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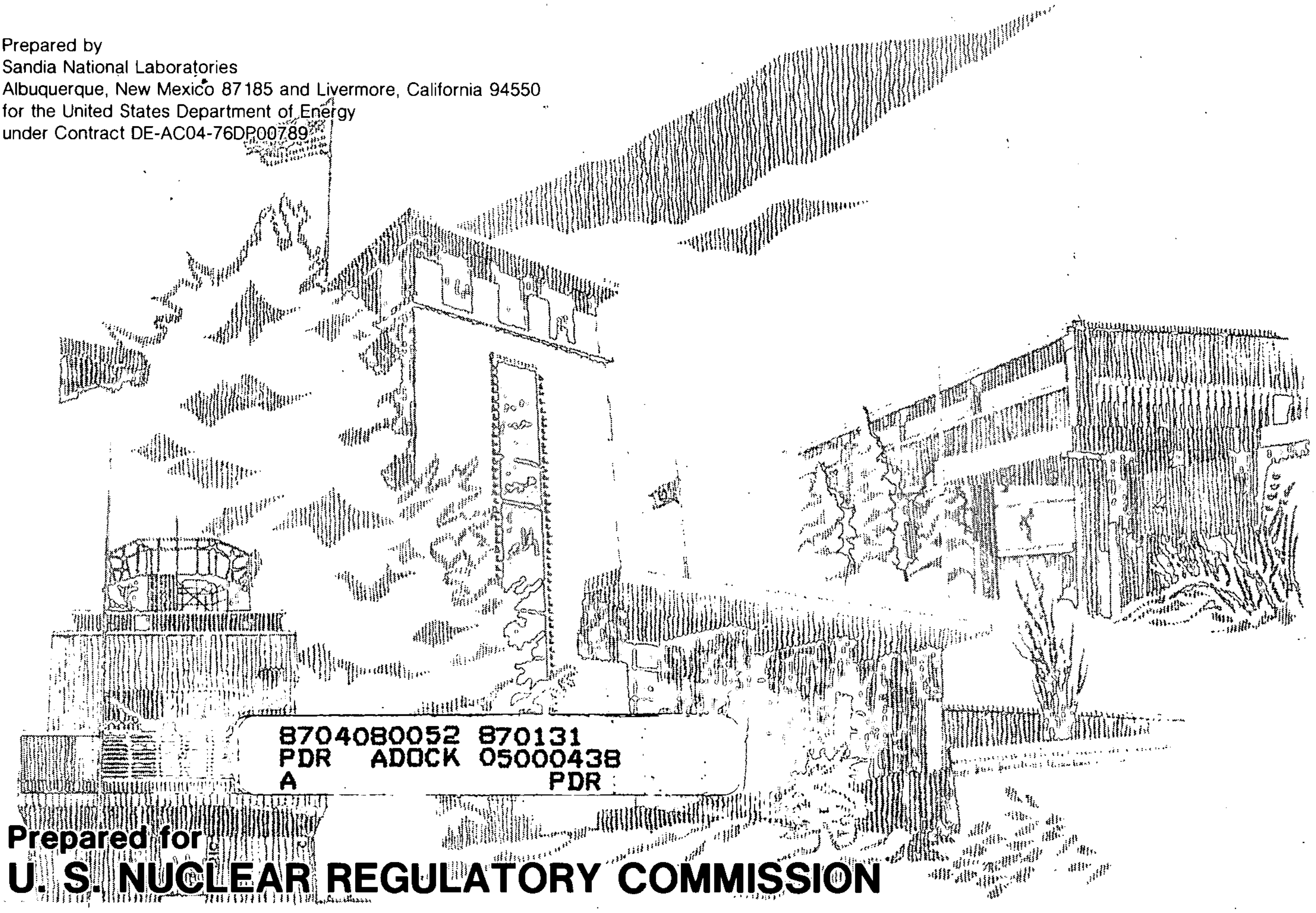

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THE POSSIBILITY OF LOCAL DETONATIONS DURING DEGRADED-CORE ACCIDENTS IN THE BELLEFONTE NUCLEAR POWER PLANT

M. P. Sherman and M. Berman

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ABSTRACT

It is possible to objectively determine whether a detonation can propagate in a given geometry (volume shape and size, obstacle configuration, degree of confinement) for a given mixture composition (concentrations of hydrogen, air and steam); this is done by conservatively equating the detonation propagation criteria with the criteria for transition from deflagration to detonation. This paper attempts to reduce the degree of conservatism in this procedure by constructing estimates of the probability of transition to detonation based on subjective extrapolations of empirical data. A methodology is introduced which qualitatively ranks mixtures and geometries according to the degree to which they are conducive to transition to detonation. The methodology is then applied to analyzing the potential for local detonations in the Bellefonte reactor containment for a variety of accident scenarios. Based on code-calculated rates and quantities of hydrogen generation and calculated rates of transport and mixing, this methodology indicated a low potential for detonation except for one volume in a few cases.

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THE POSSIBILITY OF LOCAL DETONATIONS DURING DEGRADED-CORE ACCIDENTS IN THE BELLEFONTE NUCLEAR POWER PLANT

EXECUTIVE SUMMARY

This study examines the possibility of obtaining a detonation during the course of a degraded-core accident in a large dry containment, the Bellefonte nuclear power plant. To perform the study, we used research results on the transition of deflagrations (flames) to detonations obtained in the last few years. Extrapolations of limited sets of experimental data were made to obtain a new qualitative methodology. Because the methodology used is new and of uncertain validity, the report contains considerable background material on detonations and on the method. The possibility of obtaining a detonation directly from an energetic source, such as an electric arc, or from violent turbulent mixing from a hot jet, was discussed, but not evaluated.

During the course of a severe accident in a nuclear reactor power plant, hydrogen can be generated from the oxidation of the zirconium cladding on the fuel elements by hot steam, and by other mechanisms. A major concern is that the pressure generated by the combustion of hydrogen in the containment will cause a breach in containment and a release of radioactivity. For an ordinary flame, a deflagration, the combustion is comparatively slow (several seconds), the pressure spatially uniform in containment and bounded by the adiabatic isochoric (constant volume) complete combustion (AICC) pressure. The loads on containment would be quasistatic, i.e., equal to those caused by a constant pressure of equal magnitude. The combustion of a lean, approximately 8%, hydrogen-air mixture at Three Mile Island II was such a deflagration with quasistatic loads. More dangerous mixtures are those closer to 30% hydrogen in dry air, i.e., nearer to a stoichiometric mixture with two hydrogen molecules for each oxygen molecule ($2H_2 + O_2 \rightarrow 2H_2O$).

If the hydrogen-air mixture is more energetic than the lean TMI-2 mixture, a very fast-moving deflagration or even a detonation can occur. A detonation is a combustion front moving at supersonic speed; a deflagration is subsonic. For either a very rapidly moving deflagration or a detonation, the pressure in containment will no longer be spatially uniform. The peak pressure can be higher than the AICC pressure. The loads on containment will include dynamic loads in addition to the quasistatic loads. The danger of containment breach is increased.

The method used to evaluate the possibility of deflagration-to-detonation transition (DDT) is based on existing experimental evidence and computer modelling that show the great importance of the mixture reactivity and the flame acceleration potential of the confining geometry. Obstacles in the flow path of the unburned gases greatly increase the flame speed by creating vortices which lengthen the flame front and by generating turbulence which increases the local burning rate. Hydrogen-air and hydrogen-air-steam mixtures are grouped into five "mixture classes" based on experience with lean hydrogen-air mixtures and use of a quantity called the "detonation cell width" to estimate the comparative reactivity of hydrogen-air-steam mixtures, and other mixtures for which there are no DDT data. The flame-accelerating potential of relevant volumes in the containment is grouped into five "geometric classes." The potential for DDT, from "DDT is highly likely" to "DDT is highly unlikely to impossible" is estimated for each combination of mixture class and geometric class.

