In its original form, the method permits the use of a history-dependent ignition criterion, and the solution of differential equations for the reaction rates. However, the required models for the reaction kinetics and initiation criterion (or criteria) were not available for the mixtures considered in this study.

For the simple threshold-pressure, constant-rate model, a problem is initialized with a cell, or group of cells, slightly heated; the temperature is chosen so that the initial pressure in the heated region is higher than ambient by about 0.01 times the jump to the C-J pressure. As the calculation proceeds, the original small pressure discontinuity grows, eventually reaching a significant fraction of the theoretical detonation pressure. The rate of growth and the final peak values attained can be controlled by altering the pressure threshold and reaction rate. In this study, the values of those parameters were chosen to assure smooth growth rates and pressure profiles, and avoid unreasonable numerical oscillations at the detonation front.

Figure II-1 displays pressure profiles as a fraction of C-J pressure, for a one-dimensional problem with a zone size typical of those used in the containment calculations. As shown in the figure, a propagation distance of more than 20 m may be required before the calculated peak pressure becomes reasonably constant near the C-J value, even under confined conditions.

In addition to the calculation of a peak detonation pressure somewhat lower than the C-J value, other factors have the effect of reducing the predicted boundary loads in the calculations. In a "good" CSQ calculation, several timesteps are required for a given cell to attain a peak pressure value. With the relief wave immediately behind the detonation front, a reflection at a rigid boundary results in a pressure only about 0.8 of the theoretical value. The propagation of the reflected wave into partially unburned gas also reduces the predicted boundary loads.

In all the calculations described in this report, the detonable mixture was hydrogen and dry air, with a hydrogen mole fraction of 0.2. The initial density of the mixture was about 1.25 $kg \cdot m^{-3}$; in some cases, the initial temperature of the mixture was 375 K, and in others it was 275 K. Table II-1 contains the values of various thermodynamic quantities for: the initial conditions; a C-J detonation; an isochoric, adiabatic burn; and the isentrope from the C-J state to the original density.

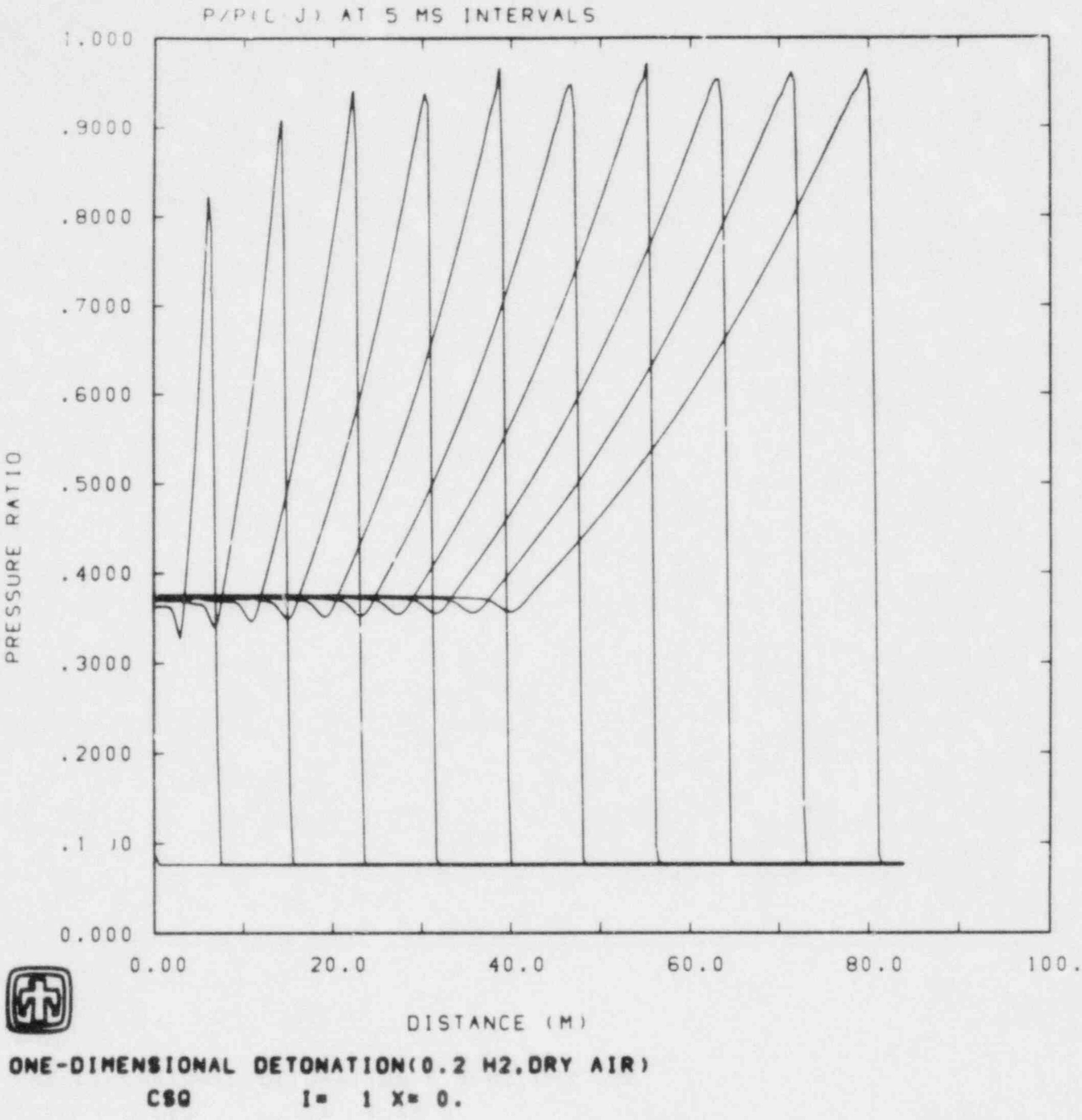

Figure II-1 Ratio of pressure to Chapman-Jouguet Pressure at 5 ms intervals

TABLE II-1

THERMODYNAMIC STATES FOR H_2: DRY AIR AT TWO INITIAL TEMPERATURES

H_2 MOLE FRACTION = 0.2; INITIAL DENSITY = 1.25 kg/m^3

INITIAL CONDITIONS		ISOCHORIC BURN		C-J DETONATIONS			ISENTROPE FROM C-J STATE TO INITIAL DENSITY	
T (K)	P (MPa)	T	P	T	P	ρ (kg/m^3)	T	P
275	0.12	2062	0.82	2282	1.58	2.18	1995	0.79
375	0.17	2253	0.90	2477	1.72	2.18	2253	0.90

III. ZION CALCULATION

In the Zion analysis, the entire containment building was assumed to be filled with the homogeneous H_2:air mixture at 375 K. (The mass of H_2 implied by a mole fraction of 0.2, given the building volume, represents a larger amount than is available from complete fuel-cladding oxidation, so the results were intended to be "conservative" in that sense.) The zones in the calculation were 0.4 m square, giving reasonably accurate spatial resolution for the 21.2 m building radius. No attempt was made to model any internal structures or components of the reactor system. This calculation was a modification of earlier ones performed for the Zion/Indian Point Study[7].

Detonation proceeds from a single cell at the center of the floor, producing a spherical wave which reflects at the wall, and the arrival of the reflected wave at the axis of symmetry results in a region of high pressure near the detonation point. (See Figures III-1 through III-4*). As may be seen in Figures III-5 through III-7, the strength of the detonation wave increases as its intersection with the wall moves upward. After the detonation wave reflects from the roof, subsequent interactions produce a region of very high pressure below the center of the roof (Figure III-8). The expansion from this region, in turn, reflects at the roof, producing the very high short-duration second pressure spike in Figure III-9.

The peak pressures observed in the Zion calculation exceed, sometimes greatly, reasonable estimates of static rupture pressure. However, the highest peaks are of very short duration (5 - 10 ms), and smaller peaks are still in the regime of dynamic, rather than static response. The results therefore give no firm answer to the question of containment integrity under the conditions postulated, but suggest the need for structural response calculations, including spatially- and temporally-varying boundary conditions.

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*In figures such as those referred to, the plotted density of dots increases with local mass density or pressure.

