An Independent Critique of Containment Loads Modeling Used in the Direct Containment Heating (DCH) Issue Resolution Effort*

David C. Williams

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ABSTRACT

The U.S. NRC's program to resolve the DCH issue depends primarily upon the two-cell equilibrium (TCE) and convection-limited containment heating (CLCH) models for estimating containment loads associated with DCH. Evaluations of these models in the present report indicates that they are not adequate for the tasks to which they have been applied. Comparison with CONTAIN code analyses of DCH experiments shows that the TCE and CLCH models omit important heat transfer effects that mitigate DCH; since the models show no consistent conservative bias, omitting important mitigating effects necessarily implies that they omit important augmenting effects. For the Zion IET experiments, processes omitted from the DCH issue resolution models appear to contribute at least 50% of the total DCH energy release. The experimental validation offered for use of these models is examined and found to be unconvincing because the DCH data base for containment pressurization exhibits a simple systematics that can be fit equally well by "models" that are demonstrably inadequate as predictors of DCH loads. Furthermore, the principal DCH issue resolution model (TCE) shows no ability at all to correlate the amounts of hydrogen produced in a DCH event except for a limited subset of experiments which are quite nonprototypic; arguments that have been offered to explain this discrepancy are examined and found to lack merit. The DCH issue resolution models assume that limited temporal coherence between debris dispersal from the cavity and the blowdown of the reactor pressure vessel (RPV) is a very important mitigating effect; however, no experimental evidence for this dependence upon coherence has been offered and some evidence to the contrary has been neglected. Methods used to estimate coherence factors in the experiments are subjective and have been applied inconsistently in a way that increases the apparent agreement between TCE predictions and experimental measurements of containment pressurization. The treatment of combustion of pre-existing hydrogen in the containment seriously understates uncertainties and is probably nonconservative. Other problems with the model include inconsistent and nonconservative definitions of the subcompartment volumes, nonconservative approximations for the atmospheric heat capacity, treatment of iron chemistry based upon an erroneous assumption that the metallic and oxide phases can form an ideal solution with one another, neglect of possible effects of ablated RPV insulation on hydrogen production and combustion, and use of a screening criterion that provides very inadequate margin for modeling uncertainties. The cumulative impact of these deficiencies is such that it is unclear what, if any, conclusions may be safely drawn from the DCH issue resolution work as it stands. More sophisticated modeling efforts and uncertainty assessments are required.

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The preparation of this report was *not* supported by the U.S. Nuclear Regulatory Commission or by the management of the Nuclear Energy Technology Center at Sandia National Laboratories. It was prepared on my own time and only I am responsible for the opinions offered and any errors therein. At the same time, I would be remiss if I did not acknowledge the benefit I have received from extensive discussion of the technical issues involved with numerous colleagues both within Sandia and outside, and some of these colleagues generously consented to review a draft of this document. While I would prefer to explicitly acknowledge some of those who have assisted me in these ways, doing so appears to be unwise at this particular time.

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Author's Preface

This document was prepared to summarize some of the reasons why I believe that the methodology used to calculate direct containment heating (DCH) loads in the U.S. Nuclear Regulatory Commission's DCH issue resolution effort is seriously deficient; that these deficiencies have not been adequately acknowledged or assessed in the DCH issue resolution effort; and that use of this flawed study as a basis for nuclear power plant regulation or plant design with respect to DCH would be unwise until these limitations have been assessed.

I acknowledge that the DCH issue resolution modeling has been subjected to a substantial review process involving a number of prestigious peer reviewers. However, I believe that the value of their review efforts has been vitiated by serious irregularities in how this process was carried out by the NRC. There have also been important irregularities in other features of the overall process used in the DCH issue resolution efforts. For example, much of the information presented in this report could have been made available to the peer reviewers before the review of the first DCH issue resolution document (NUREG/CR-6075) had been completed; however, my requests for permission to provide this information to the reviewers were not granted. Furthermore, the assessment of the CONTAIN code DCH model that was performed in support of the CONTAIN peer review revealed important conflicts with the DCH issue resolution modeling assumptions; instead of pursuing a resolution of these conflicts, the NRC responded by withholding permission to publish the CONTAIN DCH assessment report. Without these and other irregularities in the DCH issue resolution process, the technical deficiencies to be discussed in this critique would have been evaluated and addressed as part of the overall DCH issue resolution process, in which case there would have been no need for the present report. This report, however, will address only the technical issues.

It is important to understand the limitations of what I am attempting to accomplish with this critique. My goal is only to present information supporting my belief that the "resolution" of DCH that has been presented is not nearly as incontrovertible or unqualified as has been claimed. I have found that both Sandia management and the sponsoring organization (the NRC's Office of Nuclear Regulatory Research) view DCH issue resolution as a major achievement and that they are resistant to the idea that there are important limitations to the DCH issue resolution work that have not been adequately acknowledged or assessed. Hence I feel a need to make my case as strongly as possible. However, there is no intent here to develop more sophisticated alternative models or to present an alternative "resolution" for DCH. Such an effort would substantially exceed the resources available to me. For the same reason, there are limitations to the analyses presented in support of the issues addressed. With more time and resources, more sophisticated analyses might either confirm or allay some of the concerns that are raised here.

There is no intent here to impugn the integrity of the principle investigators of the DCH issue resolution effort. They appear to sincerely believe the technical issues raised here are less important than I argue; and the process irregularities noted above are the responsibility of the sponsor, not the DCH issue resolution investigators.