Based on judgments from a plant visit to Bellefonte, the relevant volumes in the plant were given values of geometric class. Using results from the HECTR control volume computer code for a small break LOCA accident and a TMLB′ accident, and a computer program which estimates detonation cell width, the mixtures in these compartments at critical times were assigned mixture classes. The results showed that, in most of the cases, "DDT is possible but unlikely" or "DDT is highly unlikely to impossible." However, for one volume, a tunnel between the steam generators, there are three cases in which the result is "DDT may occur." The mixtures in adjacent compartments are not sufficiently sensitive to propagate a detonation.

The presence of steam tended to considerably reduce the reactivity of the mixtures. As the steam condenses, the mixture class would change to higher levels of sensitivity. Hence, accurate modelling of condensation rates is an important input for this methodology.

I. INTRODUCTION

The purpose of this report is to provide guidance to the NRC concerning the possibility of local detonations during degraded-core accidents in large, dry PWR containments. In particular, this study considers the possibility of deflagration-to-detonation transition (DDT) of hydrogen-air and hydrogen-air-steam mixtures, where the hydrogen is generated mainly by the oxidation of zirconium cladding by steam in the Bellefonte nuclear power plant.

To evaluate the potential for local detonations, the analyst needs to know:

1. The composition of combustible mixtures as a function of space and time (primarily molar fractions of hydrogen, air, steam, and possibly carbon monoxide), and the thermodynamic state (temperature, pressure, etc.);
2. Detonability limits for the given composition, scale and geometry under consideration;
3. The type and strength of potential ignition sources; and
4. The potential for transition to detonation under the above conditions.

Models exist to calculate, with varying degrees of accuracy, the transport and mixing of hydrogen during postulated accident sequences. In principle, the potential ignition sources could be located and defined. As the following discussion will show, empirical relations exist to extrapolate detonability limits determined in small-scale laboratory tests to the limits that might be expected in complex, large-scale environments. However, there are no validated computer models for any of the possible modes of transition to detonation. Predictions of the occurrence of DDT in a given detonable mixture for any geometry, scale, and ignition source are still very uncertain. Large extrapolations from laboratory experiments are required, as well as subjective judgments on the part of the analyst.

In evaluating the risk due to local detonations, a conservative approach is readily available. A regulator can assume that local or global detonations may occur if the mixture falls within the detonability limits for the specified scale and geometry. The accuracy of this assumption depends on the validity of the accident-analysis codes used to model gas transport and mixing, and the validity of the detonation codes used to extrapolate the laboratory results on detonation propagation. The purpose of this report is to explore the possibility of employing a less conservative approach by estimating the potential for a particular form of DDT that involves transition of a weak deflagration to a detonation by means of turbulence-induced auto-acceleration of the flame.

A numerical probability cannot and should not be assigned to this type of DDT for two reasons. First, a validated model which could be probabilistically sampled does not exist. Second, the data base which exists is very sparse, and is limited to a small number of geometries and obstacle configurations. This type of DDT has been observed in some industrial accidents and in a few experiments, both accidentally and intentionally. The occurrences have indicated a high degree of unpredictability. Specific geometric details, local instabilities, random shock focussing, and even resonances, all lead to transitions that are difficult or impossible to forecast.

This report is intended to distill some of our knowledge and intuition into a framework that can assist the NRC in making decisions. Our guidance should be treated as qualitative. It would be an abuse to assign numerical values to the classifications described in Section III. For example, there is no basis whatever for equating the word 'unlikely' with a probability of 0.3, 0.1, 0.00001, or any other number. We do not approve of, or sanction any future use of this work which involves the conversion of the engineering judgment described in this memo into numerical values.

The main source of information on DDT used in the study was obtained from experimental results in the FLAME facility at Sandia National Laboratories. This facility has been sponsored by the NRC to investigate hydrogen combustion phenomena relevant to nuclear reactor safety. For hydrogen-air-steam mixtures direct experimental results on transition are not yet available. Experiments on DDT in ternary mixtures of hydrogen-air-steam are planned at Battelle Frankfurt in the near future. We will make use of the work on detonability of these mixtures carried out in the Heated Detonation Tube facility at Sandia, also sponsored by the NRC. Information on the energy required for direct initiation of hydrogen-air mixtures was obtained from studies in the U. K., Canada, and Sandia. In view of the subjective nature of this work and the remaining uncertainties, we feel it necessary to carefully explain the approach used in this study. The following discussion will therefore be divided into two parts. The first part will present general background and explain the approach; the second part will present the calculations and results for the Bellefonte plant.

II. BACKGROUND ON DETONATION RESEARCH

1. Chapman-Jouguet Theory

Detonations are combustion waves travelling at supersonic speeds relative to the unburned gas ahead of the wave [1]. The chemical reactions in detonations are caused by shock wave compression of the unburned gases. In contrast, deflagrations are subsonic waves. The rapid chemical reactions in deflagrations are caused by heat conduction and free radical diffusion from the hot burned gases. As early as 1900, a theory developed by Chapman, Jouguet, and others, was able to predict detonation speed and the pressure, temperature, etc., just behind the detonation wave. The C-J theory uses only thermodynamic data of the species considered. It assumes the detonation can be treated as a discontinuity. After using the conservation equations, one additional assumption is required to obtain a unique solution. It is assumed that the flow just behind the detonation front is sonic. Experimental evidence over many years, including recent work in the HDT [11], shows that the C-J theory predicts detonation speed to within ±2% in tubes large enough to minimize boundary layer effects. The pressure rise due to detonations is also reasonably well predicted.

G. I. Taylor [2] and others have developed a successful theory based on similarity solutions of the flow field behind simple one-dimensional detonations in planar, cylindrical and spherical geometries. Handling more complex geometries requires the use of computer programs such as CSQ [3] or Random-Choice method [4]. Within certain limitations, the C-J theory combined with wave-handling gas dynamics programs can predict detonation loads given the location of the initiation of the detonation.

However, the C-J theory does not predict the "dynamic parameters" of detonations, compositional limits for propagation of detonations, the energy required to directly initiate a detonation, or describe the process of DDT. In fact, much of the experimental work done on "detonation limits" and "run-up distance" for transition to detonation during these years was misleading [5]. It is only with the development of the understanding of the transverse wave structure of detonations with Mach triple-point intersections that it has become possible to develop guidelines on the compositional limits for detonation propagation.

2. Zel'dovich, Von Neumann, Döring Theory

In the 1940s Zel'dovich, Von Neumann, and Döring (ZND) developed a theory of detonation structure in which the detonation was considered as a planar front with a chemically frozen shock wave followed by a chemical reaction zone which asymptotically led to Chapman-Jouguet conditions of temperature, pressure and composition. The development of digital computers and increase in knowledge of chemical kinetic reaction rates led to the construction of numerical models of ZND shock structure [6,7]. Such models are still useful today even though we know the ZND model is not correct. Correlations of the dynamic parameters, such as the "critical tube diameter" (the smallest diameter tube in which a detonation can propagate from the tube into open space), with ZND-computed reaction-zone length have ranged from fairly good to excellent. The correlations relate a minimum geometric size to the length of the chemical reaction zone. Highly reactive mixtures have small reaction zones and vice versa. All reference to theoretical calculations of detonation cell size will use calculations based on the latest version of Shepherd's ZND model [7], carried out by Tieszen and Stamps [11].

3. Unsteady Cellular Model of Detonations

It was discovered in the late 1950s that the detonation structure was not planar, but was composed of an unsteady cellular front consisting of transverse shock waves, reflected shock waves and Mach-stem shock waves meeting at Mach triple points [1]. In a detonation wave the transverse waves are continually decaying until adjacent triple points collide and rejuvenate the waves. The locus of Mach triple points can be plotted by either or both of two techniques. The locus leaves a track on a sooted surface, and the higher luminosity of the gas at these points can be photographed. A diamond-shaped pattern is generated by the locus of Mach triple points. The transverse width of these diamonds is called the detonation cell width, λ. It has been correlated to chemical reaction length in the ZND models with surprising success. We use the empirical linear relation $\lambda = 22 \times$ ZND chemical reaction length.