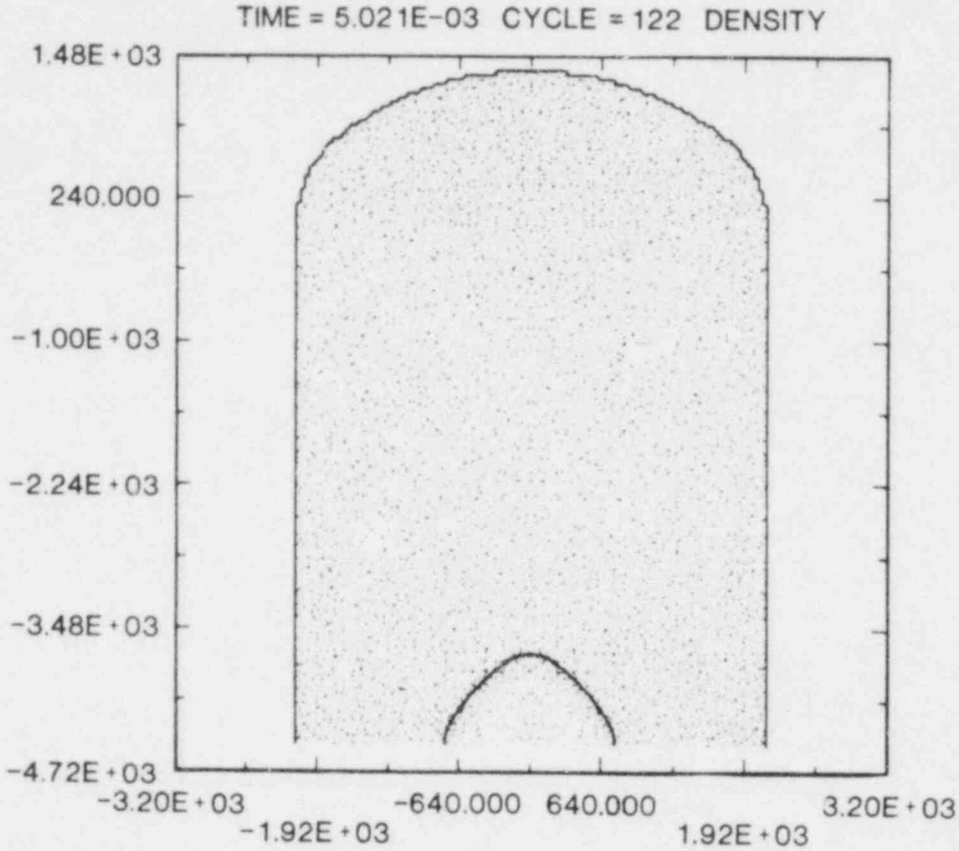


Figure III-1 Detonation wave at 5 ms in Zion Calculation

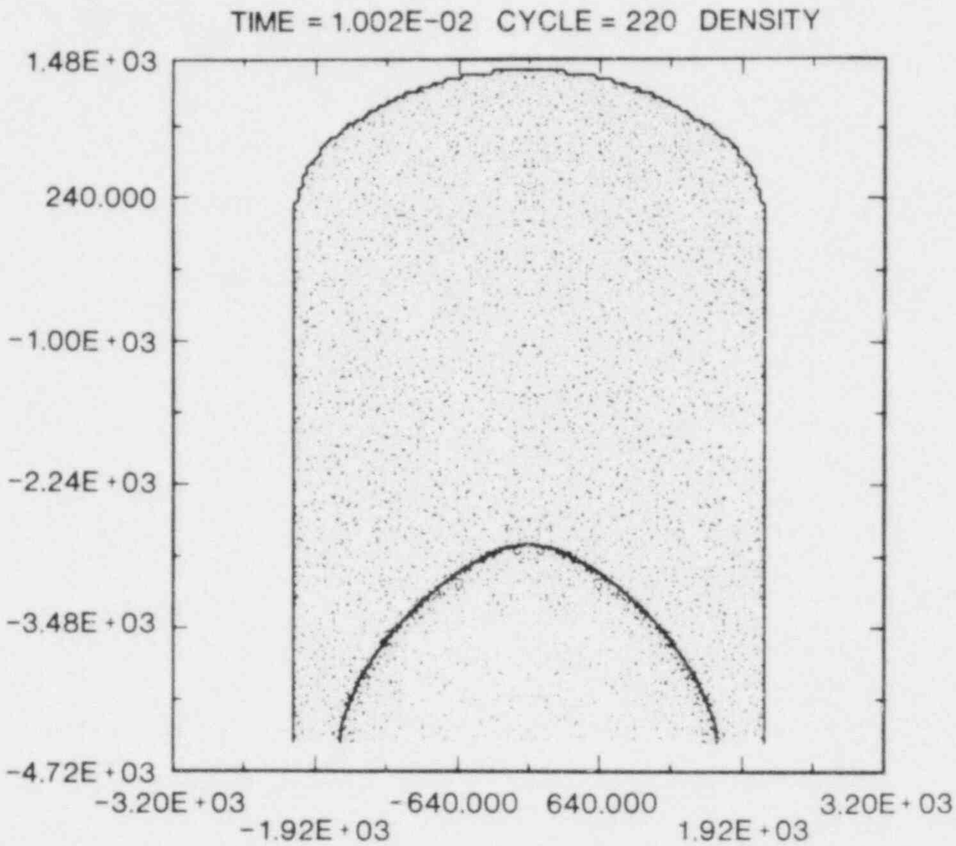


Figure III-2 Detonation wave at 10 ms in Zion Calculation

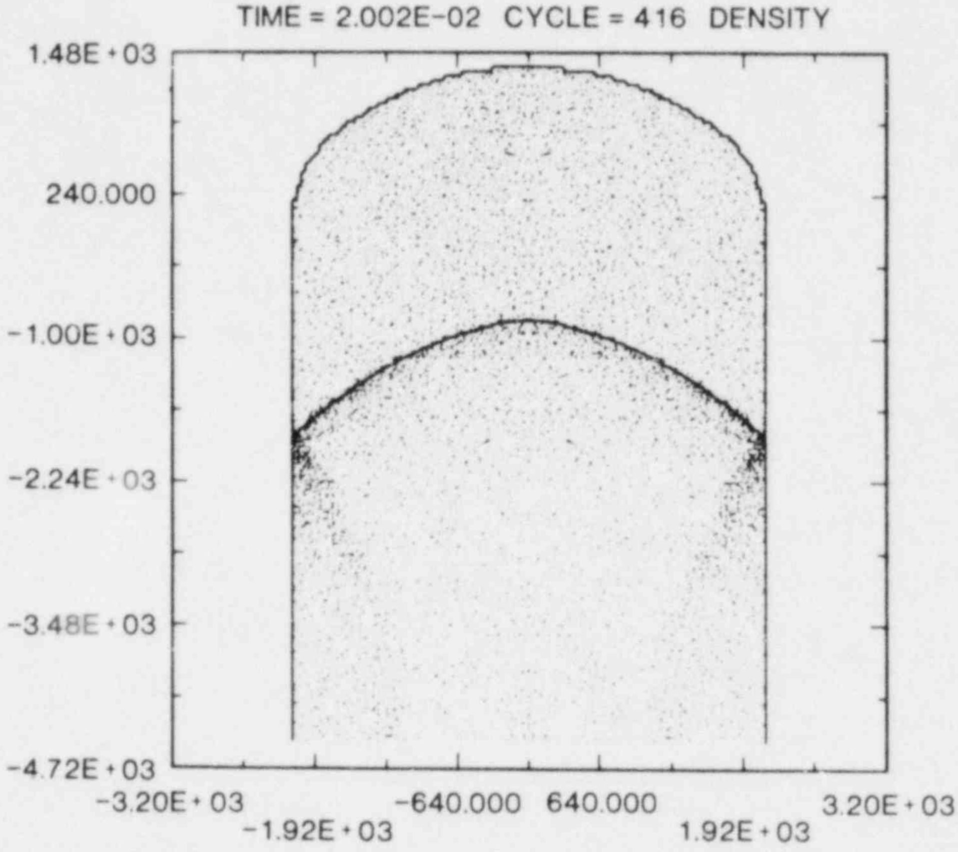


Figure III-3 Detonation wave and reflected shock at 20 ms in Zion Calculation

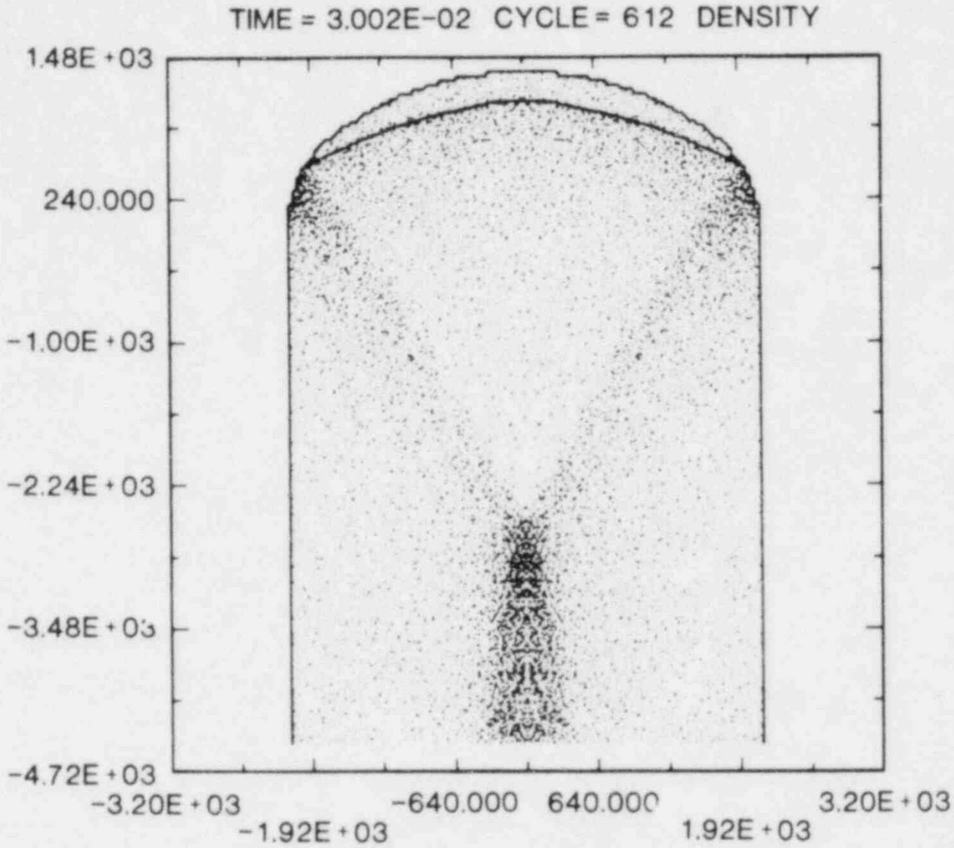


Figure III-4 Detonation wave and reflected shocks at 30 ms in Zion Calculation

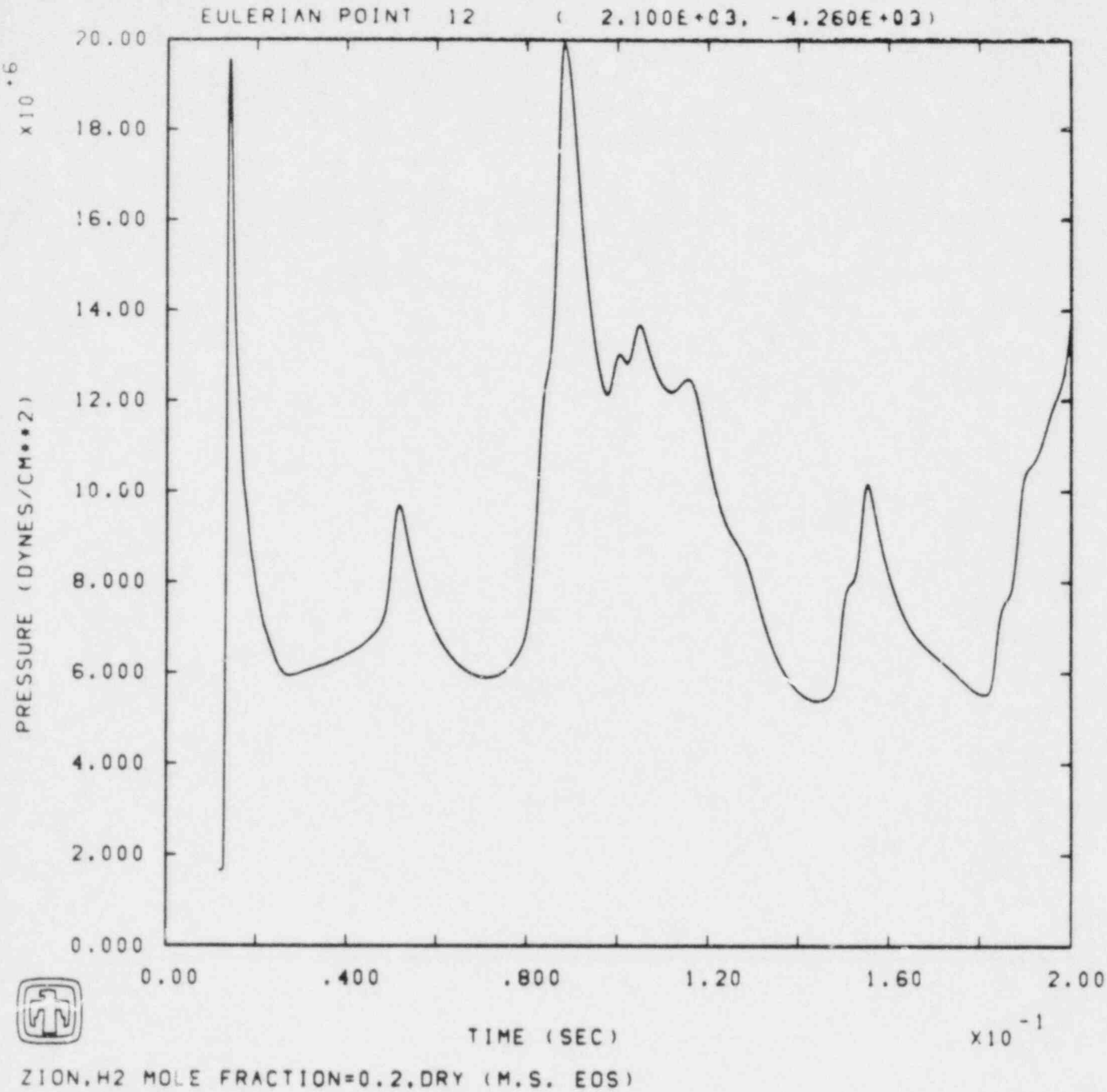


Figure III-5 Pressure History at Floor-wall Intersection in Zion Calculation

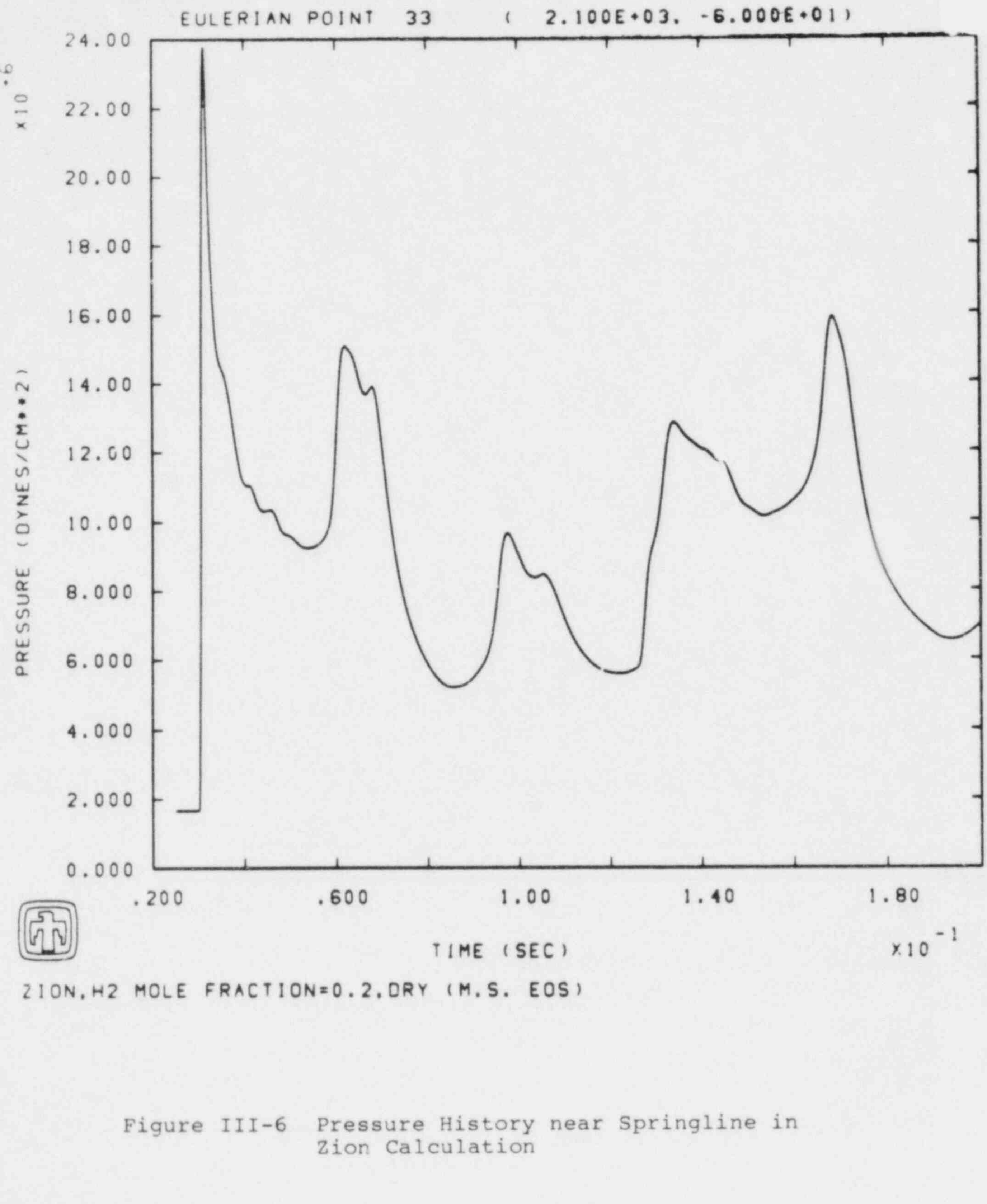


Figure III-6 Pressure History near Springline in Zion Calculation

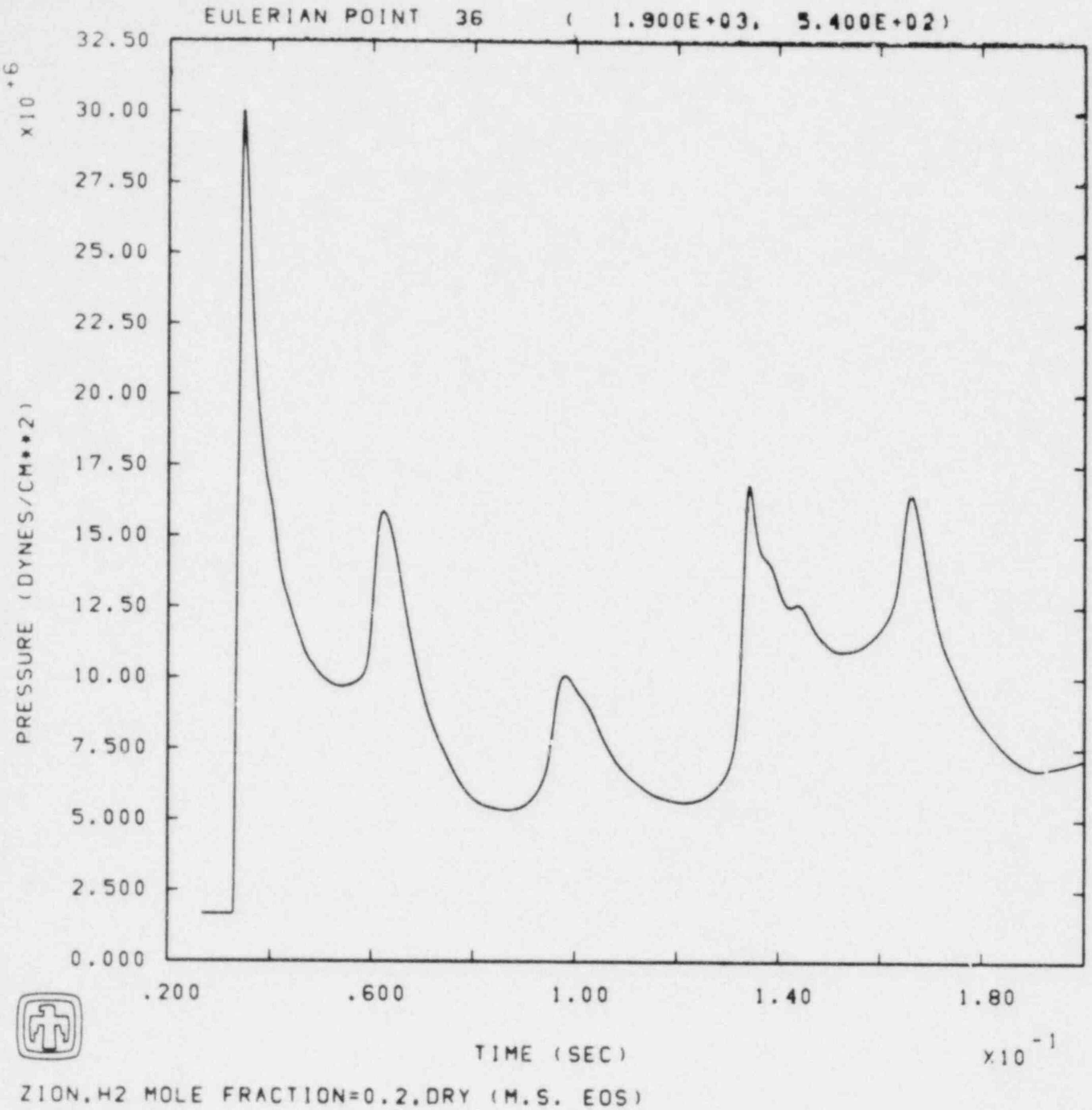


Figure III-7 Pressure History Partway up Dome in Zion Calculation

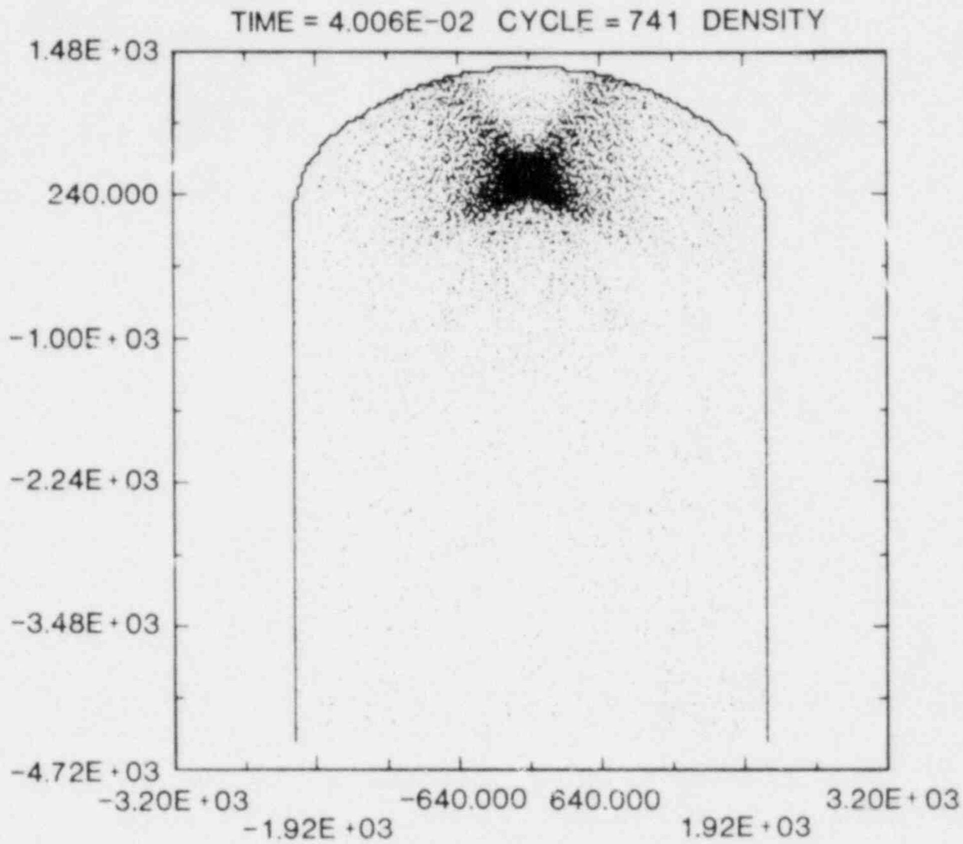


Figure III-8 Density Field at 40 ms in Zion Calculation

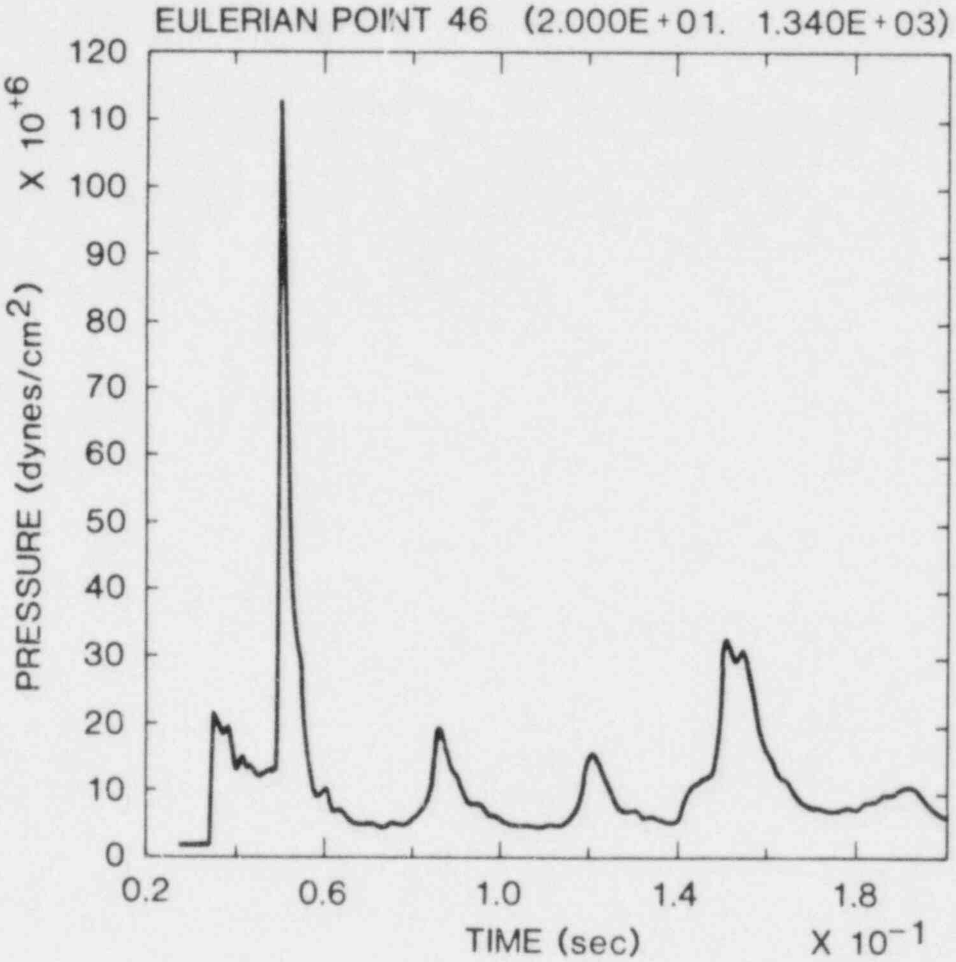


Figure III-9 Pressure at Center of Roof in Zion Calculation

IV. SEQUOYAH CONTAINMENT CALCULATIONS

Figure IV-1 presents a schematic of the Sequoyah containment building. The models chosen represented two distinct portions of containment: a lower subcompartment above the reactor vessel and below the control-rod-drive missile shield; and various regions of the upper containment compartment and ice condenser. A detonation in the lower subcompartment could threaten the integrity of containment by propelling the missile shield, or fragments of it, into the upper compartment. On the other hand, the steel containment vessel in the upper compartment has a relatively low static yield pressure (although an accepted value is somewhat uncertain), and could be vulnerable to direct loading from detonations or subsequent shock waves. In particular, the upper compartment may not be able to withstand pressures arising from an isochoric (constant