Executive Summary

In August of 1992, the U.S. Nuclear Regulatory Commission (NRC) initiated a program to resolve the direct containment heating (DCH) issue in U.S. nuclear power plants (NPP). The present report presents evidence that there are serious deficiencies in the methodology used in the DCH issue resolution work to calculate the containment loads resulting from DCH. This report deals only with the first phase of the DCH issue resolution program, which claimed to resolve the DCH issue in Westinghouse pressurized water reactor (PWR) plants with atmospheric or subatmospheric dry containments. This work is described in a series of reports designated NUREG/CR-6075, NUREG/CR-6075 Supplement #1, NUREG/CR-6109, and NUREG/CR-6638. The present critique is limited to considering these reports. The ongoing NRC efforts to analyze DCH in Combustion Engineering plants and ice condenser plants are not considered here.

It is not the intent of this work to argue that DCH actually is a serious threat in any of the plants that have been considered. What is at issue here is the validity of the claim to have *proven* that DCH is *not* a threat. Major topics to be discussed include:

- Role of the relatively mild initial conditions assumed for DCH in the issue resolution work.
- Major deficiencies in the basic assumptions of the DCH issue resolution models, and the conflicts between these assumptions and the results of CONTAIN code analyses of the DCH experiments. The models neglect processes that appear to contribute at least 50% of the DCH energy release in some important instances.
- Limitations to the experimental validation of the DCH issue resolution models, which is much less convincing than has been claimed.
- Dependence upon the unproven concept that limited temporal coherence between debris dispersal and reactor pressure vessel (RPV) blowdown plays a crucial role in mitigating DCH loads.
- Evidence that the treatment of pre-existing hydrogen in the containment seriously understates uncertainties and is probably nonconservative.
- Evidence that a number of additional modeling limitations can have significant impacts upon the results, and that the screening methodology used to analyze plants other than Zion and Surry makes a very inadequate allowance for modeling uncertainty.

It is therefore concluded that the DCH issue resolution methodology does not provide an adequate basis for regulatory and design decisions concerning DCH, and it is not adequate to support the move toward risk-informed, performance-based regulation.

Role of DCH Initial Conditions

The initial conditions for DCH assumed in the issue resolution work postulate that the melt compositions in DCH scenarios will be highly oxidic. The metal content is much lower than what was assumed in a number of prior studies including the NUREG-1150 analyses, the Severe Accident Scaling Methodology (SASM) work, and the Containment Loads Working Group (CLWG) analyses. Since combustion of hydrogen produced by metal-steam reactions during a DCH event can be a major contributor to the resulting loads, the low metallic content means that the DCH issue resolution initial conditions are quite mild compared with what has been considered in prior work.

Given these mild initial conditions, the importance of the deficiencies in the loads models identified here may be reduced (though not eliminated) in the context of PWRs with dry containments, because these containments are quite robust and it is difficult to generate threatening loads with the mild initial conditions assumed. The importance of the modeling deficiencies considered here would be much enhanced if the current DCH issue resolution methodology were to be applied to scenarios with more threatening initial conditions, or to less robust containments (e.g., ice condenser containments).

The present critique does not consider in any detail the arguments used in the DCH issue resolution work to defend the mild initial conditions that were assumed, except to note that uncertainties in the in-vessel accident progression that determines the DCH initial conditions can be substantial. The primary focus of the critique is on the modeling of containment loads.

Deficiencies in the Conceptual Basis of the Loads Models

The principal models used in the DCH issue resolution work are the two-cell equilibrium (TCE) model and the convection-limited containment heating (CLCH) model. The models are quite similar and only TCE was used after the early part of the DCH issue resolution work. Hence TCE is emphasized here. The models were developed to apply to compartmentalized containment geometries; i.e., in which the principal paths for debris dispersal from the cavity connect to subcompartment volumes delimited by structures that prevent transport of most of the debris to the main volumes of the upper containment. Most Westinghouse NPP with dry containments are compartmentalized.

Basic modeling assumptions of TCE (and CLCH) include

- Airborne debris will come into thermal and chemical equilibrium with the surrounding gas and steam.
- Only the small amount of debris transported beyond the subcompartments can interact with the main volume of the containment atmosphere in the dome.
- The remainder of the debris that is dispersed from the cavity can interact only with the portion of the reactor pressure vessel (RPV) blowdown steam that enters the cavity during the time debris is being dispersed from the cavity (called "coherent steam").
- Nonairborne debris does not interact with the gas or the blowdown steam.

- Co-dispersed cavity water and co-ejected RPV water either have no effect on DCH or have only mitigative effects; hence all effects of water are neglected.
- DCH-produced hydrogen can burn and contribute to containment loads unless the atmosphere is inert.
- Pre-existing hydrogen in the dome can burn only if certain conditions related to the atmosphere temperature and/or composition are met.
- Mitigation by atmosphere-structure heat transfer and by incomplete or delayed combustion of DCH-produced hydrogen are negligible, except that atmosphere-structure heat transfer is considered in connection with combustion of pre-existing hydrogen.

Numerous analyses of DCH experiments have been performed using the CONTAIN code, which is a systems code for analysis of containment response to a severe reactor accident. These analyses indicate that the mitigation processes neglected by TCE are actually very important in many cases. Since TCE roughly reproduces the experimental results for containment pressure rise (ΔP) without any consistent conservative bias, the fact that the model neglects important mitigation mechanisms necessarily implies that the model is also neglecting equally important processes that augment DCH energy release.

The largest discrepancies are in the Zion-geometry integral effects test (IET) experiments with noninert containment atmospheres, in which the CONTAIN analyses indicate that the processes considered by TCE contribute no more than about 50% of the total energy that is actually added to the containment atmosphere. CONTAIN sensitivity studies and stand-alone hand calculations of the mitigation effects add additional support for this conclusion. Other processes not included in TCE are evidently important contributors to the total DCH energy release, and TCE approximately reproduces the experimental ΔP values only because it also neglects the large mitigation effects. There is no reason to suppose that this cancellation of large opposing errors will apply to NPP analyses generally.