4. Detonation Limits

"Detonation limits" are the limiting mole fractions of fuel, air and diluents in a combustible mixture at a given temperature and pressure at which detonations can propagate. It was discovered that detonation limits are wider in large diameter tubes than in small ones. Hence, pure "detonation limits" which are a physico-chemical property of the mixture, do not exist, except possibly in the limit of infinitely large geometries. On the basis of experimental evidence with many detonable mixtures at a variety of initial pressures, correlations were developed between the "detonation limits" and a given geometry by the relation for possible propagation:

$$L/\lambda > C \qquad (1)$$

where L is a characteristic geometric length for the geometry, e.g. diameter of a round tube, λ the detonation cell width, and C a constant for that geometry. Values of C for some geometries are shown in Figure 1. If the above relations are correct, then with a knowledge of the detonation cell width and the various correlations, the problem of "detonation limits" is solved. Note that the above theory gives "detonation limits" that are wider for large geometric scales than small, and that are dependent on the mixture temperature and pressure as well as composition. However, it has been found that as one takes detonable fuel-air mixtures further from stoichiometric, either in the lean or rich direction, the detonation cell width increases rapidly. Consequently, for sufficiently large scales, the compositional limits for propagation of detonation change slowly with increasing scale.

The above simple theory may not be the entire picture. There is some evidence that although it generally gives the correct trends, it may not be completely accurate. There are three possible explanations. First, the measurement of detonation cell width is not very accurate. The diamond-shaped patterns caused by hydrogen-air and hydrogen-air-steam mixture detonations are somewhat irregular. Picking out the dominant cell width is something of an art. Work is being carried out to use image-processing methods to remove the subjectivity. A second possibility is that the degree of cell irregularity may be a second variable controlling detonation limits. In this view for a given mixture, detonation cell width determines minimum geometric size for detonation propagation to about a factor of two; the second variable, cell irregularity or something analogous, is required to more accurately determine the actual geometric size. A third possibility is that the main deviations from the simple theory are due to the persistence of detonations to propagate beyond the limiting compositions for stable propagation. In this view, the decay of detonations beyond the limiting mixtures is too slow to have been seen. However, these unstable detonations should be stopped by obstacles in the flow path, and should not be formed by DDT. For this report we will use the simple theory given by Eq. 1.

5. Detonation Cell Width Values

Detonation cell widths for hydrogen-air mixtures at one atmosphere pressure and 20°C have been measured over a range from 13.5% to 70% hydrogen in several different detonation tubes. Measurements of hydrogen-air mixtures at temperatures up to 100°C have been made in the Heated Detonation Tube (HDT). Finally, measurements of hydrogen-air-steam mixtures at temperatures up to 100°C have been made in the HDT. For the hydrogen-air-steam

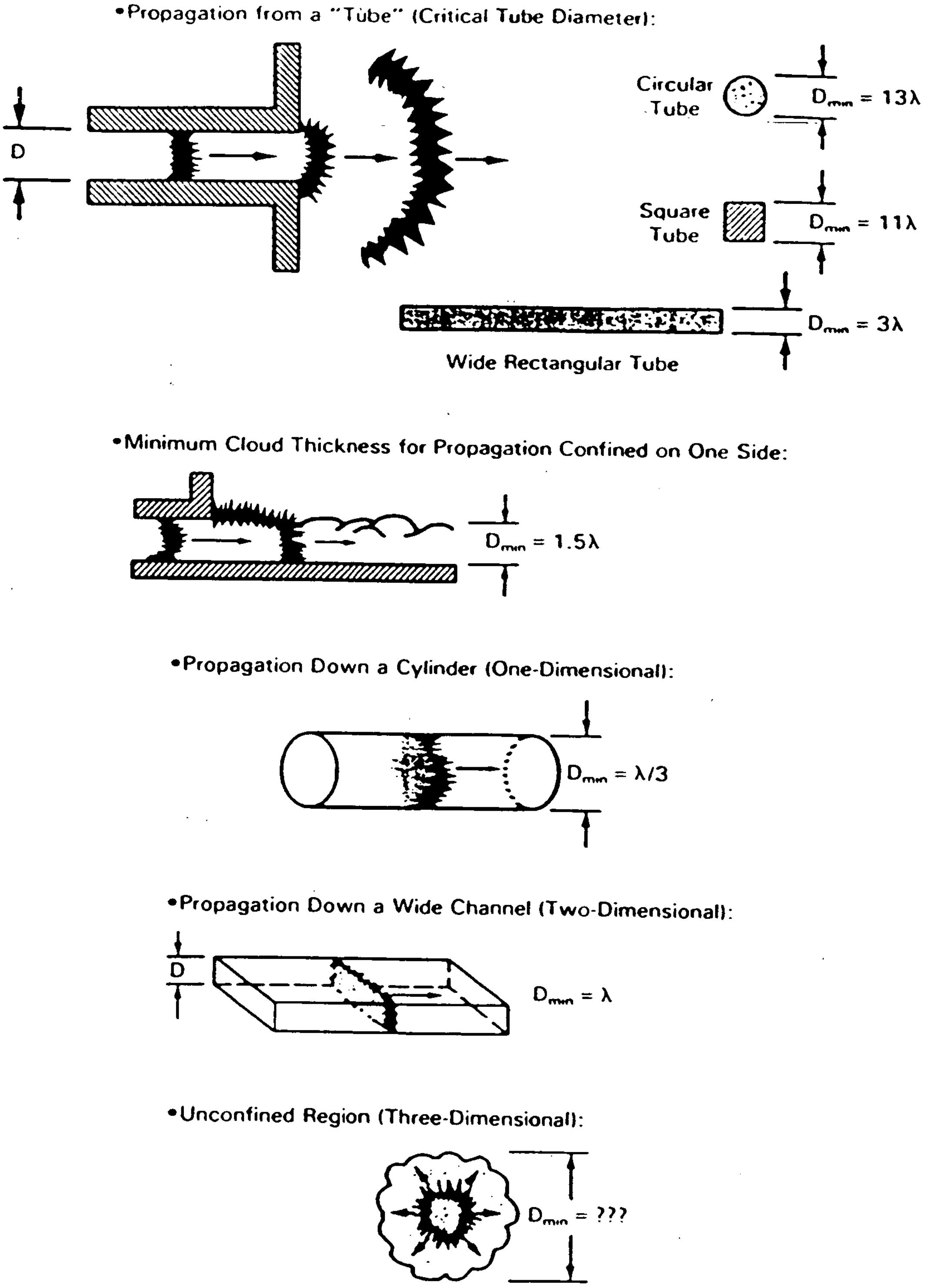


Figure 1. Schematic Illustration of the Developing Empirical Understanding of the Effects of Geometry and Scale on Detonation Propagation.

mixtures, the detonation cell width is a function of four independent variables. We take these to be:

1. Equivalence ratio
2. Steam mole fraction
3. Temperature
4. Air density

The equivalence ratio is the ratio of the fuel to oxidizer mole fraction divided by the same ratio for stoichiometric conditions. It is unity at stoichiometric conditions, above one for rich mixtures, and below one for lean. We selected it as a variable instead of hydrogen mole fraction because it is invariant to the addition of steam diluent. Hence for our mixtures, the equivalence ratio is the hydrogen mole fraction divided by twice the oxygen mole fraction. Air density was selected as a variable instead of pressure or total mixture density, because in a reactor containment, the average air density is not altered by the addition of gases or changes in temperature.

With the experimental data we have and the Shepherd ZND model [7] for interpolation and extrapolation of these data, the detonation cell width for hydrogen-air-steam mixtures is known to approximately a factor of two. We will use it in our analysis.

6. Mechanisms for Producing Detonations

A mixture of combustible gases within the "detonability limits" can be induced to detonate by making the rate of chemical reaction locally fast enough to initiate and sustain a leading shock wave. Reaction rates can be increased by increasing gas pressure, temperature, and density, or free-radical density. Mechanisms for increasing these rates include: "strong" ignition sources (high energy, high power, large size); turbulence generated by obstacles, rough walls, fans, exhaust jets, rupturing vessels, etc.; "large, hot" jets; chemical effects/sensitizers (increasing the concentration of free-radicals); energetic chemical or physical events (e.g., steam explosions or high-pressure dispersal of hot aerosols); shock waves; photochemical effects; etc.

