Conf-941011--4

Modeling and Analysis of Hydrogen Detonation Events in the Advanced Neutron Source Reactor Containment *

by

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(July 1994)

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*** Research sponsored by the U.S. Department of Energy under Contract No. DE-AC05-84OR21400 with Martin Marietta Energy Systems Inc.

Prepared for Presentation and Publication at the Third International Conference on Containment Design and Operation, October 19-21, 1994, Toronto, Canada.

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MODELING AND ANALYSIS OF HYDROGEN DETONATION EVENTS IN THE ADVANCED NEUTRON SOURCE REACTOR CONTAINMENT

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ABSTRACT

This paper describes salient aspects of the modeling, analyses, and evaluations for hydrogen detonation in selected regions of the Advanced Neutron Source (ANS) containment during hypothetical severe accident conditions. Shock wave generation and transport modeling and analyses were conducted for two stratified configurations in the dome region of the high bay. Principal tools utilized for these purposes were the CTH and CET89 computer codes. Dynamic pressure loading functions were generated for key locations and used for evaluating structural response behavior for which a finite-element model was developed using the ANSYS code. For the range of conditions analyzed in the two critical dome regions, it was revealed that the ANS containment would be able to withstand detonation loads without failure.

I. INTRODUCTION

The Advanced Neutron Source (ANS) is a user facility currently in the design stage at the Oak Ridge National Laboratory (ORNL).[1] ANS is planned to be a 330-MW research reactor using uranium-silicide cermet fuel in a plate-type configuration. A defense-in-depth philosophy has been adopted. In response to this commitment, ANS Project management initiated severe accident analyses and related technology development in the conceptual design phase. This was done to aid in designing a robust containment for retention and controlled release of radionuclides in the event of a severe accident. It also provides a means for satisfying on- and off-site regulatory requirements, accident-related dose exposures, and containment response and source-term best estimate analyses for the level-2 and -3 probabilistic risk analyses.

A hydrogen safety study (HSS) was undertaken to complement work done for the ANS conceptual safety analysis report (CSAR)[2]. As part of this effort, work was initiated to study the effect of safety of hydrogen from hypothetical severe accidents. Due to the combination of a large containment and a low hydrogen generation potential, it was found that all of the hydrogen released during a hypothetical severe accident if uniformly distributed in the containment would give rise to a concentration of less than 1 vol./o. This indicates that the ANS containment meets and exceeds the U.S. Nuclear Regulatory Commision's (USNRC's) advanced light water reactor (ALWR) requirement[3] for maintaining the containment concentration to less than 10 vol./o by a large margin. However, to accommodate recommendations[3] made by the Advisory Committee on Reactor Safeguards (ACRS), a focused study was undertaken to evaluate threats to the ANS containment from detonations in stratified configurations. The purpose of this paper is to present the salient aspects of modeling and analyses of postulated detonations under assumed stratified configurations in the high-bay volume of the ANS containment.

II. DESCRIPTION OF ANS SYSTEM DESIGN

The ANS is currently in an advanced conceptual design stage. As such, design features of the containment and reactor systems are evolving, based on insights from ongoing studies. Specifically, the 330 MW(f) ANS reactor will use about 17 kg of highly enriched uranium-silicide fuel in an aluminum matrix with plate-type geometry. The power density of the ANS will be about 4.5 MW/L. Heavy water is used as coolant/moderator with a core outlet temperature of 92 C. Total core mass is only about 100 kg, which greatly reduces the hydrogen generation potential (viz., about 10 kg of hydrogen for ANS compared to about 1000 kg for a large power reactor). The base or conceptual ANS containment design is shown in Fig. 1. As can be seen from Fig. 1, the reactor core is enclosed within a core pressure boundary tube enveloped in a reflector vessel. The reflector vessel also envelopes two cold sources that contain about 40 kg of deuterium (chemically equivalent to 20 kg of hydrogen). This reactor system is immersed in a large pool of water. The ~95,000-m^3 primary containment consists of a steel shell (varying in thickness from 12.5 to 25-mm) housed in a 0.8-m-thick, reinforced concrete, secondary containment wall with a 1.5-m gap in between. Annulus flow is exhausted through filter banks. The targeted design leak rate for the primary containment is 0.5 vol. %/d, whereas for the secondary containment, the design leak rate is 10 vol. %/d.