volume) adiabatic burn of steam:air:hydrogen mixtures with a hydrogen concentration as low as 8-9 percent[8]. In addition, a scheme of deliberate ignition of combustible mixtures has been proposed [9,10] which could conceivably lead to accelerated flames or detonations in the upper plenum of the ice condenser, with subsequent shock interactions which would threaten containment.

A. Lower Subcompartment

Two calculations modelled the region above the reactor vessel head and below the control-rod-drive missile shield. In one of the calculations, detonation was initiated in a ring corresponding to the elevation of the vent panels (A in the figure). The other calculation had detonation proceeding from a point at the top center of the vessel head (Figure IV-2). The entire region contained the detonable mixture at an initial temperature of 375 K, and the problem was assumed to be axially symmetric about the centerline of the vessel. Zones were 0.2 m square, with 20 zones to the compartment radius.

As was the case in the Zion calculation, the assumption of axial symmetry, and multiple wave interactions, resulted in boundary pressures greatly in excess of the C-J pressure. For example, in the problem with ring detonation, the detonation wave reaches the center of the missile shield after the first on-axis reflection has occurred (Figure IV-3). The boundary in that region consequently experiences a very short-duration pressure spike of about 3 times the C-J value, as seen in Figure IV-4. At the same location in the point-detonation problem, the peak boundary pressures are almost as high, but in this case, they result from shock interactions in the detonation products (Figure IV-5). The largest boundary pressures in the second calculation were observed at the missile-shield/wall intersection; the pressure history there is shown in Figure IV-6.