Limitations to the Experimental Validation Claimed for TCE

There is very little "bottom-up" analysis or experimental evidence offered to support the basic modeling assumptions made in TCE. Hence the case for using TCE is based almost entirely upon integral validation studies in which model predictions for ΔP are compared with experiment and approximate agreement is obtained. This validation is inconclusive for reasons that include the following:

- The ability of TCE to reproduce the major experimental trends is largely due to the simple systematics this database exhibits. It is shown that an almost trivial model that considers only the steam supply in the accumulator and whether DCH-produced hydrogen can burn turns out to correlate the ΔP data as well as does TCE. This total steam correlation (TSC) model is demonstrably inadequate for predicting DCH loads; it does not even include such obviously important parameters as mass and composition of the melt participating in DCH. Hence it follows that simply demonstrating reasonable agreement with the experimental ΔP data base does not in itself demonstrate adequacy for NPP application.

- The ability of a DCH model to predict hydrogen production is very important, both for the direct effect of hydrogen combustion upon containment loads and also as validation of the model's ability to predict the extent of debris-steam interactions. When the complete DCH database is considered, *TCE predictions show no correlation at all with the experimental results for hydrogen production ($R^2 = 0.01$).* The "validation" claimed is based on the model's ability to correlate a limited subset of the data in which both the containment atmosphere composition and the containment geometry were very nonprototypic. Arguments that have been given for restricting the comparison in this manner are examined in Appendix A of this report and are found to lack any independent support in all cases.

- Despite the large number of DCH experiments that have been performed, the DCH ΔP data base has a limited ability to validate DCH models, and a low resolving power to distinguish between competing modeling assumptions. One important reason is that many potentially important DCH parameters (e.g., melt mass and composition, vessel failure size, pre-existing hydrogen in the containment) have either not been varied or else have not been varied in a regime for which the parameters would be expected to have an important impact upon the results. This limitation is one reason for the simple systematics alluded to above. The resolving power of the data base is increased if one also makes full use of the hydrogen production data, which the DCH issue resolution validation effort does not do because many of the hydrogen results do conflict with TCE as noted above.

- Application of TCE to NPP scenarios involves many extrapolations beyond the existing data base; e.g., with respect to geometric scale, melt composition, hydrogen concentration within containment, and RPV water co-ejected with the melt. Uncertainties associated with these extrapolations are either inadequately addressed or not acknowledged at all.

Role of Coherence in TCE

TCE (and CLCH) assume that limited temporal coherence between debris dispersal and RPV blowdown is a "crucial mitigating factor" for DCH. However, no effort is made in the DCH issue resolution work to cite experimental evidence that supports the high importance ascribed to coherence in this work. In reality, there is some limited evidence, discussed in the present report, that coherence is not this important. In addition, some CONTAIN code calculations have been performed examining sensitivity to coherence, and this sensitivity was quite moderate in the cases considered.

In validating TCE, coherence was estimated from the experimental results and the experimental value of coherence was then input to the model. However, the methods used to estimate coherence from the experimental results are subjective and difficult to apply consistently to all the experiments. Application of an alternative method believed to be somewhat less subjective indicates that there are important inconsistencies in how coherence has been estimated in the DCH issue resolution work. It appears that correcting these inconsistencies would, in general, worsen agreement between TCE and the experimental ΔP data. In addition, these inconsistencies mask what appears to be a substantial effect of geometric scale upon coherence, based upon comparisons between the 1/40-scale and 1/10-scale IET experimental results for Zion geometry.

Combustion of Pre-Existing Hydrogen

Hydrogen released to the containment prior to vessel breach (called "pre-existing hydrogen") can make an important contribution to DCH loads if it can burn on DCH time scales. The following conclusions have been reached concerning the treatment of pre-existing hydrogen in the DCH issue resolution work:

- The treatment of volumetric combustion is based in part upon a typographical error that reversed the intended meaning of a key reference that is cited to justify the assumption of a high effective threshold temperature for substantial combustion of pre-existing hydrogen under DCH conditions. Effective threshold temperatures actually may be much lower than assumed in the DCH issue resolution work. In general, the treatment of pre-existing hydrogen likely tends to be nonconservative and clearly underestimates the uncertainties in hydrogen behavior under DCH conditions.

- Several combustion processes are considered and it is implicitly assumed in the issue resolution work that no process can contribute unless it generates energy at a rate exceeding the estimated rate of energy loss from the containment atmosphere. This assumption is not correct; the criterion should be that containment pressures can continue to rise so long as total rate of energy input from all processes exceeds the total loss rate.

- The treatment of deflagrations is likely quite nonconservative because the energy generation rate is based upon a flame propagating from a single ignition point. Multiple ignition points provided by hot debris and jet ignition effects are neglected. These effects would be expected to substantially enhance burn rates and may enhance burn completeness.

- Arguments are given that the failure to obtain complete containment mixing on DCH time scales tends to prevent combustion of pre-existing hydrogen. Incomplete mixing may be a significant effect, but the claim made in the issue resolution work that stratification will essentially prevent combustion of pre-existing hydrogen is dubious and conflicts with experimental evidence provided by the SNL/IET-11 experiment.

- The claims that the models are validated by comparison with hydrogen behavior in the IET experiments neglect the partial combustion that apparently did occur in the Zion SNL/IET experiments and also depend upon an unproven claim that pre-existing hydrogen did not burn on DCH timescales in the Surry IET experiments.

- There is no consideration of the fact that the IET experiments provide a nonconservative test of pre-existing hydrogen behavior under DCH conditions, especially when extrapolation to plants other than Zion is considered. Inferences based upon hydrogen behavior in the Surry IET experiments are very dubious because hydrogen concentrations in these experiments were only ~1/3 those expected in the NPP application.