It has been customary to distinguish two classes of detonation mechanisms: direct initiation by high explosives, and DDT resulting from a long runup in a confined tube. These two classes were convenient to distinguish between two types of laboratory experiments used to investigate detonations. However, we believe that this distinction is overly simplistic, and can be very misleading when evaluating the possibility of DDT in an industrial environment. The previous paragraph illustrates many situations in which DDT has been actually observed. The majority of accidental DDT events have not been classifiable into either of the above customary classes. In fact, analyses of the accident conditions often imply that a detonation could not have occurred (even though it did occur) because the necessary conditions for either of the above two classes were absent; i.e., there was insufficient confinement, run-up distance was too short, no high explosives were involved, etc.

An accurate assessment of the potential for DDT entails knowledge of gas composition, scale, geometry, configuration (presence of obstacles, fans, etc.), preignition flow characteristics, and all possible ignition mechanisms. This report primarily addresses the potential for a deflagration to undergo DDT due to auto-induced flame acceleration. However, we will briefly discuss some of the other mechanisms for DDT to provide additional insight and to resolve some common misunderstandings.

6.1 Direct Initiation

Figure 2 shows the critical initiation energy required to directly initiate a detonation in a wholly unconfined spherical geometry [8]. (Note that one gram of tetryl is equivalent to about 4.6 kJ.) The experiments involved the firing of a spherical charge of high explosive in a large plastic bag containing various hydrogen-air mixtures. If the charge mass is too small, the blast wave from the explosion separates from the burning hydrogen and decays, leaving only a continuing deflagration. If the high explosive is sufficiently strong, the blast wave couples with the hydrogen combustion forming a self-sustaining detonation wave.

Analysts must be very careful in using these curves. There is an obvious tendency to equate large critical charges with the impossibility of DDT in some insensitive mixtures. However, one must recognize the extreme importance of other factors on DDT, including scale, obstacles, degree of confinement, etc. As an example, an extrapolation of the data in Figure 2 implies that the critical charge mass necessary to detonate a mixture of 13.5% hydrogen in air is about 10,000 g (46,000 kJ). In reality, a detonation of this mixture was initiated in the Heated Detonation Tube with a charge of only 80 g! The huge difference is due to geometry (planar vs spherical) and degree of confinement.

In addition to the environmental effects, the specific energy, specific power, and the characteristic size or shape, and duration of the ignition source influence the potential for DDT. The characteristic size and shape can play a very important role. Benedick [12] was able to initiate a detonation in stoichiometric methane-air using 4 kg of explosive thinly spread over 2 m^2;

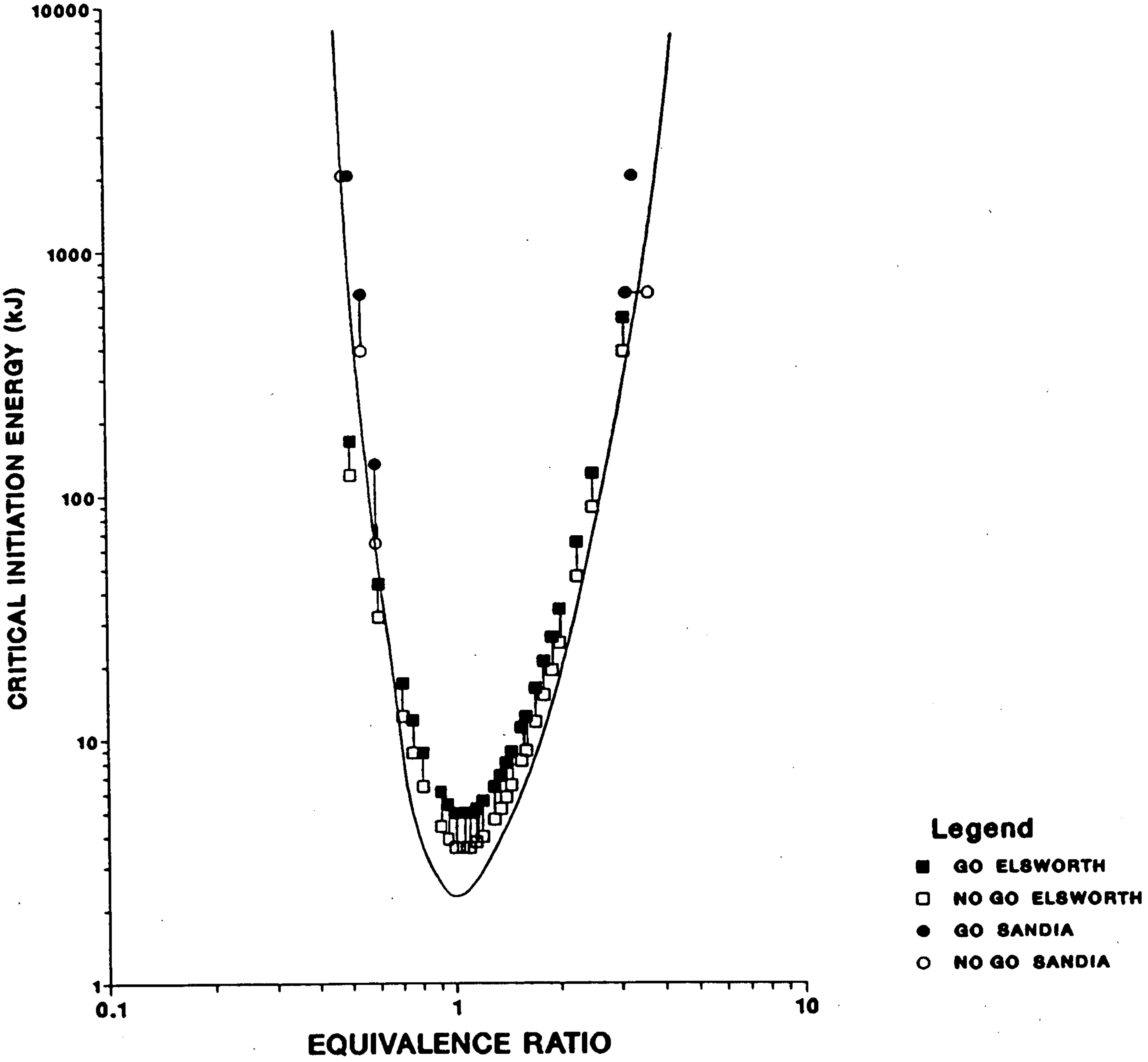


Figure 2. Critical Initiation Energy for Directly Initiating a Detonation in an Unconfined Cloud.

quantities of 22 kg or more are predicted to be required in spherical masses. A similar condition influences the potential of electric sparks to initiate detonations. Matsui and Lee [13] showed that the critical energy (joules/cm) decreased significantly with increasing spark length and increasing electrode surface area.

No analysis of the possibility of direct initiation of detonations has been made in this study. A careful analysis would require the assistance of someone familiar with the high-voltage systems in the plant. The most likely high-energy ignition source would be an electric arc. Given the characteristics of such arcs, experiments would be required to draw reliable conclusions concerning the possibility of directly initiating a detonation.

6.2 Fan-Induced DDT

Pförtner (in Reference 5) conducted experiments in mixtures containing about 40% hydrogen in air (cell width is about 5 cm) where ordinary deflagrations passed through spinning fans. He showed that DDT could be induced a short distance downstream of the fan. The fan had a diameter of 1.25 m. At 225 rpm, DDT occurred 2 m downstream of the fan. DDT did not occur for a rotational speed of 203 rpm. At 225 rpm, the fan tip speed is only about 14.7 m/s; at 203 rpm, it is 13.3 m/s. These are very low velocities compared to the flame velocities observed prior to DDT in most experiments. Similarly, the differences in tip speeds are quite small. It is possible that transition to detonation might depend on a resonance effect involving fan size and speed and the characteristic cell size of the mixture. In any case, a conservative approach would assume that the presence of a fan in the path of a deflagration could result in a rapid DDT under some conditions. Experiments would be required to establish this result quantitatively as a function of fan size, speed, configuration and the sensitivity of the combustible gas mixture.