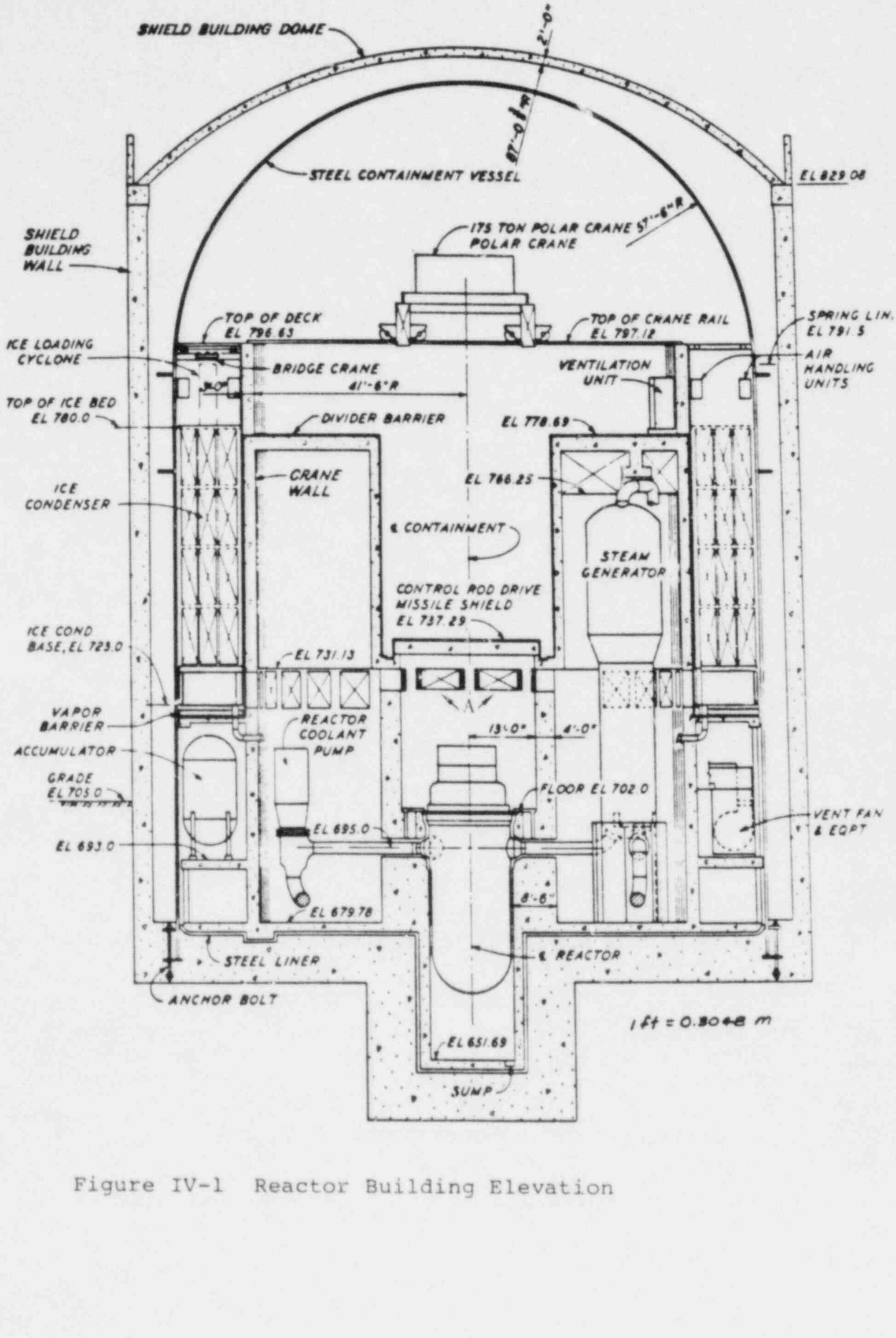
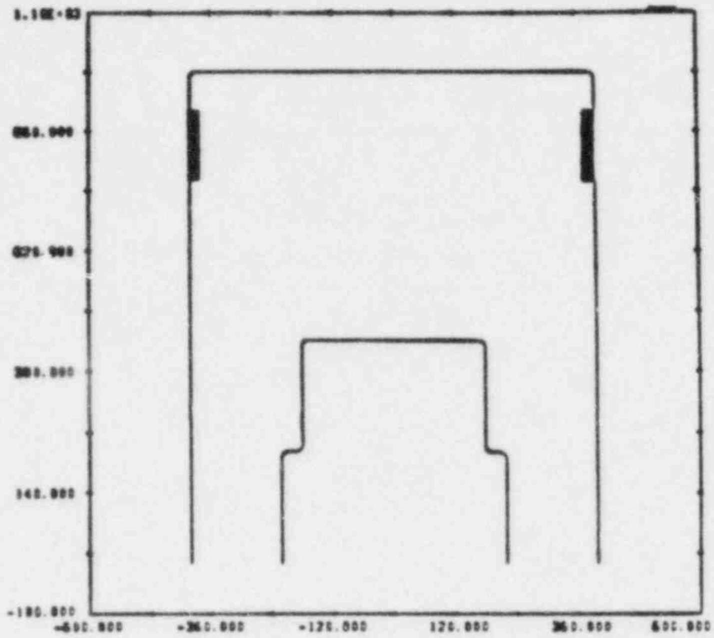
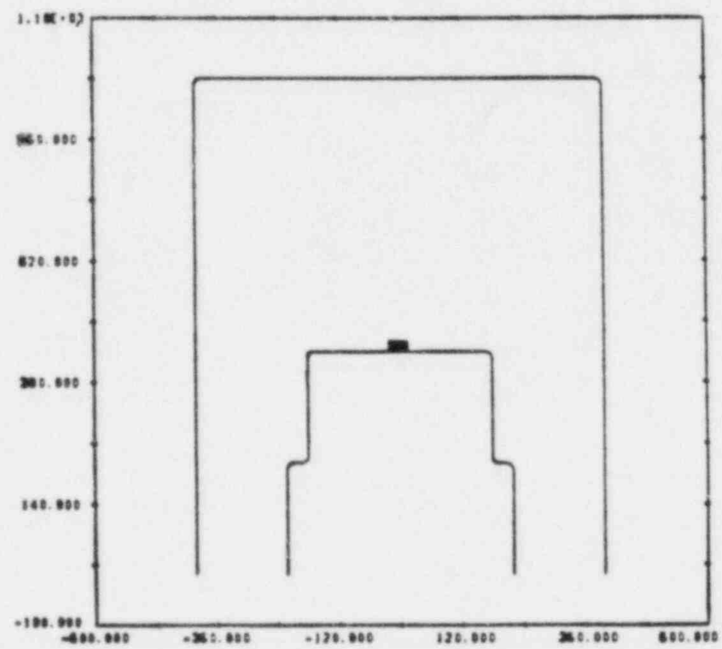


Figure IV-1 Reactor Building Elevation



a) Ring Detonation



b) Point Detonation

Figure IV-2 Sequoyah Lower Subcompartment

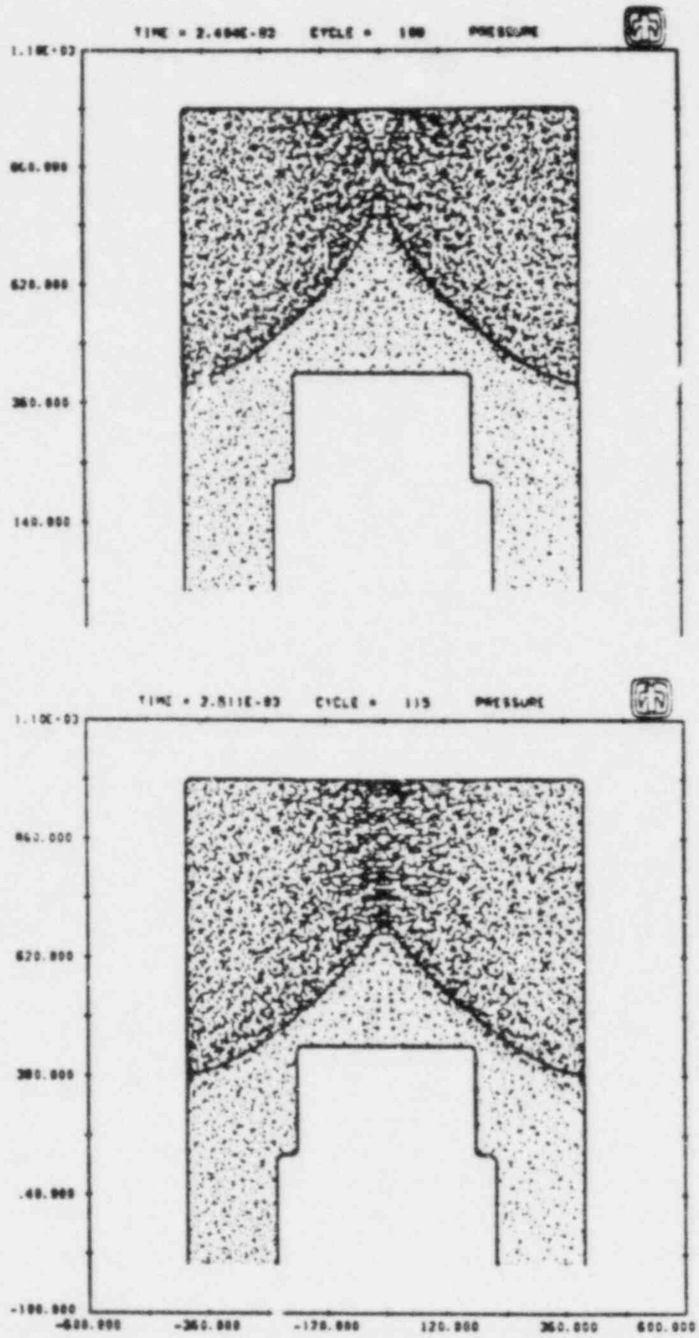


Figure IV-3 Pressure Fields at 2.4 and 2.6 ms,
Sequoyah Lower Subcompartment
(Ring Detonation)

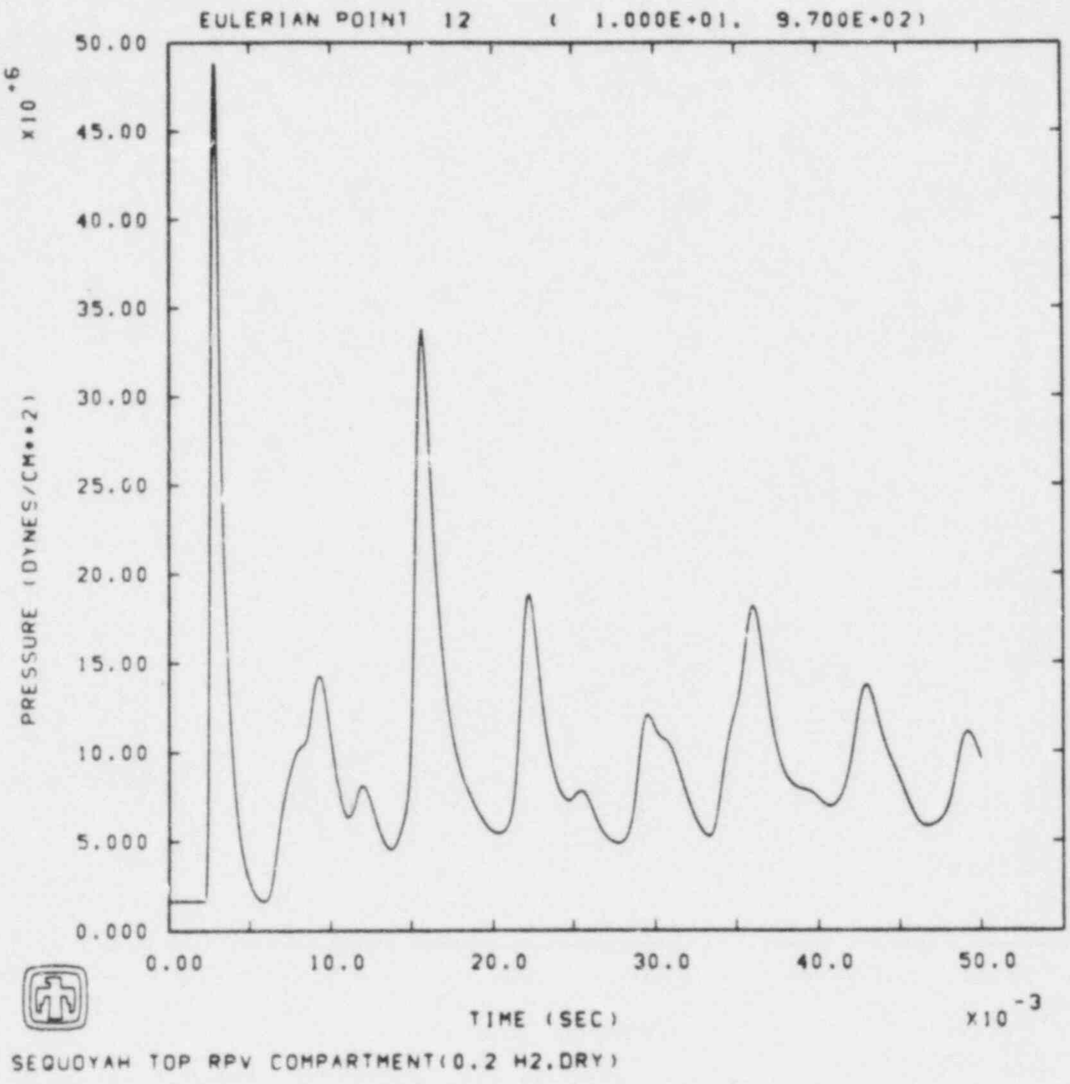


Figure IV-4 Pressure History at Center of Missile Shield Sequoyah Lower Subcompartment (Ring Detonation)

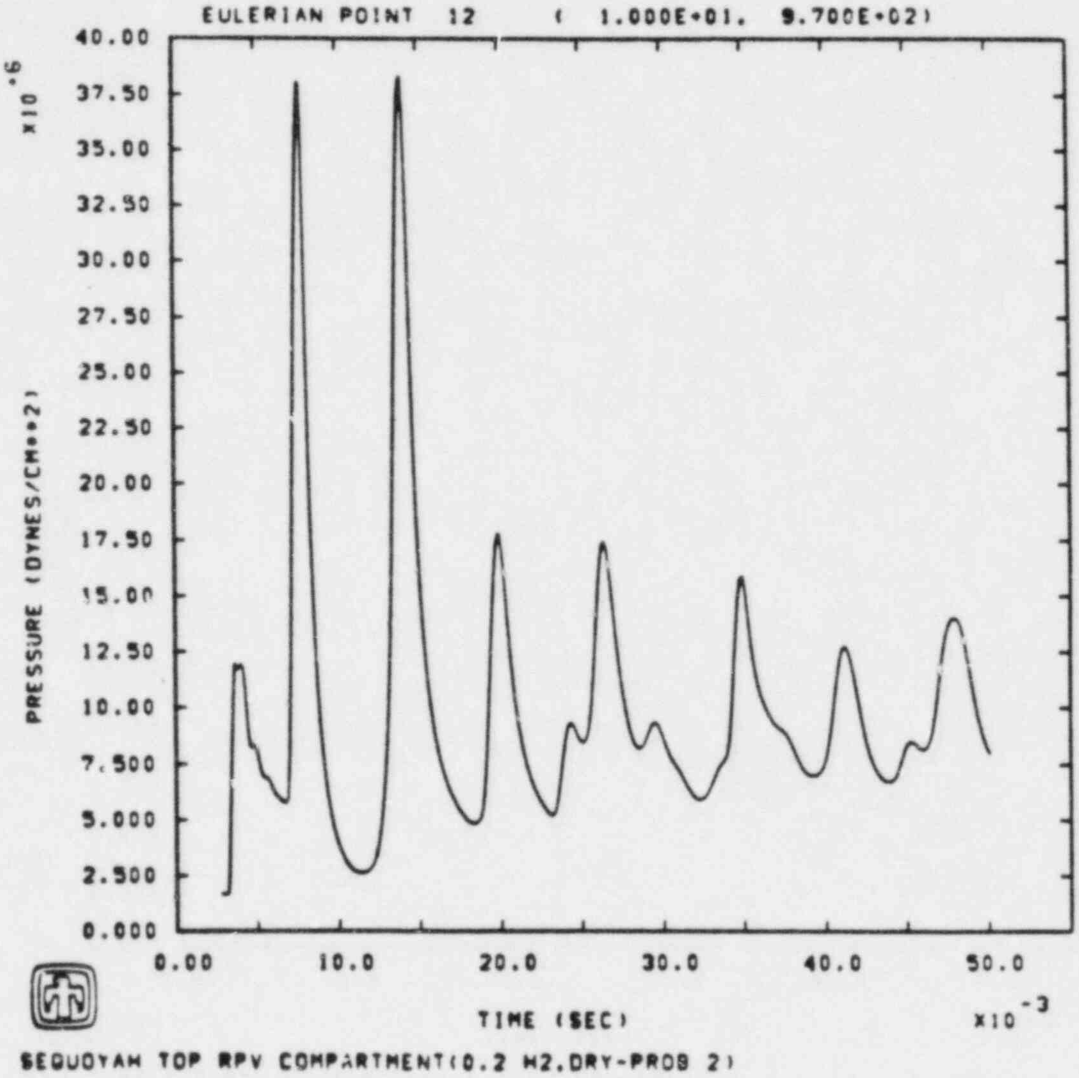


Figure IV-5 Pressure at Center of Missile Shield, Sequoyah Lower Subcompartment (Point Detonation)