III. MODELING AND PROBLEM FORMULATION

This section describes the salient aspects of modeling and problem formulation related to evaluation of dynamic loads and structural response behavior. For the initiating event, it is postulated that a hypothetical severe accident causes

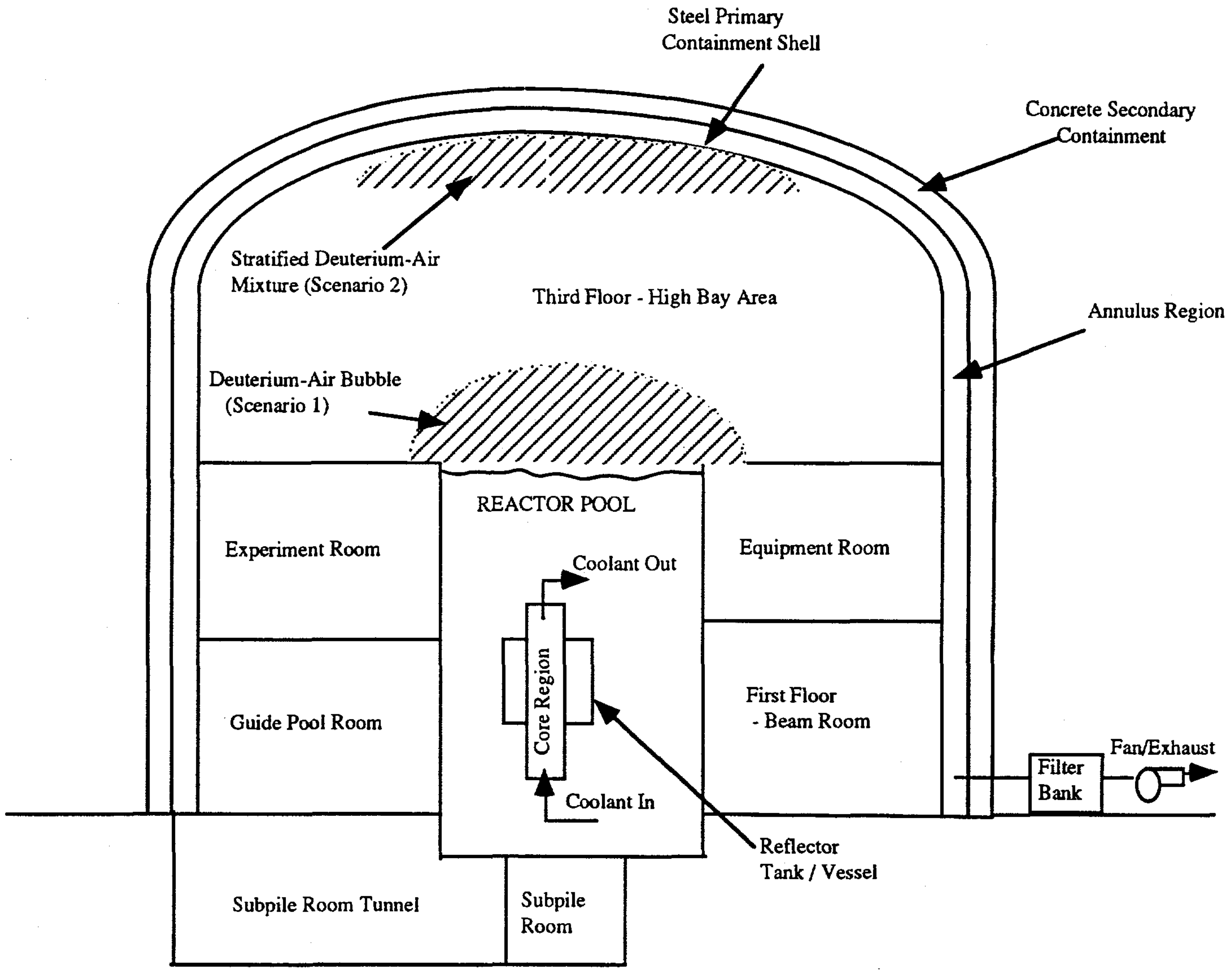

Figure 1. Schematic representation of ANS containment (showing deuterium-air mixture regions of Scenarios 1 and 2 for detonation studies)

rapid aluminum combustion of all the core fuel plates and also causes rupture of both the cold sources. This situation would give rise to about 30 kg of hydrogen (equivalent to 60 kg of deuterium) bubbling out over the reactor pool surface into the containment high-bay atmosphere volume. Two limiting scenarios were postulated. For the first scenario (SC-1) it was postulated that this bubble of hydrogen mixes with the surrounding air in various proportions before undergoing a detonation event. This was done to arrive at bounding-type estimates for detonations around the pool surface only. Calculated loads may then be used for initial estimates of structural response. The second scenario (SC-2) postulates that the hydrogen bubbling out of the pool surface rises over into the containment atmosphere and stratifies under the dome region before undergoing a detonation event there. The scenarios to be modeled and analyzed are depicted in Fig. 1.