Other Nonconservative Approximations and Inconsistencies in TCE

Some additional points of concern over the adequacy of the loads modeling in the DCH issue resolution work include the following:

- In addition to the questions summarized above concerning omission of important DCH processes in TCE, there are a number of nonconservative approximations made in the way TCE treats the processes that are modeled. These include important inconsistencies in the way the subcompartment volume is defined and used in the model; the use of constant-volume heat capacities where constant-pressure heat capacities would be more appropriate; and the use of temperature-independent heat capacities. One indication of the potential importance of these nonconservative approximations is that a CONTAIN calculation for the Surry plant was performed that included only the basic physical processes modeled in TCE, and the calculated ΔP was about 60% higher than given by TCE. These two calculations would be expected to give reasonable agreement, were it not for the nonconservative features of the TCE treatment.

- Comparison of TCE predictions and experimental results for ΔP in the Surry and Zion IET experiments shows TCE overpredicts Surry relative to Zion by about 45%; i.e., the (prediction/experiment) ratio for Surry is about 45% higher than for Zion. This indicates TCE does not capture plant-specific differences well and significant additional uncertainty should be allowed for when analyzing plants not studied experimentally. However, no such uncertainties are considered and the point is not acknowledged.

- A fundamental goal of the issue resolution study is to demonstrate that the conditional containment failure probability (CCFP) is ≤ 0.1. The study makes use of a screening criterion of CCFP ≤ 0.01 in order to provide margin for plant-specific differences not considered and for residual modeling uncertainties resulting from phenomena not modeled in TCE. The treatment neglects the fact that the margin provided by the CCFP ≤ 0.01 screening criterion shows a five-fold variation among the plants considered. For some plants the screening margin is demonstrably very inadequate to guard against just one of the important phenomenological uncertainties involved; namely, the uncertainty associated with pre-existing hydrogen combustion.

- The model used to treat chemical equilibrium in the iron-steam reaction is based upon an assumption that iron and iron oxide (FeO) form an ideal solution with each other; in reality, Fe and FeO are almost immiscible. In addition, the model neglects the dilution of FeO by other oxides present. This dilution can favor a more complete reaction of the iron.

- The SNL/IET-11 experimental results suggest that stainless steel insulation ablated from the RPV may enhance hydrogen production and combustion. The issue resolution analyses neglect this effect. The justification given for neglecting this contribution underestimates its potential magnitude by almost a factor of 4 because it erroneously assumes that only the chromium in the stainless steel can contribute. The argument that the iron cannot contribute because of "thermodynamic limitations" is incorrect.

Conclusions

The DCH issue resolution work has performed a useful service by systematizing a large amount of information concerning the DCH experimental results and concerning plant features relevant to DCH. However, the treatment of containment loads suffers from a large number of deficiencies that prevent this work from convincingly achieving its goal of demonstrating that DCH loads pose little or no threat to containment integrity in the plants that have been analyzed. The cumulative impact of the deficiencies identified here is sufficiently great that it is difficult to determine what, if any, conclusions may be safely drawn from the DCH issue resolution work as it stands.

The difficulties with the loads analysis may not be easily fixed within the framework of the simple modeling approach used in the DCH issue resolution analysis. This approach emphasizes simple bounding models for the processes that are considered together with the assumption that processes not considered will have negligible effects upon DCH loads. The present critique shows that the latter assumption is very difficult to defend in a number of important cases. Attempting to address this deficiency by including simple bounding treatments for the various processes and uncertainties that are currently neglected likely would result in calculations predicting that threatening loads *can* result from DCH, for at least some of the plants considered. Obtaining a convincing resolution may require at least supplementing TCE using more sophisticated analytical tools that allow treatment of both the mitigating and the augmenting effects neglected by TCE, as well as quantitative assessment of phenomenological uncertainties in the analysis. It might also be desirable to apply a more disciplined approach to the use of engineering judgment than has been done in the current DCH issue resolution work; e.g., formal expert elicitations might be used as was done in the NUREG-1150 study.

In its current form, the DCH issue resolution work does not provide an accurate representation of the state of the art with respect to DCH phenomenological understanding. As a result, it does not provide an adequate basis for design, accident management, or regulatory decisions with respect to DCH. This methodology would also provide a very inadequate technical basis for risk-informed, performance-based regulation of issues involving DCH.

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1 Introduction

1.1 Background

In some reactor core melt accident sequences, the reactor pressure vessel (RPV) may not fully depressurize prior to failure of the vessel lower head. In these accident scenarios, vessel breach is expected to result in molten core debris being ejected from the RPV under high pressure, a process called high pressure melt ejection (HPME). Blowdown steam from the RPV may then disperse much of the debris out of the cavity. Fragmented debris may then transfer thermal energy to the blowdown steam and/or the containment atmosphere, thereby pressurizing the containment. In addition, metallic constituents of the debris can react with steam, generating hydrogen whose subsequent combustion can add substantially to the total energy transferred to the containment atmosphere. This sequence of events is known as direct containment heating (DCH). Since the mid-1980s, both the nuclear industry and the U. S. Nuclear Regulatory Commission (NRC) have sponsored experimental and analytical programs to improve understanding of DCH phenomena and apply this understanding to assessing DCH threats to containment integrity in U. S. nuclear power plants (NPP).

In August of 1992, the NRC initiated a program specifically targeted at "resolution" of the DCH issue. This effort is still in progress; however, an important part of the effort involved resolution of DCH in all Westinghouse plants with dry containments, and this effort was considered to be essentially complete with the publication of NUREG/CR-6338 (Pilch et al., 1996). An essential part of this effort has been the modeling of containment loads that could result from a high pressure melt ejection (HPME) event with DCH. The principal models that have been used in the DCH issue resolution program are the two-cell equilibrium (TCE) model and the convection-limited containment heating (CLCH) model. The central purpose of the present report is to summarize the reasons why I believe that there are important limitations to these models that have not been acknowledged. Until these limitations have been acknowledged and their potential implications explored, it is my belief that the claim to have "resolved" the DCH issue has been substantially overstated, possibly to a degree sufficient to invite unwise decisions by the NRC and/or industry concerning HPME and DCH if the present issue resolution documents were to influence regulatory policy and/or industry decision-making. Note, however, that it is *not* the purpose of this report to argue that DCH is a serious safety threat in any of the plants analyzed to date. What is at issue here is the adequacy of the support for the claim to have *proven* that DCH is not a threat.