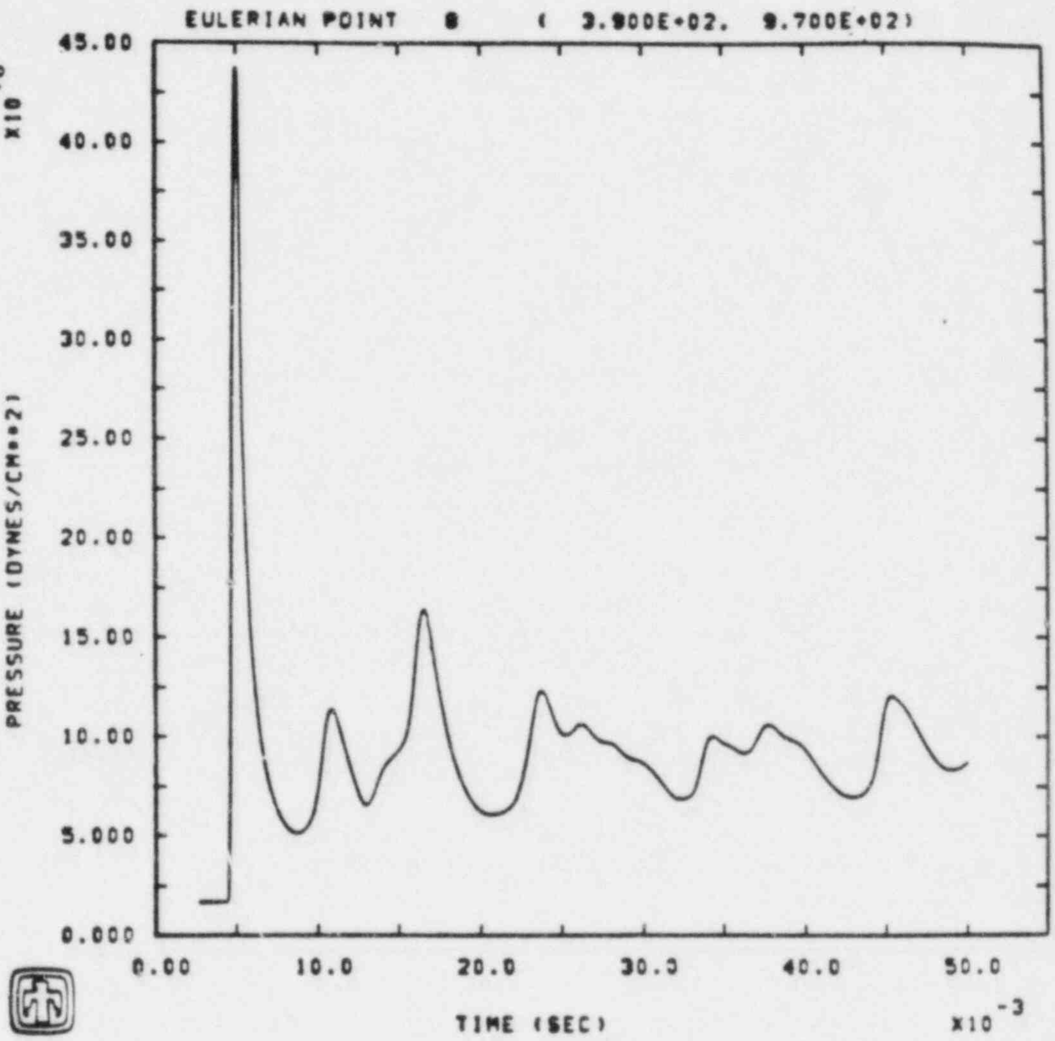


Figure IV-6 Pressure at Wall-Missile Shield Intersection in Sequoyah Lower Subcompartment (Point Detonation)

By greatly simplifying the boundary loads to a constant 1 MPa with a duration of 50 ms, it was estimated that the missile shield, if intact, would not travel far enough to strike the containment dome. In order to consider fragmentation due to spallation or complex stress states, a more detailed analysis of the shield would be required, which is beyond the scope of this work.

B. Upper-Compartment Calculations

Eight calculations were carried out for various models of the Sequoyah containment upper compartment. All concerned detonation of a dry hydrogen:air mixture in or near the ice condenser upper plenum (ICUP). As mentioned previously, if the entire upper compartment were filled with a combustible mixture, even a constant-density burn would produce pressures exceeding the estimated failure pressure. Therefore, only detonations in localized mixtures were of interest. It was speculated that an inert steam:air:hydrogen mixture could pass upward through the ice condenser, arriving at the ICUP as a detonable dry hydrogen:air mixture. This is of particular concern as glowplugs in the proposed deliberate-ignition system are located in this region.

The hydrogen:air mixture was assumed to be at an initial temperature of 275 K; C-J detonation pressure was thus about 1.6 MPa (Table II-1). Three of the calculations were axisymmetric representations of the upper compartment and ice condenser. In these cases, the ice-condenser region was filled with an ideal gas having an artificially-high density of 10 kg/m^3 (in order to model resistance to flow through the ice bed). The remaining five calculations were plan views, in Cartesian coordinates, at the elevation of the ICUP. Various combinations of boundary specifications and detonation locations were used. Table IV-1 provides a brief summary of the problem descriptions for the eight upper-compartment calculations. It was hoped that the results of this set of calculations would yield information on the relative influences of ignition location, of confinement of the detonating mixture, and of axial versus plane symmetry.

In the first axisymmetric calculation, a cloud of the H_2:air mixture was located just above the ICUP. Detonation was initiated in a single cell (i.e., a ring, considering the geometry) next to the outer wall at its juncture with the dome. Calculations 2 and 3 had the detonable mixture in the ICUP, with a rigid, vertical boundary on its inner wall; thus, the only initial interface between the air and the mixture was at the top of the ICUP. In problem 2, the ignition location was the same as in the first axisymmetric calculation; the third calculation had detonation proceeding from the same elevation, but at the mean radius of the ICUP. Figure IV-7 shows the boundaries and initial material interfaces for the three axisymmetric problems. The voids in the lower portion of the compartment were inserted to reduce the

TABLE IV-1

SEQUOYAH UPPER COMPARTMENT CSQ CALCULATIONS

Calculation	Description
1*	H_2:air above ice-condenser upper plenum. Ring detonation at outer wall.
2*	H_2:air in ice-condenser upper plenum. Ring detonation at outer wall.
3*	H_2:air in ice-condenser upper plenum. Ring detonation at mean radius of plenum.
4†	No ice-condenser inner walls. Detonation at mean radius of plenum.
5†	No ice-condenser inner walls. Symmetric point detonation.
6†	No ice-condenser inner walls. Asymmetric point detonation
7†	Completely enclosed upper plenum. Detonation at mean radius of plenum.
8†	Completely enclosed upper plenum. Symmetric point detonation.

*Axial symmetry

†Cartesian coordinates (plan view)

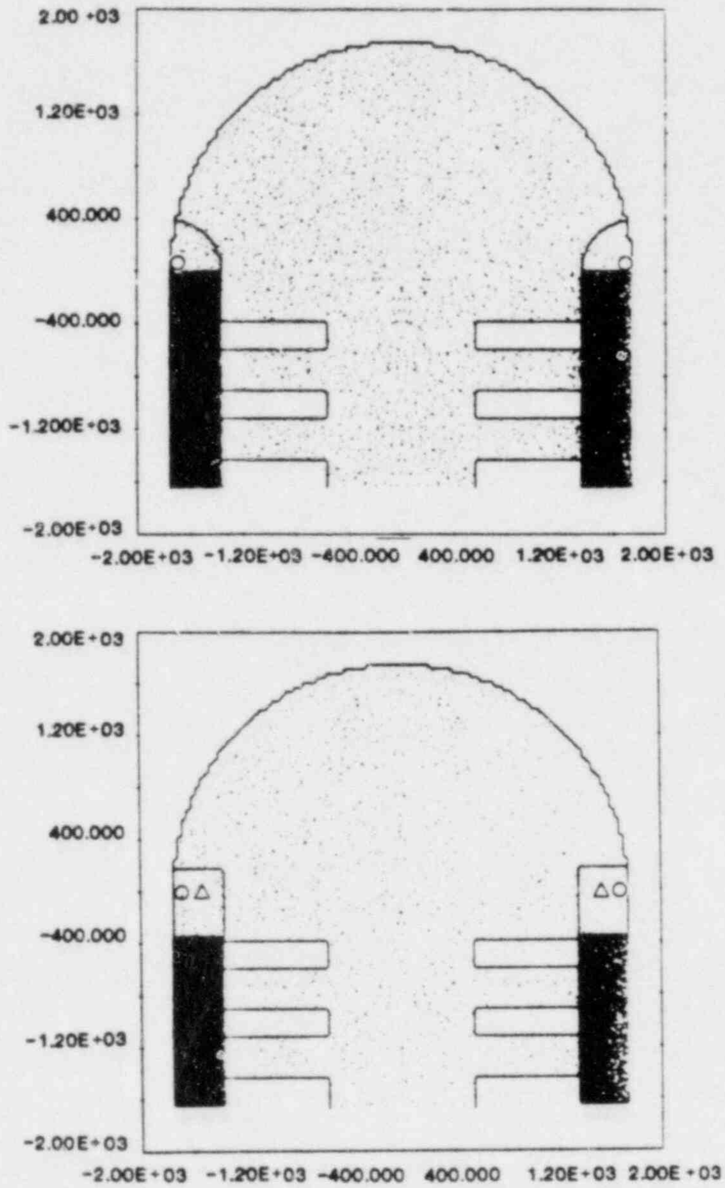


Figure IV-7 Initial Mass Density Field for Sequoyah Upper Compartment Calculations 1 (above) and 2 and 3

○ Ignition location, Calculation 1 and 2

△ Ignition location, Calculation 3

effects of strong cylindrical wave interactions, and to model the volume occupied by the steam generator enclosures. Problem 1 contained about 25 kg of the detonable mixture; in problems 2 and 3, this value was about 42.5 kg.

Predictably, the axisymmetric calculations yielded qualitatively similar results, except at early times near the ICUP. The pressure wave in the air is first attenuated and dispersed as it travels away from the detonation region, grows in amplitude as it approaches the axis of symmetry, and is strengthened by the reflection at the axis (Figure IV-8). This reflected shock arrives at the center of the dome almost simultaneously with the direct wave from the detonation region, resulting in very high peak pressures (Figure IV-9). Boundary loads exceeded the estimated static failure pressure of 0.36 MPa for more than 10 ms in all three calculations. Because of the greater available energy in calculations 2 and 3, the peak boundary pressures were approximately twice that observed in calculation 1.

The remaining five calculations for the upper compartment concerned plan views in Cartesian, rather than cylindrical, coordinates. Calculations 4-6 had the detonable mixture in the ICUP in direct contact with the air in the rest of the problem. In calculations 7 and 8, the ICUP was completely enclosed with rigid boundaries, forming a partial annulus spanning $5\pi/3$ (300°) of the plane. In problems 4 and 7, detonation was initiated in a one-cell-wide partial ring at the mean radius of the plenum; in problems 5 and 8, detonation proceeded from the point of symmetry opposite the open area between the ends of the ice condenser enclosure. For calculation 6, the ignition point was near one end of the ice condenser, so that this problem was initially very asymmetric.

In problems 4 and 5, the maximum boundary pressures observed occurred as spikes of very short duration (Figure IV-10). Because of the distributed detonation in problem 4, many points on the wall experienced virtually the same early-time pressure histories. For both calculations, the results of shock wave interactions in the air produced high pressures of much longer duration than those caused directly by the detonation wave. At the point midway between the ends of the ice condenser in problem 4, for example, multiple shock-shock and shock-wall interactions (Figure IV-11) produced pressures above the static yield pressure which persisted for tens of milliseconds, as shown in Figure IV-12.