6.3 Hot-Jet Initiation of Detonations

It has been shown that a hot jet of sufficient strength fired into a detonable gas volume can lead to the initiation of a detonation near the mixing zone between the jet and the surrounding gas [9]. The intense turbulence generated and large burning surface causes the formation of a blast wave near the jet and hence a behavior similar to the direct initiation by high explosives. Hot-jet initiation is intermediate between the almost immediate production of a detonation by a high explosive, and the comparatively slow process in DDT. It has been speculated that the hot-jet mechanism might be important in accidents. There might be a a jet produced by a small area leak from a confined burning volume, such as the gap under a door, or from a fuse box, or by the explosive rupture of a confined burning volume. However, not much is known quantitatively about the jet required or about the potential importance of this mechanism in accidents.

6.4 Deflagration-to-Detonation Transitions by Flame Acceleration

With the development of modern techniques such as laser Schlieren it was possible to observe flame-induced deflagration-to-detonation transition. The first step is the acceleration of the deflagration to high speed. It should be noted that ordinary deflagrations, even turbulent hydrogen-air deflagrations travel at speeds under 100 m/s, usually much less. However, several mechanisms can cause large increases in flame speed. The most common are the generation of vortices and turbulence around obstacles in the flow path of the unburned gases, and fluid mechanical-combustion instabilities. As the deflagration speed increases, shock waves are propagated ahead of the flame. This precompresses the gas and further speeds up the reaction. Finally, due to some local irregularity a small explosion forms and generates a detonation wave.

From a practical point of view, DDT appears to be a two step process, flame acceleration to high speeds, and transition of the fast deflagration to a detonation. One of the strongest promoters of flame acceleration is the presence of obstacles in the flow path. Both experimental evidence and numerical calculations show that the burning surface area is greatly increased by the distorted flow around the obstacles. In addition, the local burning velocity is increased due to increases in turbulence level. Even without obstacles present, combustion-flow instabilities lead to flame acceleration. All the flame acceleration mechanisms, particularly the instabilities, are much more effective at large geometric scale. A comparison of FLAME tests with similar tests in a 1/12th scale model (MINIFLAME), and with other small-scale tests, confirm the faster flame speeds, higher overpressures, and wider range of DDT at large scale. In completely open geometries, tests have shown that stoichiometric hydrogen-air mixtures do not undergo DDT. In FLAME tests with 50% top venting and no obstacles, sensitive mixtures did not undergo DDT. However, tests with obstacles, or tests without obstacles but with lesser degrees of top venting, did undergo DDT.

In FLAME and in smaller-scale tests at McGill University, it has been shown that vigorous flame acceleration can cause the deflagration to accelerate to sonic speed (relative to the burned gas), about 700 m/s for hydrogen-air mixtures. This asymptotic condition is a deflagration at the lower Chapman-Jouguet point relative to the unburned gas just ahead of the combustion wave. According to one-dimensional theory, it is the fastest possible deflagration. Test in channels with obstacles appear to indicate that DDT will then occur if the ratio of the gap between the obstacles to the detonation cell width is larger than about two. Since the geometric sizes in containment are large, this appears to indicate that large flame acceleration can lead to transition to detonation. In our analysis we will consider the flame acceleration potential of the geometries of interest. If the combination exists of sensitive mixture and large-scale geometry of high flame acceleration potential, then we will consider the mixture likely to detonate.

Since our DDT data from flame and other experiments are limited to ambient temperature, atmospheric pressure, initially quiescent mixtures, and without significant steam mole fraction present, it will be necessary to have a means of generalizing DDT experience to be able to predict DDT at elevated temperatures, somewhat elevated pressure, and with steam present. We will assume that DDT scales with detonation cell width as does detonation propagation. There is only a single series of experiments in which this was demonstrated. Pförtner and Schneider [14] scaled-up the previous experiments of Schildknecht, et al. [15] by a factor of three. For corresponding tests, Pförtner and Schneider observed a limit of DDT when their mixture had a detonation cell width three times as large as in the tests of Schildknecht, et al. This gives some experimental support to a basic assumption of our analysis, combustible mixtures having the same detonation cell width are equally likely to undergo DDT when deflagrating in the same geometry.

As discussed in Reference 5, turbulence effects are capable of either enhancing or reducing the intensity of combustion. If sufficiently strong, a detonation or deflagration could conceivably be quenched, because of the rapid addition of cold, unburned gas. Similarly, a smaller amount of turbulence could increase the burning rate enough to cause a transition from deflagration to detonation. Experiments with fans [14] have shown that even mildly turbulent gas motion can sometimes induce DDT. It is possible that high gas velocities and turbulent mixing will occur during some reactor accidents in the vicinity of the primary system break or stuck-open valve. Although we recognize the potential for DDT induced by turbulent jets, we have not included this effect in our analyses because we have no quantitative experimental data.

7. Summary of the Problem

The problem of determining the safety implications of a hydrogen detonation in containment can be divided into the following questions:

1. For given geometries, what mixtures can propagate a detonation?
2. Will such mixtures be formed in the course of a hypothetical reactor accident?
3. If ignited, will such mixtures undergo DDT or other initiation mechanism?
4. What loads will a detonation cause?
5. What damage will detonation loads cause?

The fourth and fifth questions extend beyond the charter of this study.

In our formalism, the first question involves estimating the detonation cell width of the mixtures of interest, and the geometric sizes of the compartments of interest. The answer to question one is understood to fair accuracy.

The answer to the second question comes from the results of accident-analysis codes such as HECTR and HMS. The authors have used results from the HECTR control-volume code run by A. Peterson and D. King [10], and the HMS finite-difference code run by J. Travis [16]. Control-volume codes such as HECTR are subject to certain limitations. They can not correctly model turbulent plume behavior and may, in some cases, overestimate the speed and degree of hydrogen mixing with the containment atmosphere. Finite-difference codes in principal are less subject to this objection, but because of computer limitations, must use very coarse nodalization. Consequently, the authors wish to remind the reader that our analysis may be limited by the accuracy of the information used to answer question 2.

The answer to question 3, the DDT problem, is the primary contribution of this study. First, given mixtures were graded on their sensitivity. For hydrogen-air mixtures this can be based on experimental results for transition. For hydrogen-air-steam mixtures we make the assumption that such a ternary mixture is as sensitive as a corresponding binary hydrogen-air mixture of the same detonation cell width. This is equivalent to assuming the sensitivity to flame acceleration is proportional to the detonation sensitivity.

Jaung, Berlad and Pratt [17] also investigated the sensitivity of potentially detonable mixtures in containment by considering the chemical reaction length in a ZND-type model. They considered a detonation as possible if the length was below a critical value. Their chemical length is related to the detonation cell width. However, they did not consider the flame-acceleration potential of various geometries in containment, nor use the ratio of chemical length to characteristic geometric length as a detonation propagation criterion.

Second, given geometries were qualitatively graded on their flame acceleration potential. The presence of obstacles such as pipes, wiring, cabinets, pumps, etc., was a main factor. The type of confinement was the second parameter. Scale is important, but all the volumes of interest are large. The effects of these factors are semiquantitatively known from the limited experimental base. For this analysis we estimated the quantitative effects of the parameters to come up with a ranking of flame acceleration potential. Note also that we have non-conservatively neglected the effects of preignition gas motion and turbulence, because of the absence of appropriate experimental data.

III. THE FORMALISM FOR ESTIMATING DDT

1. Grading the DDT Sensitivity of Mixtures

We qualitatively define the following classification scheme for lean hydrogen-air mixtures at ambient pressure and temperatures. The extrapolation of the classification scheme to hydrogen-air-steam mixtures, elevated temperatures, etc., can be approximated by detonation cell width equivalence as previously discussed.

Table 1.

Classification of Hydrogen-Air Mixtures
At 20°C and 1 atm Pressure

Mixture Class	Mole Fraction %	Equiv. Ratio	Cell Width mm	Mole Fraction %	Equiv. Ratio
1	24 -30	.75-1.0	20-15	38-30	1.5-1
2	21 -24	.63- .75	40-20	48-38	2.2-1.5
3	15 -21	.42- .63	320-40	63-48	4.1-2.2
4	13.5-15	.37- .42	1200-320	70-63	5.6-4.1
5	<13.5	<.37	no data	no data	>5.6

The mole fractions and equivalence ratios in Table 1 are shown for dry hydrogen-air mixtures. For mixtures that include steam, experimental data and code calculations are used to calculate the corresponding cell widths. Figure 3 shows the dependence of cell width on hydrogen and steam concentrations. Hence, the mixture class in Table 1 corresponds to cell widths; the equivalence ratios/mole fractions shown are illustrations for the dry case.