The detailed modeling and analysis of every stage of hydrogen-air explosions can become a formidable task. Considerable uncertainties associated with complex thermal-hydraulic issues such as mixing patterns, stratification, effect of obstructions on enhancement of turbulence, randomly occurring ignition sources, and transition from deflagration to detonation. Several of these issues are still in the research stage. Hence, for the sake of evaluating conservative end-effects from possible detonations, several simplifying assumptions had to be made. The key assumptions are as follows:

1. Any hydrogen-air mixture (i.e., one that may also include deuterium) in a concentration range of 15 to 58 vol./o would be assumed to undergo a classical Chapman-Jougeot (C-J) detonation. While making this assumption, we verified that the masses and dimensions under consideration would (based upon detonation cell-width requirements) indeed support a deflagration-to-detonation transition.
2. The hydrogen-air mixture would be assumed to be instantaneously and uniformly distributed in the explosion zone. That is, no concentration gradients will exist.
3. For evaluation of structural response conditions, a detonation would begin as a point source and propagate outwards hemispherically. This assumption was relaxed for parametric studies. Additional cases to investigate volumetric heating (e.g., due to distributed spark) conditions are also investigated; the details of which are described later.
4. Fluid-structure interactions at boundaries and within the air volumes are negligible, and boundaries are treated as being perfectly reflecting. Thereafter, dynamic loads evaluated will be used as forcing functions in a separate structural response analysis model using finite-element modeling techniques. While this may miss some important feedback information, such an assumption has also been used[4] in making safety cases for power reactor containments.
5. A two-dimensional (2-D) symmetric simulation of the shock wave generation and transport is adequate for capturing effects in the high-bay region.

The principal tools being utilized for evaluations are the CTH [5]and CET89 [6]computer codes. CTH is a highly sophisticated tool developed to evaluate shock wave physics, fluid-structure interactions, missile penetration dynamics, along with multimaterial motion and response in one, two and three dimensions. A previous version of CTH (viz., CSQ) has also been used[4] in the past for analyzing hydrogen detonations in power reactor containments. CET89 is a chemical equilibrium thermodynamics code developed to evaluate thermodynamics of reacting substances. For best-estimate evaluations of hydrogen detonation studies, CET89 results were utilized at the front end to set up appropriate CTH modeling input for simulating a high explosive burning process. Some of these are given in Table 1. C-J detonation parameters were obtained for three hydrogen-air volume fractions (viz., 15, 29 and 58 vol./o) representing (in dry air and standard atmospheric conditions) the lower detonation limit, stoichiometric composition, and the upper detonation limit, respectively.

Table 1. Key thermodynamic parameters from CET89 for detonation calculations

	Hydrogen concentration (vol./o) / Hydrogen Mass (kg)		
Parameter	15 / 30	29 / 30	58 / 30
Post-burn mixture density (kg/m3)	1.78	1.57	0.96
Post-burn to pre-burn mixture density ratio	1.72	1.81	1.73
Post-burn specific heat ratio	1.26	1.17	1.25
Ratio of post-burn to pre-burn specific heat ratios	0.898	0.839	0.897
Detonation velocity (m/s)	1510	1971	2234
Shock burn energy (MJ / kg)	1.74	4.68	3.89

III.1 Scenario 1 (SC-1) - Detonation in high-bay volume above reactor pool surface

Initially, efforts were made to set up an appropriate 2-D CTH model of the ANS containment high bay volume and steel shell, to evaluate combined fluid-structure response behavior. However, due to the very large air space and the relatively minuscule curvilinear thickness of the steel dome, it was concluded that conducting a coupled calculation would be impractical. This is primarily due to the approximately 12,000 by 12,000 matrix of spatial mesh nodes that would be required for a proper simulation of fluid-structure interaction and structural response. Due to this feature, it was decided that CTH would be used to provide time- and space-dependent pressure variations. These values would then be used (as done conventionally for power reactor analyses) by the ANS Project architect-engineering firm Gilbert Commonwealth (GC) as forcing functions to evaluate structural response of the ANS steel dome. Such an approach has been used for power reactor hydrogen detonation simulations[4] and is deemed conservative because the absorption characteristics of the steel dome shell and air outside are not directly factored into the shock wave physics calculations.

It was decided to represent the detonation process in a 1-D spherical framework before embarking on a 2-D modeling effort. This was done primarily to optimize nodalization and to study effects of parametric variations without having to wait long periods of time (hours to days) before a result is obtained.