The sixth calculation, with detonation initiated near one end of the ice condenser, showed behavior due entirely to the simple detonation criterion that was used. As the detonation wave travels away from the ignition point, the pressure wave induced in the air travels across the compartment. Because the pressure jump necessary to trigger the detonation calculations is very

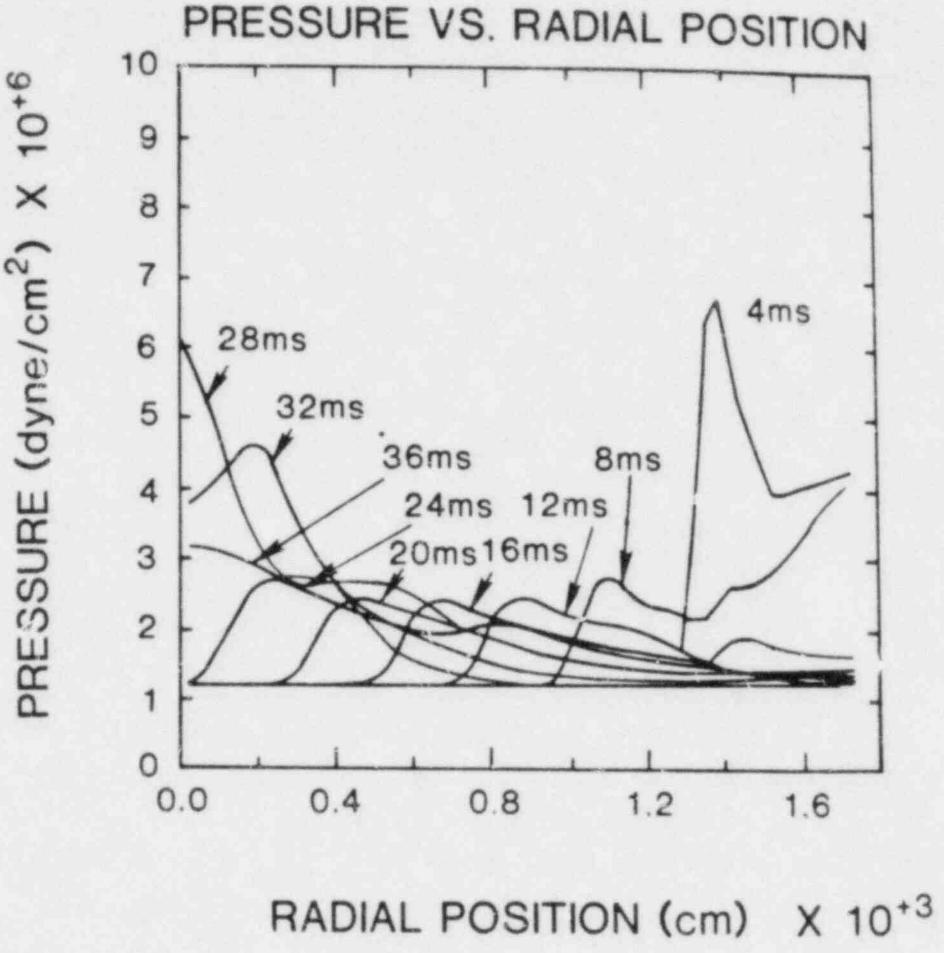


Figure IV-8 Pressure Distributions at Elevation of Ignition Point for Sequoyah Calculation 1 (0-36 ms).

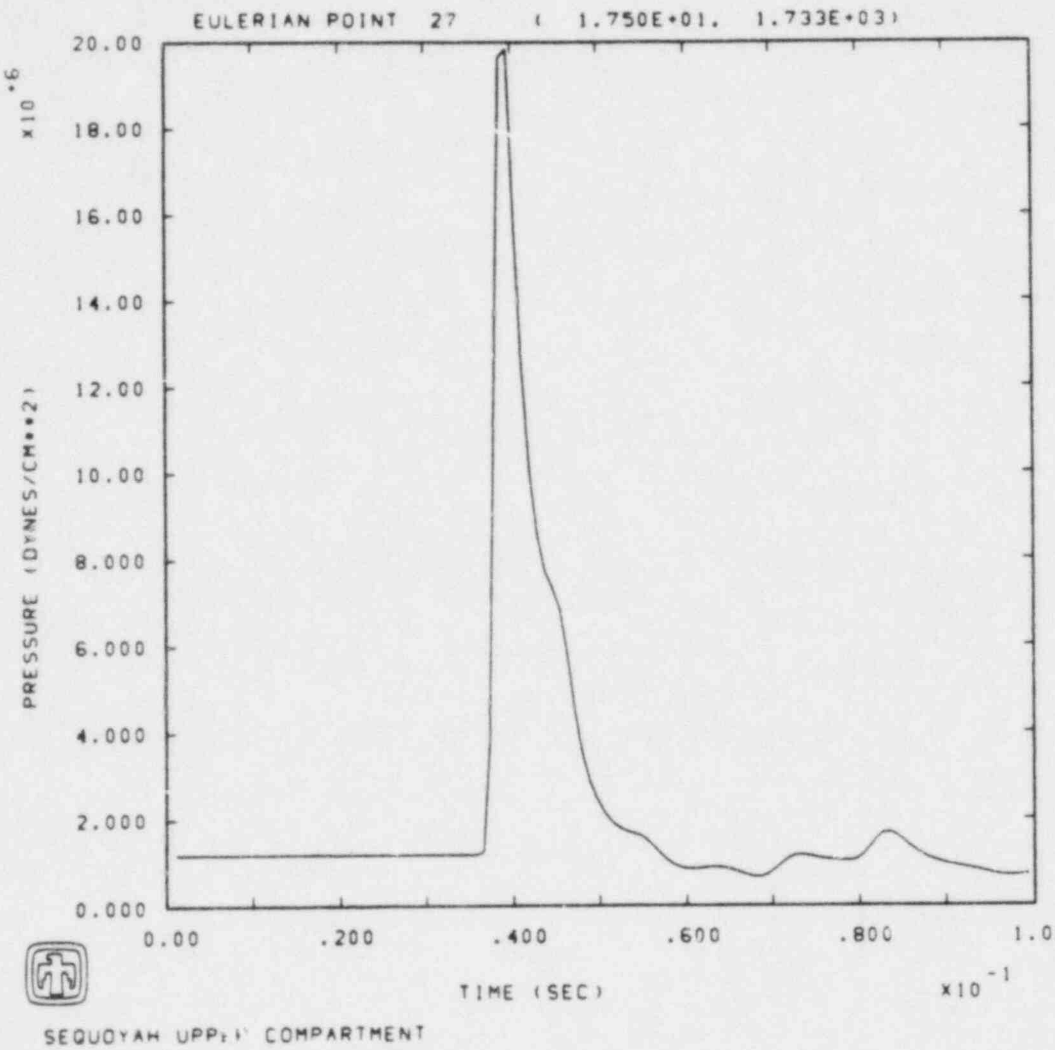


Figure IV-9 Pressure History at Center of Sequoyah Dome, Calculation 1

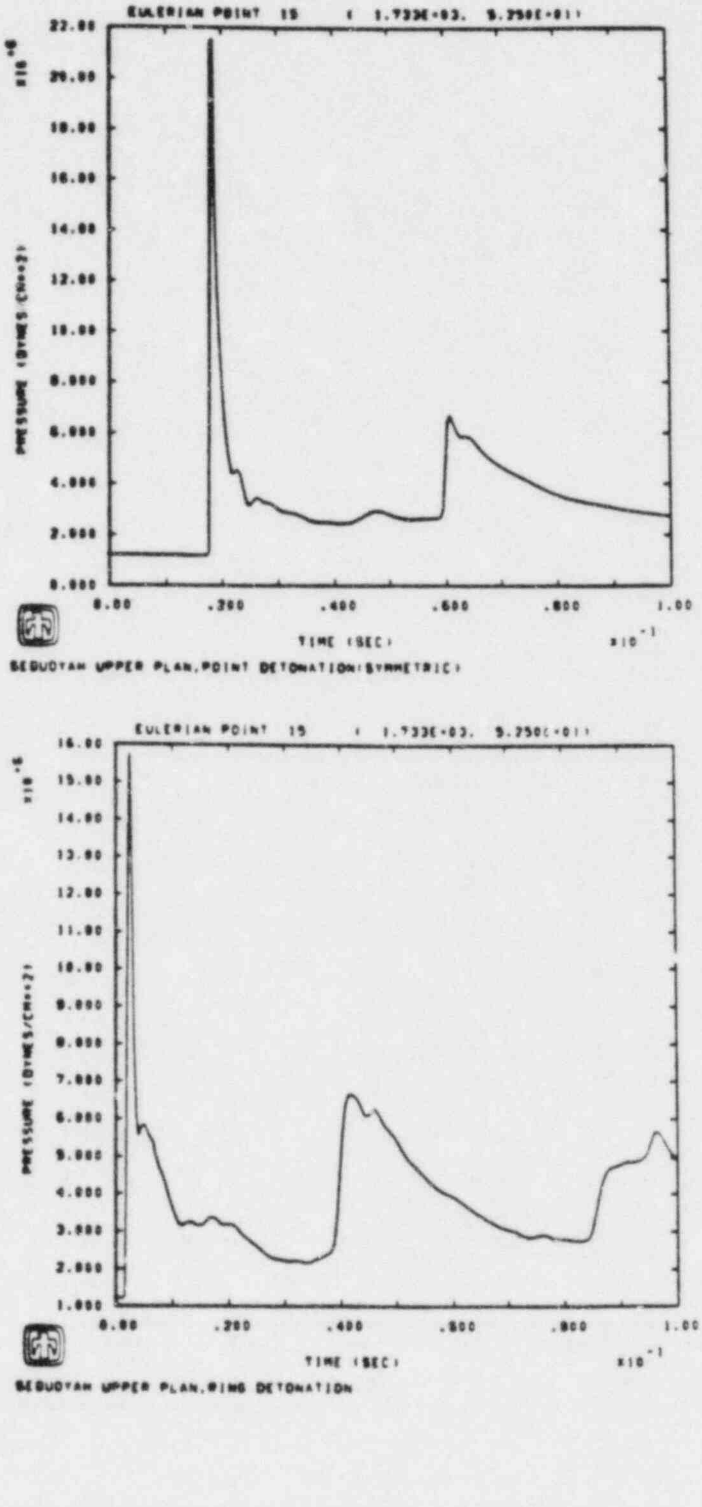


Figure IV-10 Pressure Histories at Maximum X, Sequoyah Calculations 4 and 5

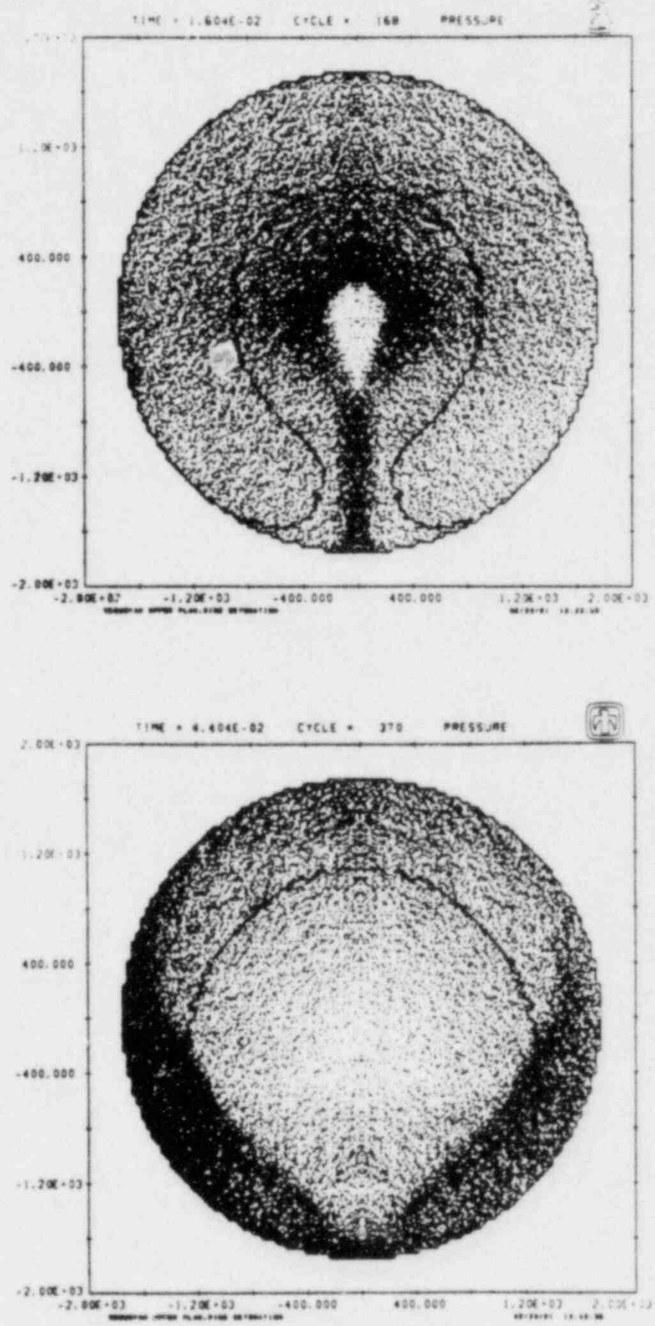


Figure IV-11 Pressure Fields at 16 and 44 ms in Sequoyah Calculation 4

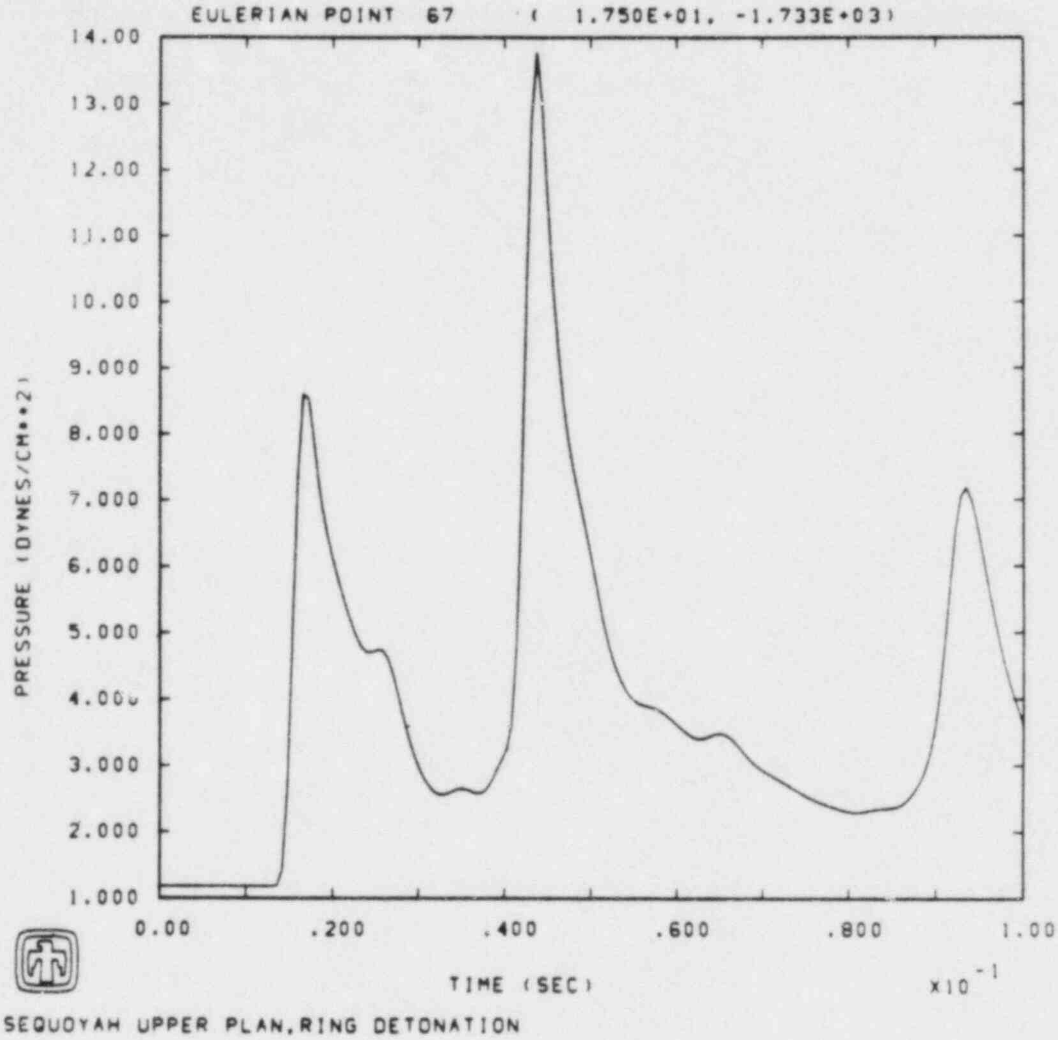


Figure IV-12 Pressure on Wall Midway between Ice Condenser Ends, Sequoyah Upper Compartment Calculation 4 small, a second detonation begins in the opposite end of the mixture (Figure IV-13). The two detonation waves collide shortly after 40 ms (see Figure IV-14), producing the high, short-duration pulse in Figure IV-15. The sensitivity of the detonation criterion thus causes unrealistic predictions of the magnitude, location, and time of occurrence of the peak boundary load in this calculation. However, the results demonstrate that the model is capable of describing flow-induced detonations, and could do so realistically if a better detonation criterion were used.