Class 1 mixtures are extremely detonable. They are very likely to undergo DDT in most geometries of interest. Class 2 mixtures are slightly less likely to detonate. Class 3 mixtures have been observed to undergo transition in geometries which favor flame acceleration. Detonations have been propagated through class 4 mixtures, but to date, DDT has not been observed for a hydrogen concentration less than 15%. Class 5 mixtures are unlikely to undergo DDT, although a detonation has been propagated in a 13.5% H_2 in air mixture at STP [5,18].

2. Classification of Flame Acceleration Potential of Geometries

Geometric Class 1. Large geometries with obstacles in the path of the expanding unburned gases. Partial confinement favors gas expansion past the obstacles. A large tube with numerous obstacles, and with ignition going from a closed end to an open end is an example. Class 1 geometries are the most favorable to large flame acceleration.

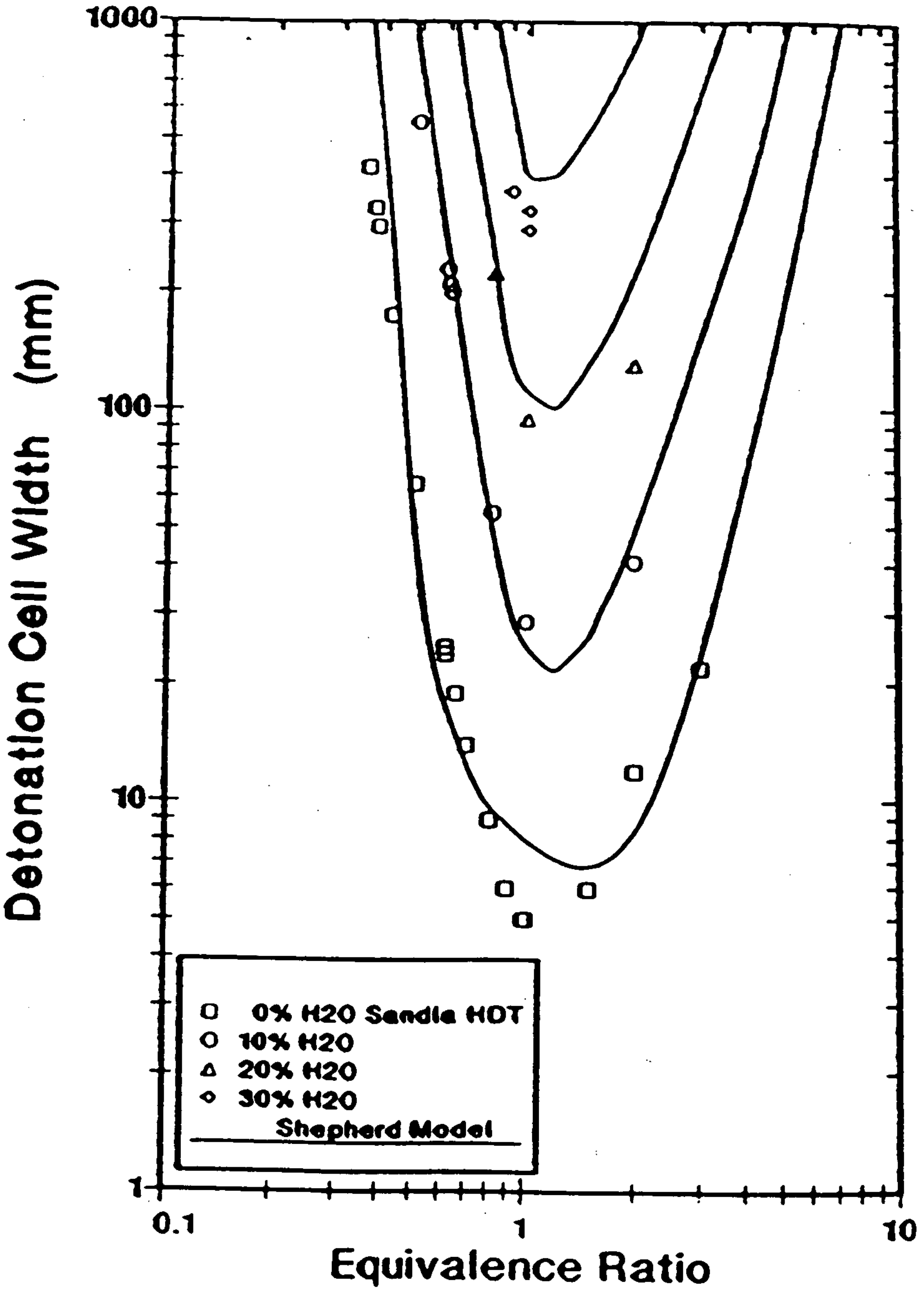


Figure 3. Detonation Cell Width vs. Equivalence Ratio for Various Concentrations of Added Steam.

<u>Geometric Class 2</u>. Geometries similar to class 1 but with some feature which hinders flame acceleration. Examples would be a tube open on both ends or large amounts of transverse venting.

<u>Geometric Class 3</u>. Geometries that yield moderate flame acceleration but are neutral to DDT. Examples are large tubes without obstacles, small tubes (several inch diameter) with obstacles.

<u>Geometric Class 4</u>. Geometries unfavorable to flame acceleration. Examples are large volumes with hardly any obstacles and large amounts of venting transverse to the flame path, or small volumes without obstacles. DDT will not usually occur in a class 4 geometry.

<u>Geometric Class 5</u>. Geometries so unfavorable to flame acceleration that not even large volumes of stoichiometric hydrogen-air mixtures are likely to detonate. The only examples are totally unconfined geometry at large scale, or a small spherical geometry without obstacles and central ignition.

3. Classification of the Probability of DDT

<u>Result Class 1</u>. DDT is highly likely.

<u>Result Class 2</u>. DDT is likely.

<u>Result Class 3</u>. DDT may occur.

<u>Result Class 4</u>. DDT is possible but unlikely.

<u>Result Class 5</u>. DDT is highly unlikely to impossible.

4. Results Table

Table 2.

Matrix of Results

Results →		Highly Likely	Likely	May Occur	Unlikely	Highly Unlikely
Mixture Class →		1	2	3	4	5
Geometric Class ↓						
Very Favorable	1	1	1	2	3	4
Favorable	2	1	2	3	4	5
Neutral	3	2	3	3	4	5
Unfavorable	4	3	4	4	5	5
Very Unfavorable	5	4	5	5	5	5

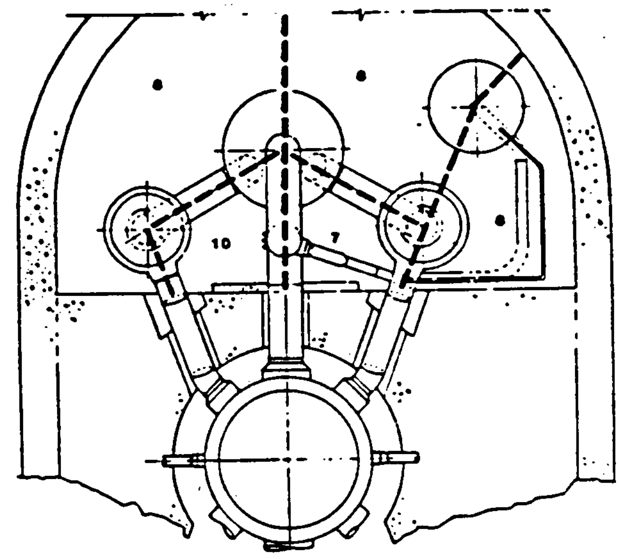
5. The Bellefonte Compartment Classes

A. Peterson and D. King took a trip to Bellefonte, bringing back photographs and technical drawings of the plant. Since the authors have not visited the plant, they are relying on the information supplied to them.