To date, the published work on DCH issue resolution deals with Westinghouse PWR plants with large dry or subatmospheric containments. The Zion plant was first considered in detail in NUREG/CR-6075 (Pilch et al., 1994a) and its Supplement (Pilch et al., 1994b), and the Surry plant was analyzed in NUREG/CR-6109 (Pilch et al., 1995). The methodology was then extrapolated to treat all PWRs with Westinghouse dry containments in NUREG/CR-6338 (Pilch et al., 1996). Most of the Westinghouse containments are characterized as "compartmentalized", meaning that the dominant exit path for debris dispersal from the cavity communicates to lower-containment compartments defined by structures that present barriers to debris transport to the main volume of the containment dome. [In a few of these containments, line-of-sight paths do exist for substantial debris transport from the cavity to the dome (Pilch et al., 1996).] Except where otherwise noted, compartmentalized geometries are assumed in this discussion.

The main points to be considered deal with limitations to the modeling of DCH loads. However, the importance of these limitations depends upon the DCH initial conditions assumed, and this subject is considered in Section 2. Section 3 reviews the conceptual basis for the TCE model and presents evidence for believing that the model omits several effects that are important to DCH and that the validation claimed for TCE depends heavily upon the cancellation of opposing errors. Similar conclusions apply to the CLCH model although it is considered in less detail because it was used only in the first of the issue resolution reports, NUREG/CR-6075 (Pilch et al., 1994a); only the TCE model has been used in all subsequent work. Section 4 further considers the limitations to the validation claimed for the TCE model, and notes the potential significance of the TCE model's almost total inability to correlate the data for hydrogen production during DCH. Both the TCE and CLCH models are heavily dependent upon the concept of "coherence", and some questions concerning the importance of coherence and how it has been estimated from the experimental results are considered in Section 5. In Section 6, arguments are given for believing the treatment of the combustion of pre-exiting hydrogen within the containment seriously underestimates the uncertainties involved and is very likely nonconservative. Additional modeling issues are summarized more briefly in Section 7. In Section 8, it is concluded that the cumulative impact of the deficiencies noted is sufficiently great that it is very doubtful whether the present form of the DCH issue resolution work should be used at all as the basis for decision-making concerning DCH threats.

Appendix A of this report considers the arguments that have been advanced for explaining away the inability of TCE to correlate the DCH hydrogen production data and concludes that these arguments are not well founded. Appendix B discusses some problems with the means used to estimate coherence from the experimental results in more detail than is done in Section 5. Section 3 alludes to evidence that there are important DCH phenomena not treated by the TCE and CLCH models, and Appendix C presents additional analyses supporting the importance of these phenomena. Appendix D provides a summary of the major experimental investigations of DCH that are relevant to this work, for the convenience of readers not intimately familiar with the DCH experimental program.

Readers of this document should understand that its purpose is to examine deficiencies in the DCH issue resolution modeling in order to correct the overly optimistic picture of DCH understanding given in that work; there is no attempt to provide a complete and balanced review of the entire DCH issue resolution effort. Hence the focus is necessarily on the negative, and the more positive features of the DCH issue resolution work are generally not discussed. For example, one noteworthy achievement of the DCH issue resolution work is that it has systematically summarized a large amount of information concerning the DCH experimental results and concerning plant features relevant to DCH. Comparable compilations of relevant information are not available for most severe accident issues.

1.2 Methodology of this Critique

Analysis of reactor severe accident issues typically requires consideration of strongly coupled complex and nonlinear phenomena, and DCH is a prime example of this difficulty. It is therefore inevitable that any attempt to "resolve" an important severe accident issue must make a number of approximations and assumptions that introduce significant uncertainty. Provided that this uncertainty is properly acknowledged and allowed for, this is not grounds for criticism, since the only alternative is to attempt no analysis at all. Unfriendly critics of severe accident analyses usually find it possible to generate a long list of deficiencies and oversights that sound impressive so long as one does not demand any *quantitative* demonstration that the deficiencies could have important consequences for the results of the study. Properly done, qualitative critiques of this type can be useful, but they can also be unfair because virtually any severe accident analysis is potentially vulnerable to such attacks and practitioners of the technique can be rather selective in choosing their targets.

In the present critique, therefore, the emphasis is on providing a more detailed discussion of several specific topics for which there is significant quantitative evidence, experimental or analytical, that the deficiencies noted could have a significant impact in one or more of the following three areas:

- Calculation of containment loads;
- Analysis of phenomena such as hydrogen combustion that are known to be important to containment loads; and
- Assessing the fundamental physical validity of the TCE and CLCH models.

In Section 7, there is also a secondary emphasis on identifying approximations or assumptions that are erroneous and that could be corrected without significantly complicating the model, even if it is not established that these errors could have a major quantitative impact upon the calculations.

As a result of this emphasis, some potentially important issues are not considered in this report. One example is uncertainty in the amount of debris transported to the dome. This uncertainty received considerable discussion in the peer review of NUREG/CR-6075 (Pilch et al., 1994a; Pilch et al., 1994b). Although it might yet turn out to be important, quantitative evidence that this uncertainty could have a substantial impact upon containment loads is considered to be insufficient to justify a detailed discussion here.

It is also important to understand that the goal of this critique is to establish that the "resolution" of DCH that has been presented is not as nearly incontrovertible or unqualified as has been claimed. There is no intent here to develop more sophisticated alternative models or to present an alternative "resolution" for DCH. Such an effort would greatly exceed the resources available for this work.