In calculations 4 and 5, the peak pressures on the boundary occurred at the first arrival of the detonation wave. The seventh and eighth problems (like 4 and 5, but with the detonating mixture completely enclosed) exhibited the same behavior, so the peak pressure values were about the same in the corresponding problems. Of course, with the complete enclosure of the ICUP, pressures remain higher and show reverberations of higher frequency (Figure IV-16).

In all the upper-compartment calculations, the peak pressure on the boundaries occurred as sharp spikes of very short duration. Even though the pressures far exceed the static yield pressure of the Sequoyah containment, the threat posed to containment is uncertain, because of the short duration. In the absence of detailed dynamic structural analyses, some approximate criterion is needed by which to judge the severity of the calculated results. Mark(11) has used such a criterion for impulsive loading in examining the effects of a detonation in Sequoyah. Assuming spatially-uniform loading of the Sequoyah structure, Mark calculated an acceptable impulse of 2.6 kPa·s. The calculation uses the natural period of the structure and the pressure giving the maximum elastic displacement. Mark terms his calculated value "very conservative" for the Sequoyah containment. This criterion can be applied for loads delivered during the first quarter-period of the structure, which Mark takes to be 6 ms.

Because significant boundary loads in the CSQ calculations are observed to occur at times and places other than the first arrival of a detonation wave, the results were analyzed by calculating impulses for every 6 ms interval after the arrival of a pressure pulse, rather than just the first such interval. The calculations in most cases do not exhibit spatially-uniform loading, but that question would have to be addressed by means of detailed structural analyses.

In the axially-symmetric calculations, the maximum impulses ranged from 7.8 to 13.0 kPa·s - i.e., 3 to 5 times Mark's acceptable value - with the largest value occurring at the center of the dome. In calculation 1, for example, the calculated impulse exceeded 2.6 kPa·s to a radial position of almost 4 m (Figure IV-17). In the plan-view calculations, peak impulses ranged

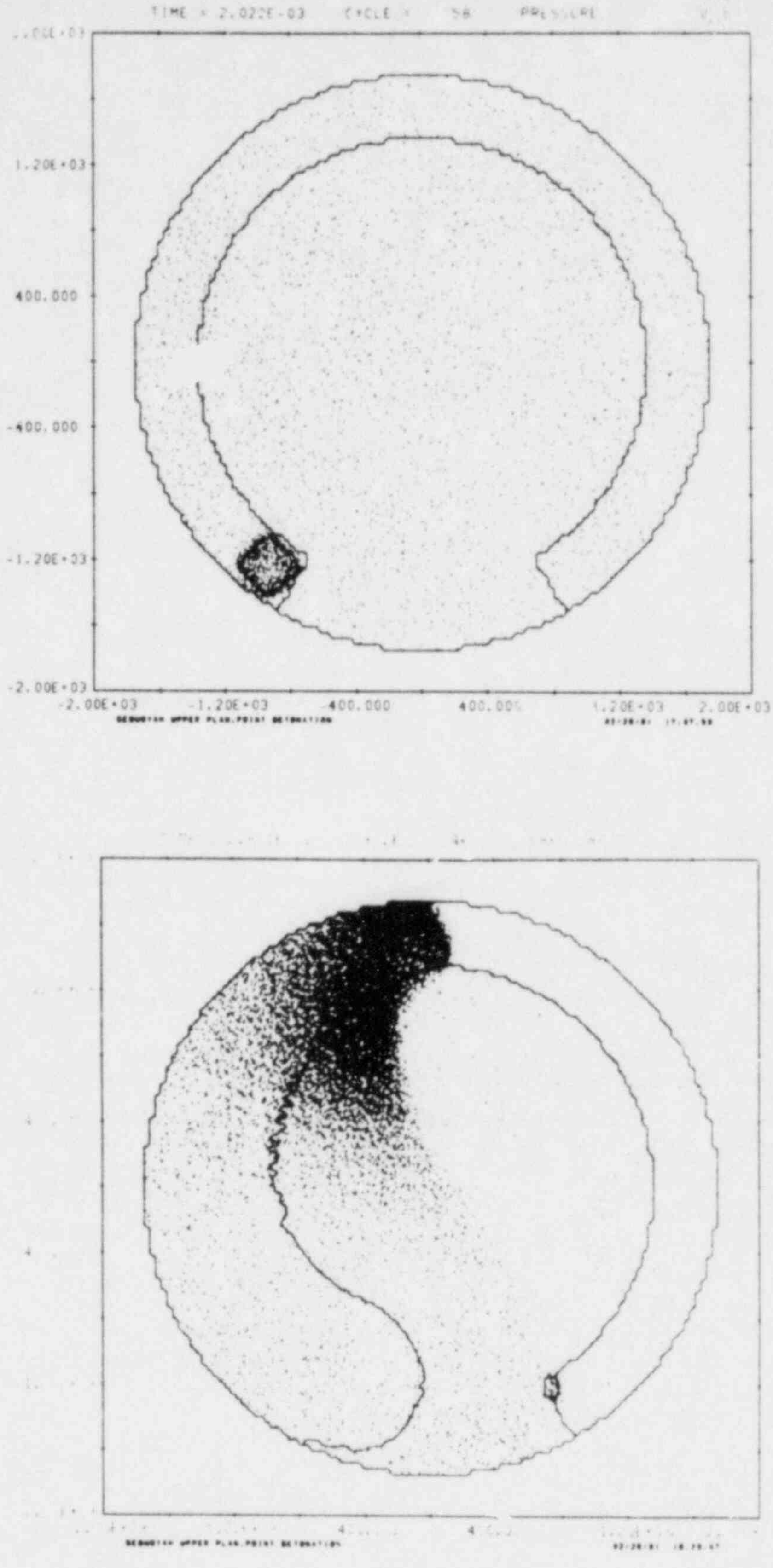


Figure IV-13 Pressure Fields at 2 and 28 ms in Sequoyah Calculation 6

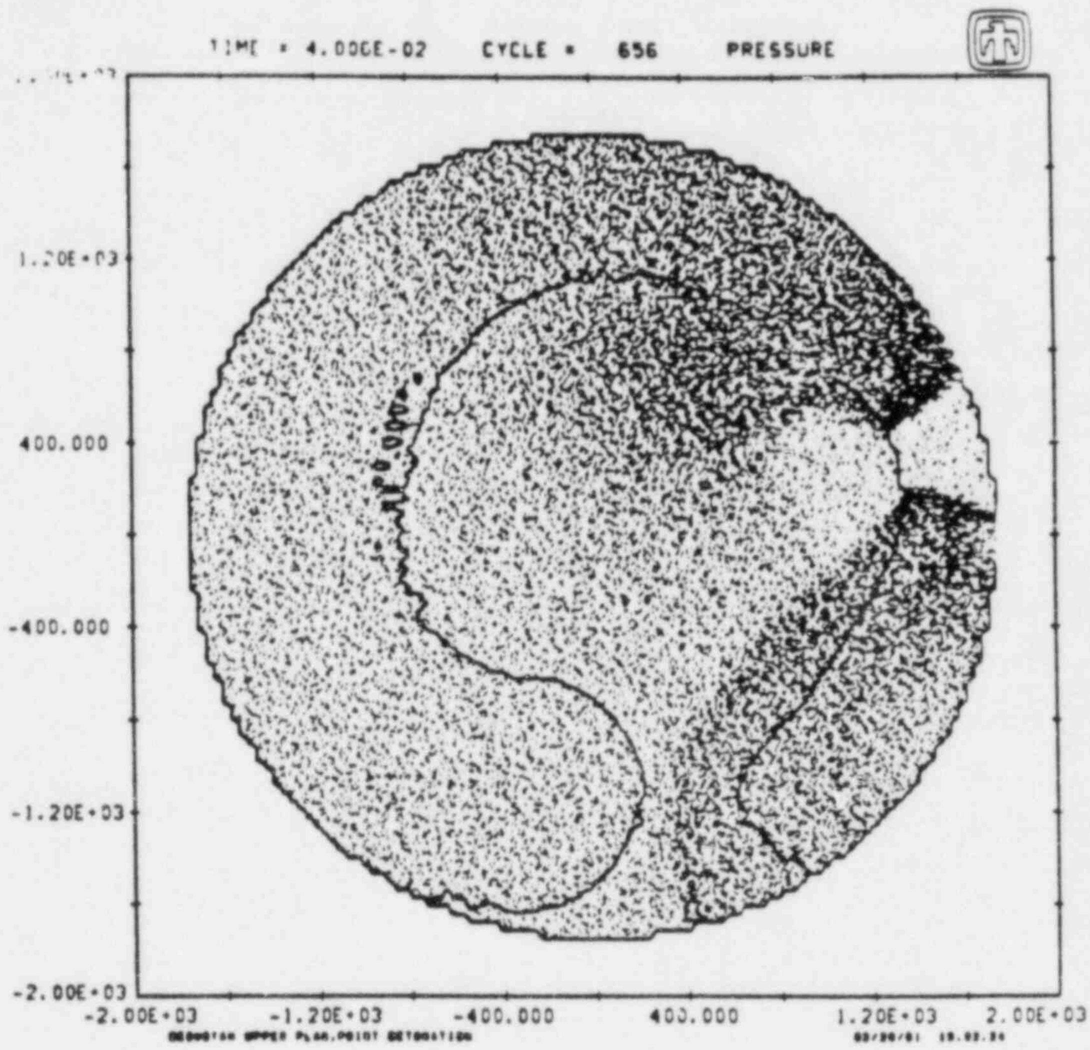


Figure IV-14 Pressure Field at 40 ms, Upper Compartment Calculation 6

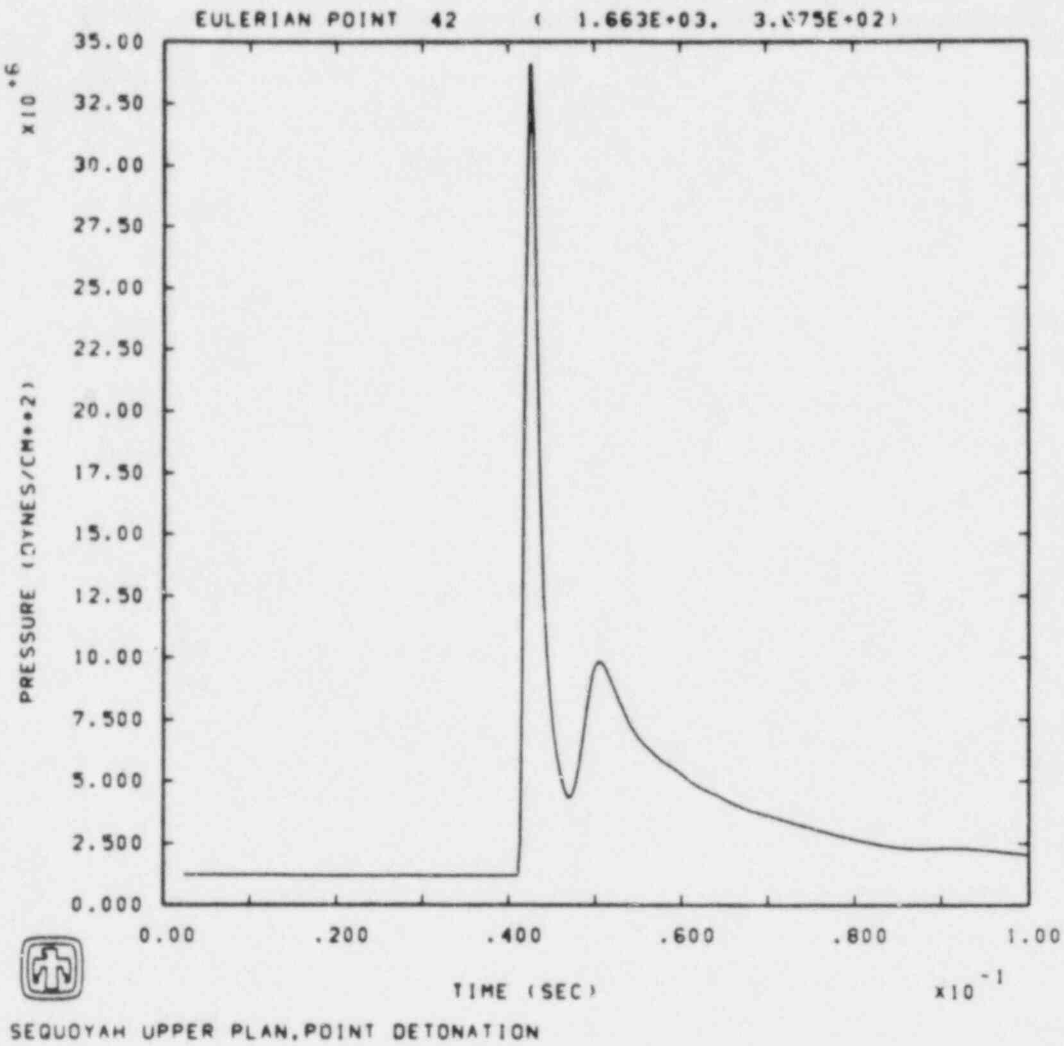


Figure IV-15 Pressure Near Collision of Detonation Waves, Upper Compartment Calculation 6