The volumes of interest are shown in Figures 4-6. Volume 1 is the annular region around the reactor pressure vessel. It is bare of obstructions. It is rated as a class 3, neutrally encouraging of flame acceleration. This volume is usually steam inerted.

Volume 5 is at the bottom of the D rings. It is very cluttered with pipes and other obstructions and confined on the bottom and sides. It is considered class 2, encouraging to flame acceleration.

Volumes 6, 8, and 9 are above volume 5 in the outer parts of the D rings. Volumes 7 and 10 are above volume 5 in the inner part of the D rings. All these regions are confined on some sides. All contain some gratings and other obstructions. It was felt that the outer regions, volumes 6, 8, 9 are geometry class 2. Regions 7 and 10 are more open and are between classes 2 and 3.



661A ELEVATION 525.5 - 570

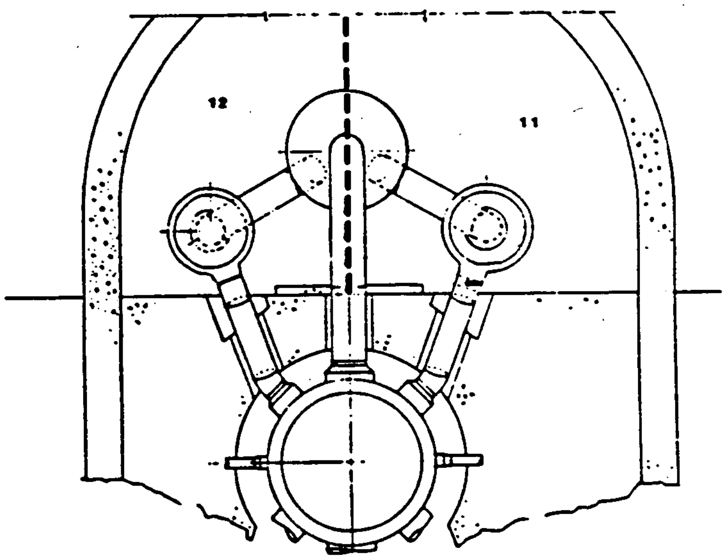


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Figure 4. Plan View of Bellefonte Showing Some of the Volumes Used in the Analysis.

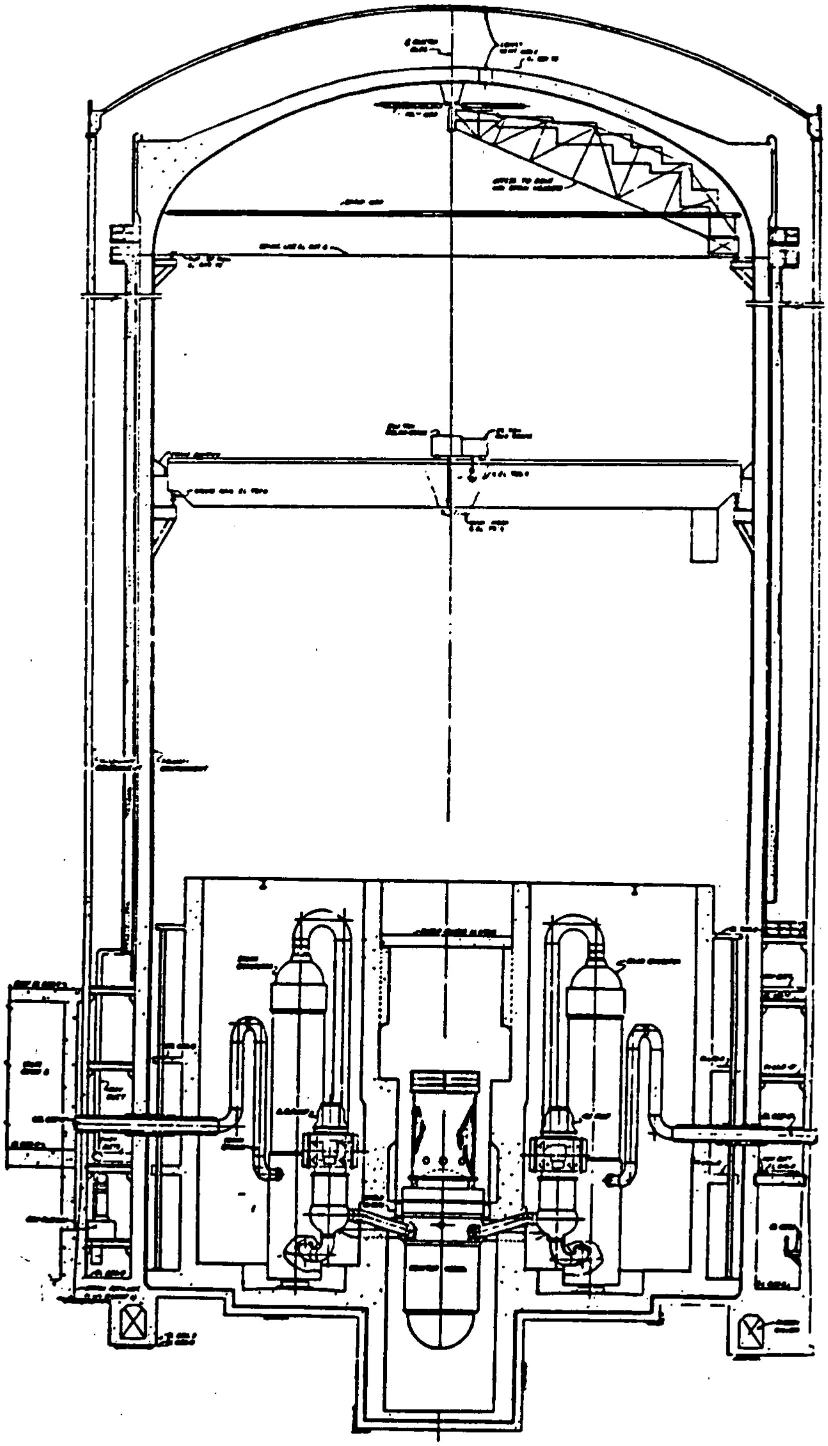
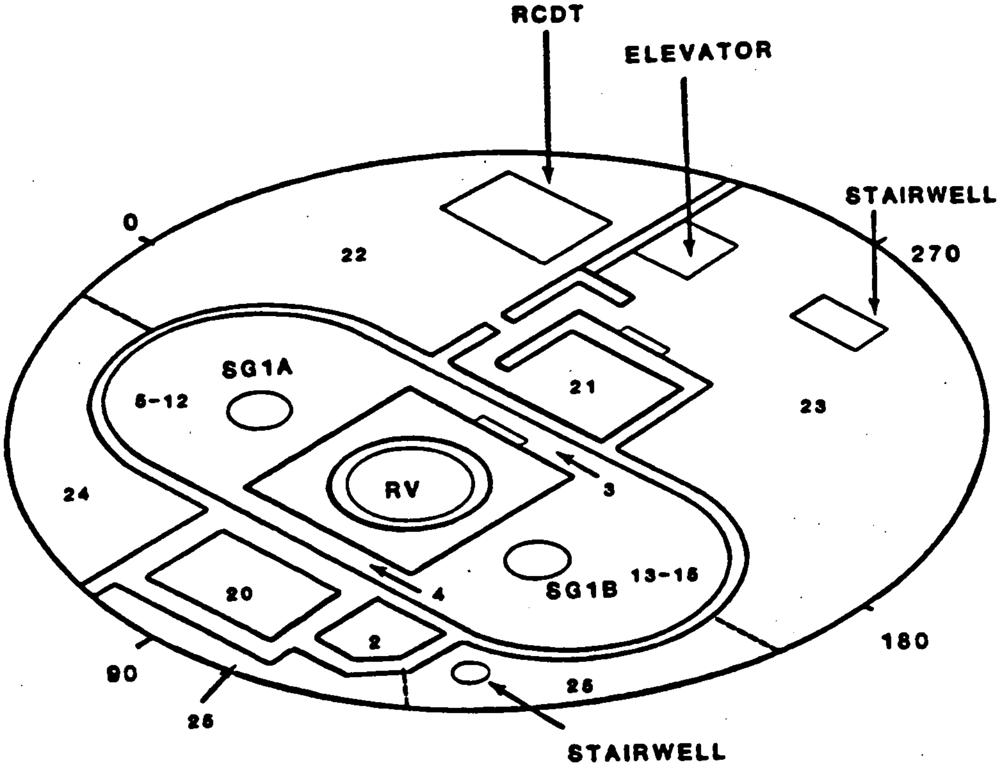


Figure 5. Elevation View of Bellefonte Nuclear Power Plant.