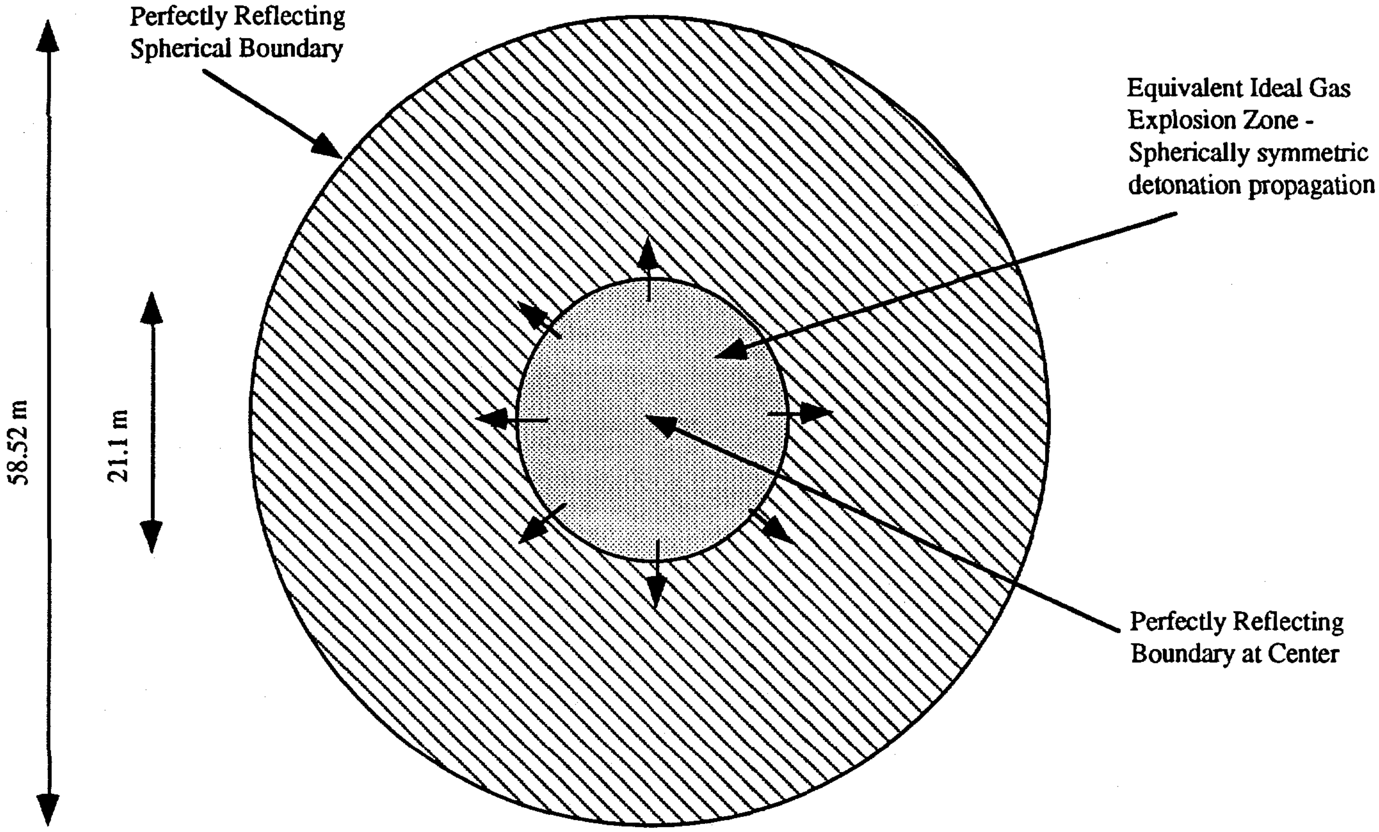

Fig. 2. 1-D spherical geometry CTH model for 15 v/o hydrogen-air detonation analysis

Several 1-D spherical geometry evaluations were made. For 1-D simulations a spherical geometry representation was developed. This geometry, shown in Fig. 2, tends to represent best (albeit in 1-D) the overall geometry of the ANS containment dome. It is realized that reflections off the floor regions are not simulated in this geometry. However, the 1-D cases provide valuable lessons for modeling in 2-D geometry later on. For CTH simulations, the explosion zone, consisting of hydrogen-air mixtures, is represented as an equivalent ideal gas mixture where suitable modifications are made using state properties from CET89 calculations. Energetics of the hydrogen detonation process are represented in two different ways to represent two different modes of ignition. In the first mode (mode 1), we represent energy generation via time dependent energy deposition over the entire explosion zone volume. This tends to represent the situation wherein multiple sparks may be available randomly located in space. Variations about this base case were set up to investigate effects of nodalization, and time over which energy is deposited in the explosion zone. In the second mode (mode 2), it is assumed that a single ignition source would be available at the focal point of the hemispherical volume right above the center of the reactor pool. A detonation beginning from this point would then propagate outward hemispherically. Once again, variations about this base case (i.e., for mode 2 energy insertion) were set up to investigate effects of nodalization and variation of detonation velocity. An additional case was also evaluated to see what loadings were generated if a reduced quantity of hydrogen were available for detonation. For this, the case where the hydrogen content was reduced 50% to 15 kg was also modeled for CTH calculations. For simulated hydrogen calculations it is not very obvious what should represent the ideal-gas mixture (which simulates the hydrogen-air-detonation product material mixtures). That is, should the overall mixture be represented with values for thermodynamic parameters of the initial mixture or of the final mixture (i.e., C-J conditions)? To evaluate the impact of such a choice, we also investigated the case of representing the gas explosion zone mixture by using the thermodynamic parameters for the C-J conditions of the mixture (i.e., after reaction completion).