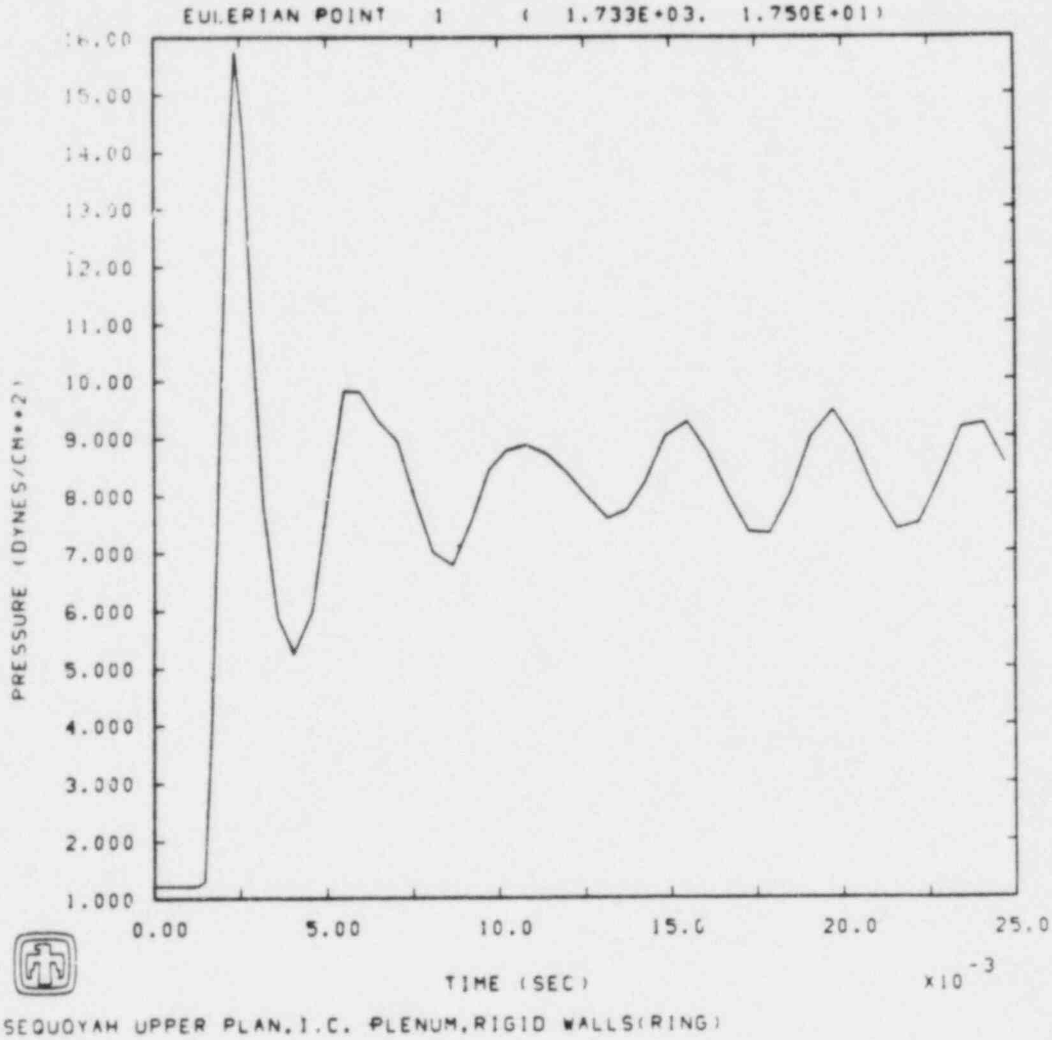


Figure IV-16 Pressure on Outer Wall, Upper Compartment Calculation 7

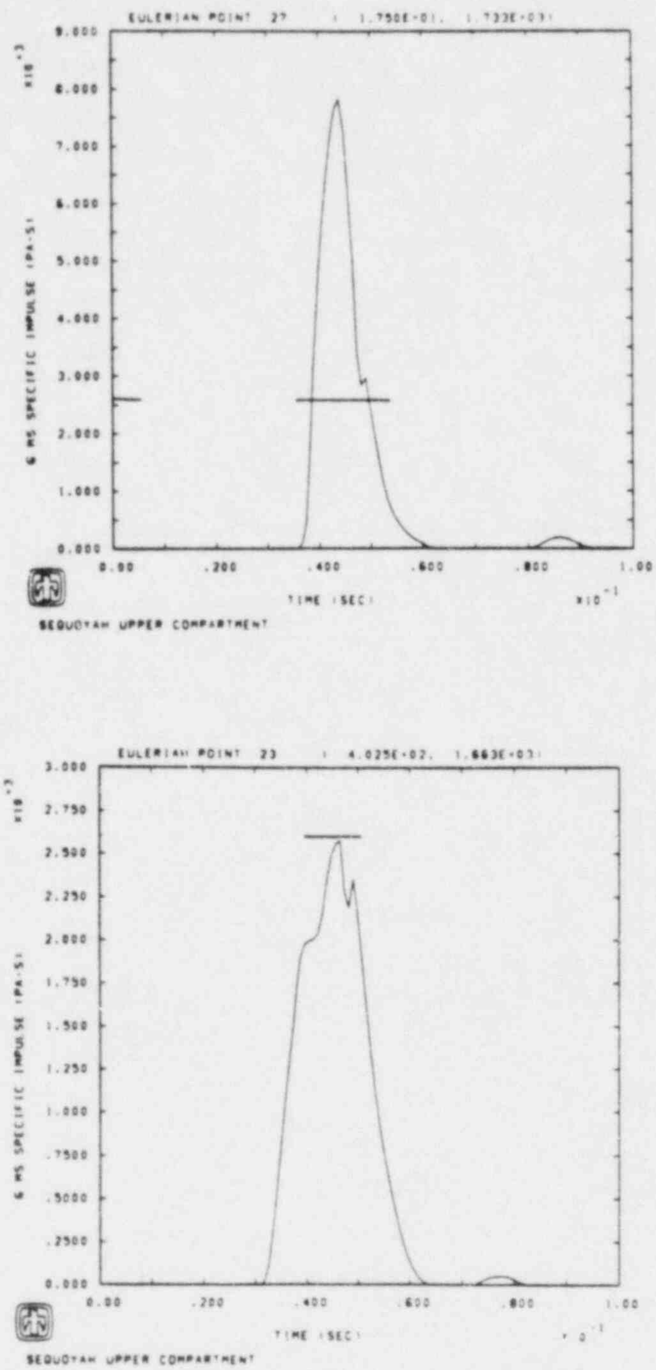


Figure IV-17 Impulse Histories at Center of Dome (above) and 4 m Radius, Sequoyah Calculation 1 from 5.0 to 11.1 kPa·s. The maximum impulse values did not always occur at the location of maximum pressure. In calculation 4, for example, the peak impulse was calculated at the point midway between the ends of the ice condenser, as a result of the multiple wave interactions alluded to earlier (see Figure IV-18). Table IV-2 summarizes the peak pressures and impulses for the upper-compartment calculations.

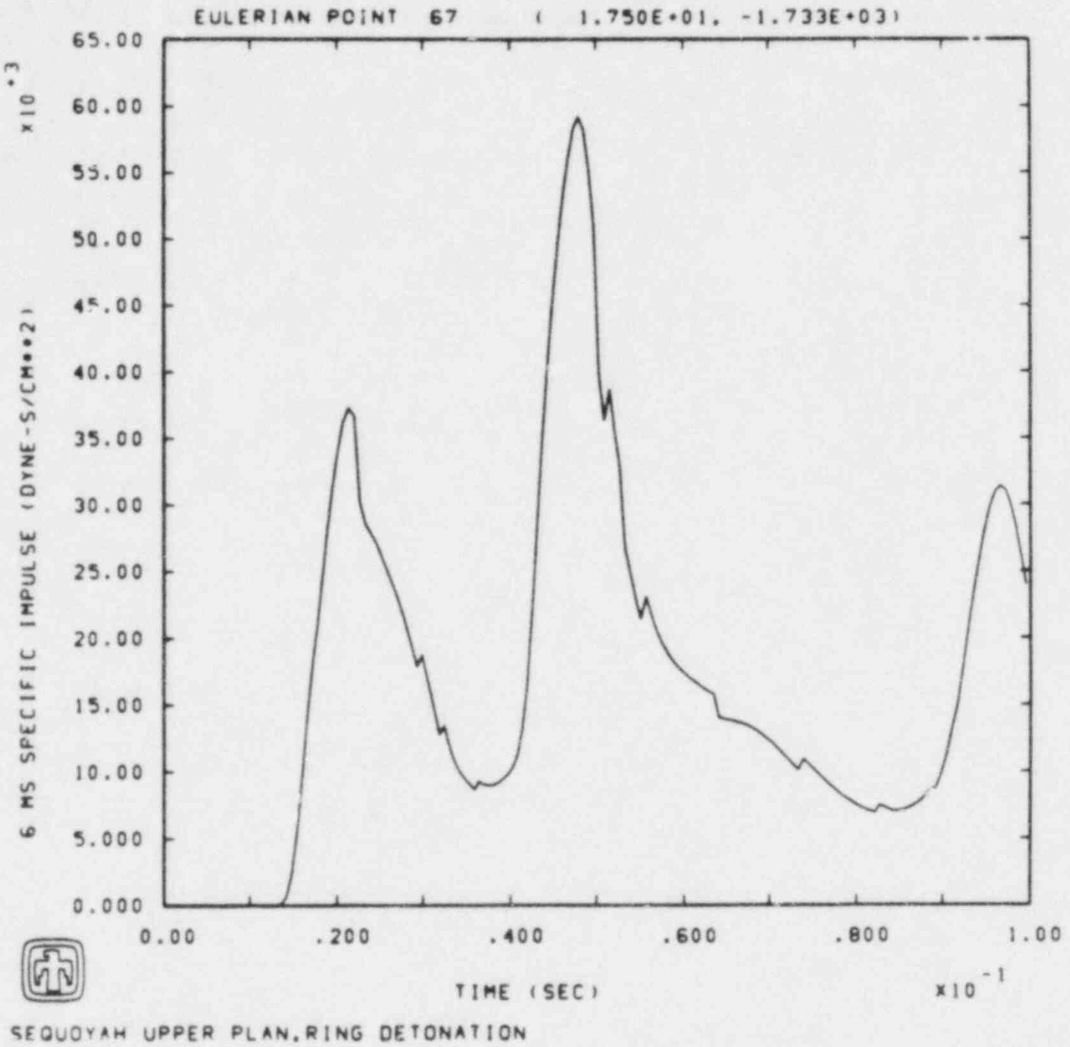


Figure IV-18 Impulse on Wall between Ice Condenser Ends, Upper Compartment Calculation 4

TABLE IV-2

PEAK PRESSURES AND 6 MS SPECIFIC IMPULSES

Calculation (see Table IV-1)	Peak Pressure (MPa)	Peak 6 ms Impulse (kPa·s)
1	2.0	7.8
2	4.0	13.0
3	4.0	13.0
4	1.6	5.9
5	2.4	8.8
6	3.4	7.5
7	1.6	5.0
8	2.4	11.1

V. CONCLUSIONS

In the CSQ calculations described in this report - 10 for Sequoyah and 1 for Zion - the most severe threats to the integrity of containment were seen in axisymmetric calculations for the Sequoyah upper compartment. Detonations of relatively small amounts of a hydrogen:air mixture produced, by means of subsequent shock interactions, very high pressure and impulsive loads on the boundaries modelling the building walls. The detonable mixtures were in regions where conceivably they might be present during an accident, and be deliberately ignited by a proposed mitigation scheme. In calculations for a lower subcompartment of the Sequoyah containment, and for the Zion containment, the results did not seem to be so severe. The assumption of axial symmetry did not uniformly produce the highest calculated boundary loads, in terms of either pressures or specific impulses. In cases where direct comparisons could be made, the relative effects of confinement of the detonating mixture, and of distance travelled by the detonation wave, were as expected.

The area of major uncertainty in treating detonations of hydrogen:air mixtures with CSQ is in a detailed (or reasonably so) treatment of the onset of detonation and treatment of reaction kinetics during the detonation process. The model used here was adapted from one which has been used successfully in a more sophisticated manner; however, the current state of experimental knowledge does not allow the full capabilities of the model to be employed.

Because rigid boundaries were used to model building and compartment walls, the results of the calculations cannot give a firm indication of whether or not failure would occur in the situations analyzed. For the Sequoyah upper compartment, a simple model for an acceptable impulsive load yields a value which was exceeded in every case. The CSQ-predicted loads appear to be too complex, both spatially and temporally,to admit the confident application of any very simple failure criterion.

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