RCDT - REACTOR COOLANT DRAIN TANK

RV - REACTOR VESSEL

SG - STEAM GENERATOR

Figure 6. Cross-Section at Elevation 622 of Bellefonte Showing Some of the Volumes Used in the Analysis.

Volumes 11, 12, and 13 are near the top of the steam generators. Because they are fairly open and free of obstructions, we classify them class 3.

Volumes 19, 20, and 21 are higher up. These are also cluttered regions with some transverse confinement. They are classified as being between class 2 and 3, closer to class 2.

6. Results

Mixture cell sizes, λ, in Tables 3a, 3b and 3c, were computed in Reference 11.

Table 3a

Likelihood of Detonation in Bellefonte - Type 1 Accident

Run	Times,'s	Vol. No.	Geom. Class	Mixture λ,mm	Mixture Class	Result Class
1A	5156	6	2	6690	5	5
	5248	7	2-3	2.8E5	5	5
	5246	8	2	3.7E5	5	5
1B	5248	9	2	8.2E5	5	5
	5155	10	2-3	627	4	4
1C	5155	1	3	----	5	5
	5163	3	2	1120	4	4
	5163	4	2	143	3	3
1D	5156	6	2	1.3E4	5	5
	5248	7	2-3	----	5	5
	5444	8	2	----	5	5
1E	5165	6	2	1.6E4	5	5
	5165	7	2-3	----	5	5
	5248	8	2	----	5	5

---- indicates the detonation cell width is very large

Table 3b

Likelihood of Detonation in Bellefonte - Type 2 Accident

Run	Times,s	Vol. No.	Geom. Class	Mixture λ,mm	Mixture Class	Result Class
2A	6382	7	2-3	----	5	5
	12570	7	2-3	2.3E5	5	5
	6382	9	2	----	5	5
	12570	9	2	1.3E4	5	5
	6382	10	2-3	1.3E4	5	5
	12570	10	2-3	2170	4	4
2B	6330	7	2-3	----	5	5
	12561	7	2-3	3.3E4	5	5
	6330	9	2	----	5	5
	12561	9	2	2.0E4	5	5
	6330	10	2-3	2040	5	5
	12561	10	2-3	453	4	4
2C	6330	4	2	50	2-3	2-3
	12561	4	2	43	2-3	2-3
	6330	5	2	----	5	5
	12561	5	2	4.1E5	5	5
	6330	9	2	----	5	5
	12561	9	2	4.7E3	5	5

Table 3c

Likelihood of Detonation in Bellefonte - Type 3 Accident

Run	Times,s	Vol. No.	Geom. Class	Mixture λ,mm	Mixture Class	Result Class
3A	5163	19	2	2.3E3	5	5
	5163	20	2	----	5	5
	5163	21	2	----	5	5
3B	5164	10	2-3	----	5	5
	5164	11	2	7280	5	5
	5164	12	2	1720	5	5
	5164	13	2	----	5	5
3C	5160	10	2-3	2330	5	5
	5160	11	2	----	5	5
	5160	13	2	4.3E4	5	5
3D	5144	10	2-3	----	5	5
	5144	11	2	2.6E4	5	5
	5152	12	2	2.6E4	5	5
	5160	13	2	6820	5	5
3E	5141	10	2-3	2600	5	5
	5141	11	2	----	5	5
	5141	12	2	----	5	5
	5141	13	2	----	5	5
3F	5192	10	2-3	----	5	5
	5192	11	2	2240	5	5
	5192	12	2	----	5	5

Table 3d

Likelihood of Detonation in Bellefonte - Type 4 Accident

Run	Times,s	Vol. No.	Geom. Class	Mixture λ,mm	Mixture Class	Result Class
4	5567	19	3	4600	5	5
	5567	20	3	----	5	5
	5583	21	3	4.7E5	5	5
4A	5566	19	3	6250	5	5
	5566	20	3	----	5	5
	5566	21	3	----	5	5

Volume number 4, the tunnel between the steam generators, is the only one which contains mixtures in results class between 2 and 3, "DDT may occur," or "DDT likely." The detonation cell width was computed in the adjacent compartments for the cases with results class 2-3 in volume 4. In all cases, the mixtures in these adjacent compartments were mixture class 5. Consequently, a detonation in volume 4 probably would not propagate into adjacent volumes.

IV. CONCLUSIONS

There are no codes capable of quantitatively analyzing the probability of a local detonation for a given set of initial conditions in a complex three-dimensional geometry. Such codes may not be developed for many years, and even then the cost of computer calculations might be prohibitive. However, experiments in various geometries have been conducted, and empirical relations have been developed which link dynamic detonation properties to the prevailing chemical and fluid mechanical conditions. This paper presents a qualitative methodology for estimating the likelihood of transition to detonation as a function of geometry (scale, obstacle configurations, degree of confinement) and chemical sensitivity (concentrations of hydrogen, air and steam).

The methodology discussed here is currently incomplete. We have not attempted to estimate the probability of directly initiating a detonation by a strong ignition source (e.g., a strong spark or a hot jet issuing from a "small" confined or semi-confined region). We have also not attempted to determine the effect of preignition gas turbulence due to jets or fans, or the presence of multiple ignition sources (e.g., deliberate ignitors or hot aerosolized material). These questions have not been addressed because of a lack of appropriate data and analysis, and not because we believe that they are unimportant.

The data upon which the various geometric classes are based, are very sparse. Only a small number of experiments have been conducted to investigate the effects of geometry, obstacle configuration and degree of confinement on the probability of transition to detonation. Hence, caution should be employed when extrapolating these results to untested geometries and obstacle configurations.

The Bellefonte containment was chosen as an example to illustrate the methodology. The set of accidents analyzed dealt only with degraded-core accidents, and not severe accidents involving core melt.

This study should not be considered a definitive work on the possibility of local detonations in the Bellefonte containment. Rather, it is intended to illustrate a qualitative methodology for conducting such an analysis, with a containment type and group of accident scenarios selected as examples of application of the methodology. The assessment of the mixture, geometry and result classes depends strongly on the experience and knowledge of the person making those assessments. Different "assessors" may indeed produce different numerical values of the three classes, and it may be difficult to compare the degree of "expertise" among the various assessors. The most prudent approach would be to treat the predictions of classes very conservatively when making decisions concerning local detonations.

On the basis of the compositions, temperatures, and pressures given in Reference 10, the evaluation of the flame-acceleration potential of the compartments from the photographs, drawings and description by King and Peterson, and the methodology described, the "results classes" were obtained. These indicate detonation by flame-induced DDT is unlikely or impossible for most of the cases considered. Detonation is possible for run 2C, in volume number 4, at two times, 6300 s and 12562 s, and for run 1C in compartment 4. However, such a detonation probably would not be able to propagate into adjacent volumes.

The low sensitivity of most of the mixtures often results from the presence of high steam concentrations. If steam were to condense locally with little mixing, a volume that is a more detonable mixture might result.

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It is possible to objectively determine whether a detonation can propagate in a given geometry (volume shape and size, obstacle configuration, degree of confinement) for a given mixture composition (concentrations of hydrogen, air and steam); this is done by conservatively equating the detonation propagation criteria with the criteria for transition from deflagration to detonation. This paper attempts to reduce the degree of conservatism in this procedure by constructing estimates of the probability of transition to detonation based on subjective extrapolations of empirical data. A methodology is introduced which qualitatively ranks mixtures and geometries according to the degree to which they are conducive to transition to detonation. The methodology is then applied to analyzing the potential for local detonations in the Bellefonte reactor containment for a variety of accident scenarios. Based on code-calculated rates and quantities of hydrogen generation and calculated rates of transport and mixing, this methodology indicated a low potential for detonation except for one volume in a few cases.

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