A 2-D representation of the ANS containment high bay region was evaluated. As mentioned previously, representing the 12.5 mm-thick shell of the ANS steel dome would need a 12,000 by 12,000 matrix of nodes, making it impossible to conduct practically feasible CTH calculations. Therefore, an alternate representation was modeled with CTH. This model, in 2-D cylindrical geometry, essentially carves out the shape of the ANS containment spherical dome and vertical structure from a given block of metal. Two different metals were experimented with for this purpose. The first one was steel, whereas, the second one was lead. As a mathematical device in code input lead was experimented with to allow use of a denser material and to reduce computational time significantly (due to sonic wave propagation constraints entering the Courant limit). In reality, some absorption of energy would occur in either the thick lead or steel boundaries adjacent to the air zone inside. From this view, the use of lead provides a better reflecting boundary. Similar to the 1-D case, the explosion zone was modeled as an equivalent ideal-gas mixture. Figure 3 schematically shows the model used for this purpose.

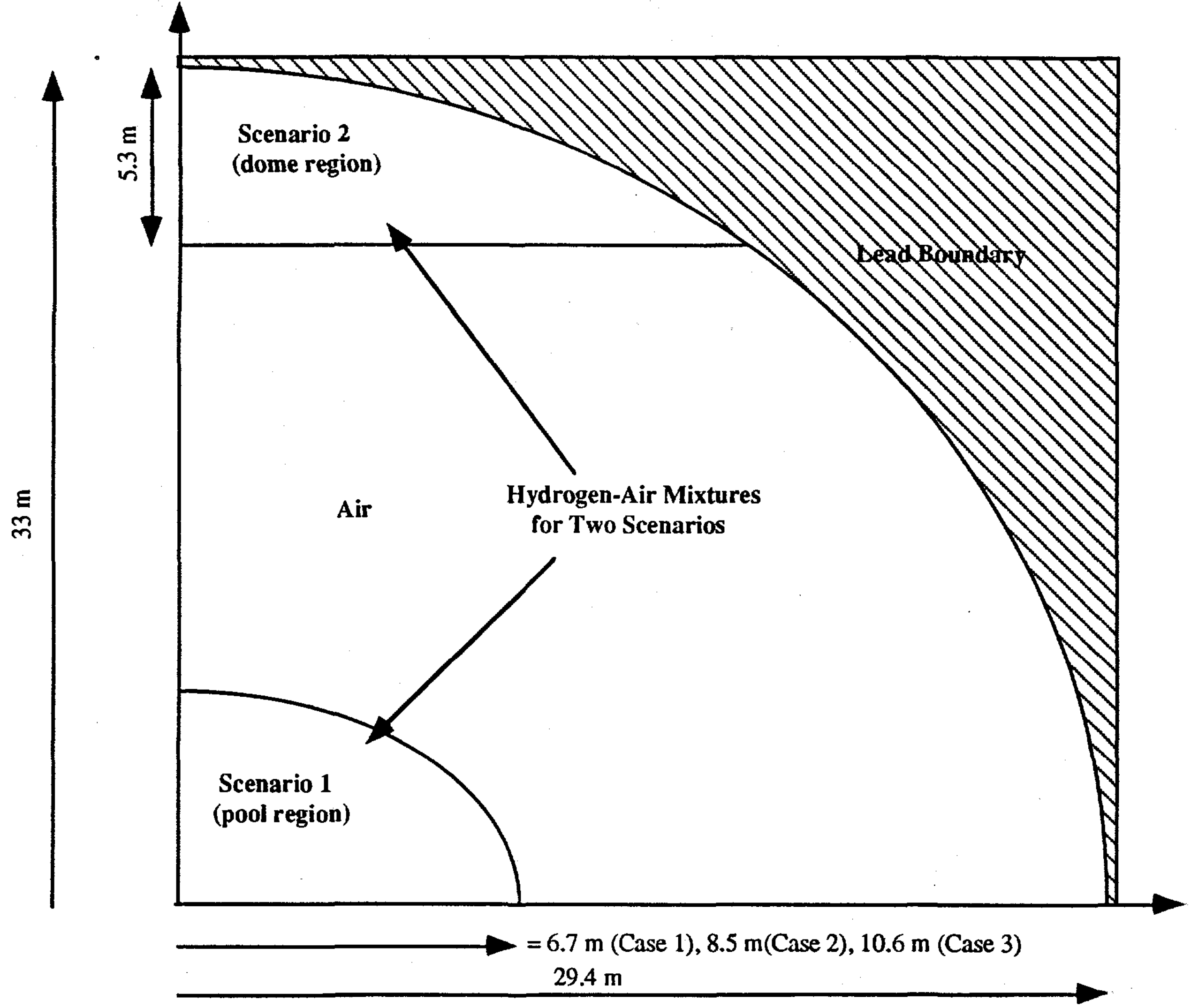

Figure 3. 2-D cylindrical geometry CTH model for best-estimate load evaluations

III.2 Scenario 2 (SC-2) - Detonation in high bay volume in upper dome region

SC-2 is modeled and analyzed for the situation wherein the 30 kg of H_2 rises through the high bay volume and stratifies under the steel dome. From a practical perspective, it was decided that any such rise would involve significant dilution of the hydrogen concentration. Therefore, it was assumed that a stratified mixture under the dome would be a lean detonable mixture at the lower end of the detonation limit (viz., 15 vol./o). For this configuration, the 2-D CTH model developed for SC-1 was modified to locate the explosion zone to be under the dome region, as shown in Fig. 3. To represent the pressure profile on the surrounding structures better, node widths were halved.

III.3 Structural response modeling and failure strain criteria

The dynamic loading functions evaluated using the 2-D CTH model were utilized to drive a containment shell finite-element structural analysis model developed by GC staff. GC staff conducted modeling with the ANSYS code[7]. Nonlinear effects of elastic-plastic material properties along with bilinear kinematic hardening model were included. It is not the intent of this paper to present modeling details of the nonlinear transient dynamic ANSYS model, but to present only the key assumptions and results, the details of which have been documented elsewhere[2]. For determining shell failure, guidelines developed for severe accident conditions for steel containments (such as the Mark I steel containment) were utilized, rather than use of American Society of Mechanical Engineers guidelines which are more appropriate for design basis accidents. Using these criteria, dynamic strain limits (to avoid failure) for the ANS containment were set as being 1% for membrane strain, 2% for surface strain and 5% for peak strain. Failure from buckling was considered incredible for ANS containment.