1.3 Role of the CONTAIN Code

The CONTAIN code has been developed for the NRC as an analysis tool for evaluating containment response to reactor severe accidents (Murata et al., 1989; Washington et al., 1991). Modeling of DCH has been an important focus of the CONTAIN development program (Washington and Williams, 1995). Results of a detailed independent peer review of the CONTAIN code, including a review of the CONTAIN DCH models, were published recently (Boyack et al., 1995). The DCH experimental data base was extensively analyzed using the CONTAIN code during the period August 1993 - March 1994, with more limited analyses being performed since that time. A draft report (SAND94-1174) describing this work, commonly referred to as the "CONTAIN DCH Assessment Report," was prepared and released for review in May of 1994 and subsequently revised to take into account review comments (Williams et al., 1997). Much of this analysis was performed in support of the CONTAIN peer review effort (Boyack et al., 1995). The critique of TCE and CLCH given here makes considerable use of the results given in SAND94-1174, especially in Sections 3 and 4 of this report. However, in the context of understanding the arguments concerning the adequacy of TCE and CLCH, it is very important to recognize the following two points:

1. Although the CONTAIN code is used here to provide quantitative estimates of the importance of the effects omitted from the DCH and CLCH models, understanding the issues involved does not require a complex computer code. Furthermore, one does not have to accept the adequacy of all features of the CONTAIN DCH modeling in order to recognize the potential importance of the limitations to the modeling of DCH given by TCE and CLCH.

2. There is no intent to imply that DCH could be neatly "resolved" if only CONTAIN were substituted for TCE. On the contrary, the work described by Williams et al. (1997) indicates that there are important phenomenological uncertainties in the analysis of DCH, and analysis based upon CONTAIN could be as unreliable as one based upon TCE or CLCH if these uncertainties are ignored. The CONTAIN code does provide various means of quantifying the impact of these uncertainties, and in this sense CONTAIN could have made a valuable contribution to the DCH issue resolution process. The DCH issue resolution work based upon TCE and CLCH, however, largely ignores these uncertainties and makes essentially no effort to quantify them; where they are discussed at all, it is usually only to deny that they could be important.

Because SAND94-1174 does present results that conflict with basic modeling assumptions of TCE and CLCH, publication of this report has not been authorized by the NRC and/or SNL management. The report has been through the standard SNL internal technical review process, and is available in draft form upon request. A paper summarizing the results was presented at the 1995 ANS Winter Meeting (Williams et al., 1995). It should be noted that neither the report nor the ANS paper makes any actual mention of the conflicts with the modeling assumptions used in TCE and CLCH, although the existence of these conflicts likely would be apparent to knowledgeable readers of SAND94-1174 who are also familiar with the DCH issue resolution models.

2. Initial Conditions for DCH

The initial conditions assumed in NUREG/CR-6075 were generally characterized by the peer reviewers as tending toward the "optimistic" and as making inadequate allowance for uncertainties (Section 3.1, Pilch et al., 1994b). On May 16-17, 1994, a "Working Group" meeting was held in Albuquerque, NM, to discuss both the initial conditions and DCH modeling issues. This Working Group included a selected subset of 6 out of the original 13 reviewers of NUREG/CR-6075. The initial conditions were redefined in this meeting. Whether the new sets of initial conditions have been perceived as being more credible than the old, except by those defining the new initial conditions, is difficult to say; only the members of this Working Group have been included in the documented review of all subsequent DCH issue resolution documents.

The Working Group defined four scenarios for DCH initial conditions, two of which had highly oxidic melts with little metallic content and two of which had higher metallic content but relatively low RPV pressure at vessel breach. Based in part upon subsequent calculations performed at INEL using the SCDAP/RELAP5 (SR5) code, the two scenarios having the higher metallic contents were eliminated on the grounds that the hot leg or surge line would fail well before the vessel lower head, thereby completely depressurizing the RPV and precluding DCH. Hence only the two scenarios with low metallic content were considered in the NUREG/CR-6075 Supplement and all subsequent DCH issue resolution work. These were designated "Scenario V" and "Scenario VI" and were first described in the NUREG/CR-6075 Supplement (Pilch et al., 1994b), with some minor modifications in subsequent reports (Pilch et al., 1995; Pilch et al., 1996).

The two scenarios that remained under consideration are actually substantially *milder* than some that were originally included in NUREG/CR-6075. For details of these scenarios, the documents cited above should be consulted. Key features include:

- Total melt masses comparable to, or somewhat less than, what has been assumed in prior work (24-36 metric tonnes (mt) median, 59-84 mt upper bound for a Zion-type core, with the larger values corresponding to Scenario VI).

- Metallic constituents in the melt much less than assumed in most previous work; e.g., <20% of what was assumed in the Severe Accident Scaling Methodology (SASM) work (Appendix G, Zuber et al., 1991). The NUREG-1150 (NRC, 1991) and the Containment Loads Working Group (CLWG; NRC, 1985) studies also allowed for substantial metallic content.

- Water overlying the melt (~70 mt and ~10 mt in Scenarios V and VI, respectively) at the time of vessel breach, with this water being co-ejected with the melt.

- RPV pressure 16 MPa and 8 MPa in Scenarios V and VI, respectively.

- RPV slightly superheated in Scenario V, substantially superheated in Scenario VI ($T \approx$ 1000 K).

- A relatively small vessel breach area (~0.2 m^2 or less).

Of these characteristics, the low metallic content may be the most important because combustion of DCH-produced hydrogen generated by metal-steam reactions can be a major contributor to DCH loads; for example, it contributed over half the total containment pressure rise (ΔP) associated with DCH in some of the Zion-geometry Integral Effects Test (IET) experiments (Allen et al., 1994a). Reducing the metallic content of the core debris can reduce this contribution to DCH loads. The small vessel failure size assumed is also worth noting because CONTAIN, TCE, and CLCH all tend to predict increasing loads with increasing vessel failure size. The reasons for this dependence differ for the different models and the magnitude of the effect depends heavily upon other parameters of the DCH scenario.