IV RESULTS & DISCUSSION

Significant quantities of data were generated from these models and evaluations. From space limitations it was decided to graphically highlight only those results used for determining structural response of the ANS containment. The results and discussion section is divided into sub-sections for each of the two scenarios mentioned earlier.

IV.1 Detonations above pool surface (SC-1)

As mentioned earlier, it is not practical (from space limitations) to show plots of all the various quantities affecting shock generation and transport. For 1-D simulations, only summary descriptions are given for some of the important results.

Insights from simplified 1-D simulations

One-dimensional simulations indicated that mode 1 (i.e., volumetric heating which may represent multiple sparks or detonation initiation points) of energy deposition gives rise to impulse loadings which can be different from those of mode 2 (i.e., point initiation of combustion). In the center of the explosion zone, the peak pressure buildup was greater (by 50%), as may be expected for mode 1. However, the pulse does not last as long. Total impulse impressed at the center of the explosion zone is somewhat larger for mode 2 deposition than for mode 1. Despite the similarities in total impulse delivered, it is realized that such a variation in actual pressure buildup may become important for structural response calculations. For other locations the pressure traces looked remarkably similar. Nodalization was seen to play an important role. Doubling the number of nodes from the base case was seen to result in higher pressure spikes. However, these spikes get very narrow above the pressure levels seen for the base case, giving rise to impulse loading levels which are quite the same. However, reducing the number of nodes by a factor of 2 can give rise to considerable dissipation. It was further found that pressure buildup is not significantly affected by inaccuracies in knowing the precise rate of energy deposition or detonation velocity. Reasonably large levels of uncertainties (+/-25%) in detonation velocity will not affect significantly the predicted pressure-time histories at vulnerable locations. An important safety consideration deals with high temperatures. Very high (5000 K) temperatures may be reached during hydrogen detonation events. The impact of these flame temperatures on safety and non-safety related equipment may become a cause of concern and will be examined for relevance as the containment design and associated severe accident analyses evolve. Finally, upon comparing pressure and temperature traces, it was seen that specification of the gas mixture values upon initial or final conditions does not give rise to results which are significantly different. Actually, values for pressurization with post-burn parameters are slightly lower than those seen using preburn conditions. Therefore, to stay on the conservative side, the 2-D simulations for the ANS HSS would be conducted with specification of the initial mixture based upon properties before combustion.