There is an important relationship between the initial conditions and the requirements for adequate loads modeling. If the range of initial conditions postulated in the NUREG/CR-6075 Supplement is accepted as a valid representation of the credible range, one may not require sophisticated DCH models in order to conclude that the threat to containment integrity is minimal in most PWR dry containments. Except for uncertainties involving the behavior of pre-existing hydrogen in the containment, simple bounding models similar to those used in the early CLWG work would predict minimal threats to containment integrity for at least some PWR plants with dry containments. Indeed, if initial conditions as mild as those assumed in the DCH issue resolution work had been accepted at the time of the CLWG review, it is questionable whether DCH ever would have emerged as a major safety issue.

Given the postulated initial conditions, it could be argued that the limitations of the containment loads models used in the issue resolution effort are academic, insofar as the PWR dry containments are concerned. This argument would be equivalent to arguing that DCH had been resolved based upon a consideration of the in-vessel accident progression alone. However, this is not the claim being made in the issue resolution work; in fact it has been claimed that DCH has been resolved based upon a *consideration of containment loads alone* (Pilch et al., 1996). Thus the issue resolution work includes a claim to present a validated methodology for assessing containment loads, and the unacknowledged limitations in this methodology will be a serious concern if it were to be applied to DCH scenarios in which the large margins characterizing the existing applications were not available.

In the past, uncertainties in the in-vessel accident progression have been considered to be major contributors (even dominant contributors) to the overall uncertainties in DCH loads. It is not the purpose of this report to examine the adequacy of the initial conditions assumed in the issue resolution work in any detail (the in-vessel analysis is not my principal area of expertise). However, it is not difficult to cite specific reasons for concern as to whether the uncertainties in the initial conditions have been adequately accounted for, e.g.:

- The PHEBUS FPT-0 experiment (Schwarz and von der Hardt, 1995) on in-vessel accident progression resulted in substantially larger and earlier fuel melting than predicted. This result illustrates the large uncertainties involved in the analysis of the in-vessel accident progression.

- The Advisory Committee on Reactor Safeguards (ACRS) recently raised questions as to the validity of SCDAP/RELAP calculations of natural circulation under severe accident conditions (INRC, 1996). These questions were raised in connection with the issue of whether steam generator tube failures could occur before primary system failure results in system depressurization; DCH was not explicitly at issue. However, the prediction that primary system failure will result in depressurization prior to vessel breach and thereby prevent DCH in many scenarios also depends, in part, upon the ability of the code to calculate natural circulation under severe accident conditions.

- The initial conditions do not explicitly consider phase diagram information for core materials which indicates that, even if there is little free metal in the melt, the oxidic components may be substoichiometric, possibly highly substoichiometric.* Interaction of the substoichiometric materials with steam could release chemical energy and enhance hydrogen production substantially, much as would the presence of free zirconium metal.

- Under some conditions, even UO_2 can interact with steam and water to generate hydrogen. In a recent experiment in the FARO facility simulating in-vessel conditions (5 MPa pressure), estimated hydrogen production from melt-water interactions was considerably greater than what would be allowed by the NUREG/CR-6338 melt compositions, even though this melt consisted of only UO_2 and ZrO_2, with no metal at all (Magallon et al., 1995). This result may raise questions as to whether there can be additional sources of pre-existing hydrogen and/or DCH-produced hydrogen not allowed for in the DCH issue resolution work.

- The first experiment performed in an ongoing program studying lower head failure modes, though not fully prototypic, yielded a vessel failure size an order of magnitude larger than what would be implied by the assumptions used in the issue resolution work, which could imply increased DCH loads as noted above. Other experiments in this series have yielded results more nearly consistent with the small failure sizes assumed in the DCH issue resolution work.

It is acknowledged that the results cited above cannot be uncritically extrapolated to DCH scenarios at plant scale. They are cited as a caution that uncertainties in the phenomenology controlling the in-vessel accident progression may be larger than is implied by the DCH issue resolution work; they do not necessarily prove that the initial conditions assumed in the issue resolution work are in gross error.

A more fundamental reason why the containment loads issues cannot be dismissed as being moot is that nuclear safety has traditionally been based upon the defense-in-depth

*The documentation includes statements (Pilch et al., 1996) that the melt composition includes an allowance for substoichiometric oxides; without this, the specified Zr content of the melt would have been even smaller. However, even with this allowance, the Zr content of the melt corresponds to $\leq$ 10% of the initial core inventory as an upper bound, and $<$ 5% as a median estimate. Alternatively, the melt composition could be viewed as corresponding to a uranium oxide stoichiometry of about $UO_{1.83}$ with no elemental zirconium present at all.

concept. In the case of DCH, this has meant both addressing the in-vessel accident progression that determines the DCH initial conditions and also understanding the phenomena controlling containment loads. To ignore important deficiencies in the loads modeling methodology simply because the in-vessel accident progression may be more favorable than formerly believed would be to accept a serious degradation of the defense-in-depth concept.

3. Limitations to the Conceptual Basis of TCE and CLCH

The TCE and CLCH models are both dependent upon some basic assumptions concerning the dominant phenomena of DCH; these assumptions are referred to here as the "conceptual basis" of the models and are summarized in Section 3.1. The detailed description of the models appear in Appendices D and E of NUREG/CR-6075 (Pilch et al., 1994a) for CLCH and TCE, respectively, except that the modeling of the combustion of pre-existing hydrogen in TCE was subsequently changed to that described in Appendix E of the NUREG/CR-6075 Supplement (Pilch et al., 1994b). Some reasons for believing that the conceptual basis of these models does not capture all the major phenomena controlling DCH loads are then summarized in Section 3.2.