Results from 2-D simulations for detonations above the pool surface

Based upon 1-D simulation results, it was decided to conduct analyses with point source alone and the mixture conditions were defined with preburn conditions. Using the 2-D CTH model of Fig. 3, the impact of specifying the reflecting shell material by steel versus lead were examined. For the atmosphere region, it was found that pressure traces calculated with use of lead as a boundary versus use of steel are almost exactly the same. The only difference noted was in the CPU time required, which was lower by more than a factor of two for lead than that required for steel. Therefore, to conserve computational resources, lead was chosen as a boundary material.

The 2-D CTH model was exercised for three cases covering the detonability range (viz., Case 1 for the upper detonation limit of 58 vol./o, Case 2 at the stoichiometric limit of 29 vol./o and Case 3 for the lower detonation limit of 15 vol./o). Sample pressure trace results from the 2-D model for Case 3 (viz., 15 vol./o) are shown in Fig. 4. Locations at which pressure traces have been shown are the top of the pool surface, intersection of the steel shell with the floor and right underneath the top of the containment dome. From Fig. 4 we note that significant differences in timing of pressure front arrival at different structural boundaries should be expected.

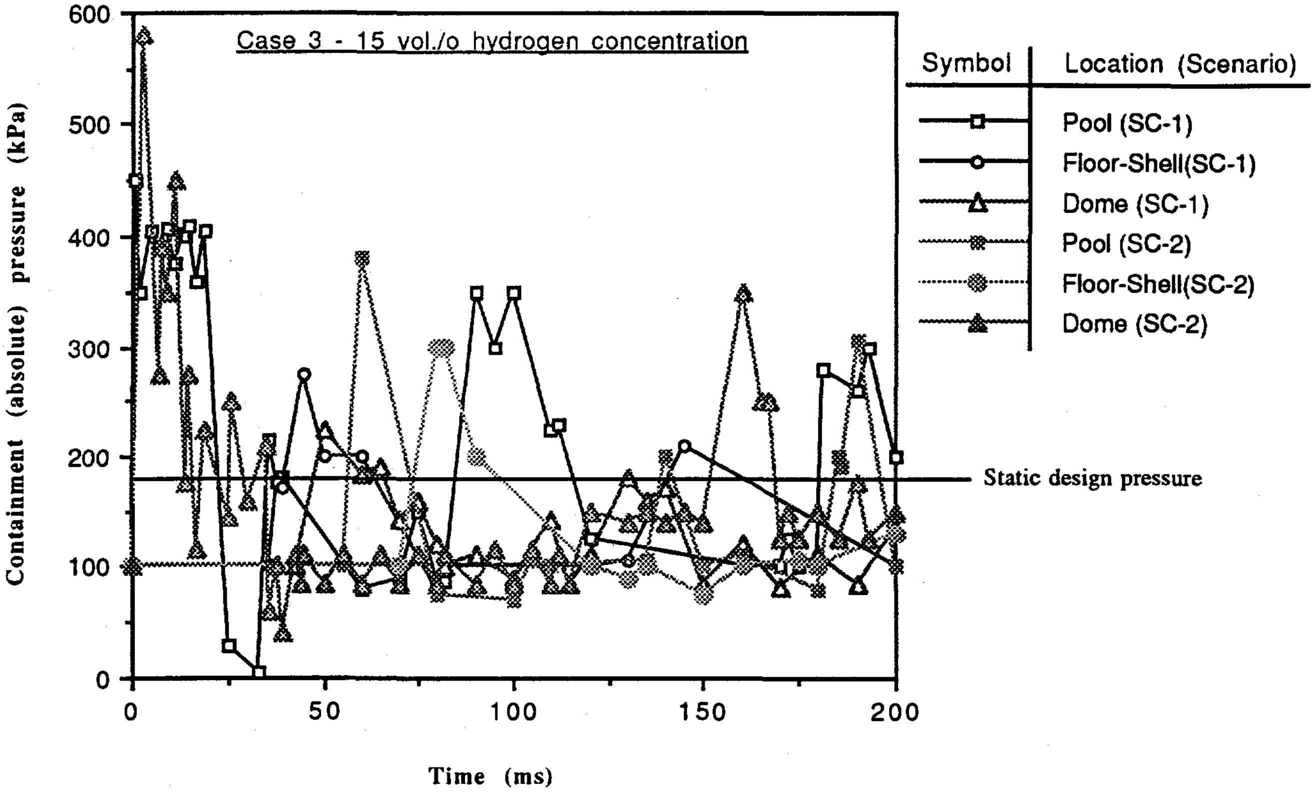

Figure 4. Variation of pressure with time during hydrogen detonations in ANS containment (SC1 - Scenario 1; SC-2 - Scenario 2)

Very significant variation in pressure variation along the high bay floor was calculated. Pressure levels can vary significantly from one region of containment to another. For example, for Case 3 (viz., 15 vol./o) pressures vary from more than 500 kPa at the region directly above the pool region to about 250 kPa at the containment wall-floor boundary. Such information clearly can not be obtained from 1-D simulations, which underscores the importance of conducting multidimensional modeling. Overall, the pressures at the containment shell boundary and also in the explosion zone were evaluated to be significantly lower than those observed from 1-D evaluations, indicating the effects of multidimensional dissipation.

Across the containment shell boundary, the (absolute) pressure levels vary from 220 to 275 kPa. The "static" design pressure of the ANS containment is 171 kPa (or 10 psig). The dynamic pressures (indicated by triangular symbols) lasting about 40 ms are above this limit, however, this does not mean that the steel shell integrity will be compromised. Only a dynamic structural response study can properly determine whether allowable strain limits are exceeded, and whether failure will occur.

Overall, it was found that the Case 2 conditions (i.e., stoichiometric H_2 concentration) give rise to the most challenging loadings on the structural boundaries, followed by Case 3 and Case 1, respectively. Case 1 conditions give rise to incomplete combustion due to the relative lack of oxygen, and account for the resulting low pressures at the structural boundaries, which are even lower than the ANS static pressure difference design limit of 10 psig (or 71 kPa gage). Maximum vertical displacements evaluated by GC with the ANSYS model were, 110 mm (4.5 in.) for Case 1, 160 mm (6.3 in.) for Case 2, and 140 mm (5.4 in.)for Case 3 respectively. Membrane and surface strains were found to be sufficiently below the 1% and 2% limits, respectively. Therefore, we conclude that containment shell integrity is not compromised.

IV.2 Detonations under top of dome (SC-2)

For SC-2, 1-D simulations were not considered useful to conduct due to lack of symmetry, and the many insights already gleaned from earlier work reported above. Results of pressurization for SC-2 (where only the lean mixture detonation is examined) are also shown in Fig. 4. Compared with SC-1, significantly larger (i.e., 600 kPa vs. 225 kPa) pressure levels are evaluated under the top region of the steel dome. Due to complex shock wave interactions, it was found that the actual pressure level right under the top of the dome (midplane) is somewhat lower than at adjacent points. However, the pulse lasts for a longer duration and hence, may be in a position to cause more damage. Relatively minor loads are evaluated on the reactor floor level above the pool surface. The structural analysis results indicated a maximum vertical displacement of 250 mm (~10 in.) for the steel shell. Membrane and surface strains were found to be sufficiently below the 1% and 2% limits, respectively. Therefore, containment shell integrity is not compromised even for this case.

V. SUMMARY & CONCLUSIONS

To summarize, this paper has presented salient aspects of modeling and analysis results for evaluating detonation loads and containment response behavior in selected regions of the ANS containment during hypothetical severe accident conditions. As mentioned earlier, the ANS containment meets USNRC ALWR requirements for avoiding detonations on a containment-wide basis by a wide margin. Stratified configurations were studied based upon following the intent of ACRS recommendations to evaluate detonations above the pool surface and also below the top of the containment dome. Major tools employed were the CTH and CET89 codes. The modeling and analysis work was done systematically. First, insights were derived on required degree of nodalization, inaccuracies associated with knowledge of detonation velocities and pre- and post- burn mixture representation, and detonation front modeling from 1-D simulations. Nodalization was seen to have a pronounced influence with relatively minor dependence on other parameters. Volumetric versus point spark initiation of detonation does give significant differences in predicted peak pressures, however, the resulting impulse levels are approximately the same. Use of lead versus steel for the containment boundary model significantly reduces the computational time for 2-D simulations with no noticeable difference in pressure time-position history for the atmosphere regions of the containment. Significant spatial effects were possible to capture with 2-D simulations which was not possible from 1-D simulations. From 2-D simulations, dynamic pressure loadings were generated for key locations and used for evaluating structural response behavior for which a finite-element model was developed using ANSYS. Even though the static design pressure limit is exceeded for short durations of time, dynamic structural analysis indicated that, for the range of conditions analyzed in the two critical dome regions the ANS containment would be able to withstand detonation loads without failure. Detonation loadings are most severe for stoichiometric mixtures, followed by mixtures at the hydrogen lean and rich limits, respectively.

Acknowledgments
Much useful insights were provided by Kevin Boyack and Doug Stamps of Sandia National Laboratory for initiating model development. Also acknowledged are D. Krause and G. Kowal of GC who provided consultation during problem formulation. The support and guidance provided for this work by R. M. Harrington, D. L. Moses and C. D. West of the ANS Project office are gratefully acknowledged.

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