3.1. Conceptual Basis of TCE and CLCH

Both the CLCH and the TCE models were originally developed for analyzing DCH loads in containments with compartmentalized geometries. By "compartmentalized geometry" it is meant that the dominant exit path from the cavity communicates to lower-containment compartments defined by structures that present barriers to debris transport to the main volumes of the containment (i.e., to the dome). Containments in which the dominant exit path communicates directly to the dome are said to possess an "open" geometry. Most Westinghouse plants with dry containments, including the Zion and Surry plants, have compartmentalized geometries; for a limited number of these plants, there is sufficient line-of sight communication from the cavity exit to the dome that categorizing these plants as being "compartmentalized" is questionable.

The major features of the conceptual basis of TCE are the following:

- Only debris that is dispersed from the cavity as airborne particulate is assumed to contribute to DCH, and it contributes only as long as it is airborne; for debris which is not transported beyond the subcompartments, de-entrainment in the subcompartments is assumed to be instantaneous.

- Only blowdown steam that leaves the RPV during the time that debris is being dispersed from the cavity is assumed to interact with debris; this steam will be called the "coherent steam" here. Steam entering the cavity after dispersal terminates ("noncoherent steam") is assumed to undergo no interaction with debris. The coherent steam is parameterized in terms of the so-called coherence ratio. In validating the TCE model, the coherence ratio for each experiment is estimated from the experimental data and input to the model (see Section 5 and Appendix B of this report for more details).

In plant applications, coherence is estimated from an empirical correlation fit to available experimental data together with the assumption that coherence does not depend upon facility scale. The role of coherence is considered further in Section 5.

- Debris that is dispersed from the cavity, but is not transported beyond the subcompartments, equilibrates (thermally and chemically) with either the subcompartment atmosphere or the coherent steam, whichever has the larger heat capacity. In practice, the subcompartment volume in the model has been set to 1% of the total containment volume in most plant analyses (Pilch et al., 1996) and thus the interaction with the coherent steam controls.

- Debris that is carried beyond the subcompartments can equilibrate with the dome atmosphere. The amount reaching the dome is an input to the model. In comparisons with experimental data for validation, this quantity has been taken directly from the experimental results. Pilch et al. (1996) describe the approach used for plant applications.

- All energy transferred to the gas and steam in the cavity and/or the subcompartment is assumed to transport to the dome and contribute to DCH pressurization.

- All DCH-produced hydrogen is assumed to be transported to the dome and burn with 100% efficiency, assuming the containment atmosphere is of a composition that can support combustion. Pre-existing hydrogen in the containment atmosphere can also "autoignite" if a user-specified ignition temperature is exceeded in the dome volume, or if criteria for a propagating deflagration are satisfied. The latter conditions are controlled by correlations that depend upon atmosphere compositions and temperature (Appendix E, Pilch et al., 1994b).

- Effects of debris interactions with cavity water and/or water co-ejected from the RPV are assumed to be either negligible or unconditionally mitigative.

- Certain mitigation effects are assumed to be negligible. These include:

  1. Incomplete equilibration between airborne debris and the gas it interacts with.

  2. Incomplete or delayed combustion of DCH-produced hydrogen; e.g., due to temporary oxygen starvation in the subcompartments.

  3. Heat transfer between the atmosphere and the containment heat sinks, except that a correction for heat transfer during a deflagration of pre-existing hydrogen is applied. This correction has no effect on the pressurization resulting from combustion of DCH-produced hydrogen, which is assumed to be adiabatic.

At this level of description, the conceptual basis of CLCH is similar except for the following:

- Airborne debris interacts only with the coherent steam, never the subcompartment atmosphere.

- Debris remaining in the cavity can chemically react with (but not transfer heat to) the noncoherent blowdown steam, generating additional hydrogen; however, this additional hydrogen cannot burn in the model unless the threshold ignition temperature for pre-existing hydrogen in the dome is exceeded. In all applications for both experimental analysis and plant calculations, this threshold was never exceeded.

- CLCH is described in terms of rates of blowdown and debris dispersal while TCE is described in terms of integral quantities of coherent steam and dispersed debris; however, the level of detail in the time-dependence of the rates assumed in CLCH is insufficient for this distinction to be significant.

In actual application, the TCE subcompartment volume was defined to be sufficiently small that it was always the coherent steam that controlled the interaction with airborne debris. Furthermore, the CLCH ignition threshold temperature for hydrogen in the dome was set sufficiently high that it was never exceeded. Hence the TCE - CLCH differences noted had no effect upon the results for ΔP. Other differences in how the models were implemented and applied did have some effect; however, these differences are at a level less fundamental than what I am calling the "conceptual basis" of the models. Hence, no further discussion of CLCH is needed here.

3.2. Inadequacies of the Conceptual Basis of TCE

Although many of the discussions in the issue resolution documentation of the TCE and CLCH models refer to them as "conservative" or even "bounding", it is very important to note that the experimental comparisons presented by Pilch et al. (1994a) for model validation show little evidence of any conservative bias. Instead, the plots for the predicted versus experimental values of ΔP are what might be expected for a best-estimate model, with about as many data points lying below the agreement line as above it; see Section 4 for more details. It necessarily follows that demonstrating there are important *mitigating* processes neglected by the model represents as serious a deficiency as would demonstrating that there are important *augmenting* processes neglected by the model. This conclusion follows from the fact that the model predictions show no consistent conservative bias; hence, if the models are omitting important mitigation effects, it clearly must be omitting important augmenting effects that are making up for this mitigation. In what follows, we discuss only the TCE model. Although some details differ for CLCH, the same basic arguments would apply for it also.

To examine this question further, it is useful to consider some of the results from SAND94-1174 (Williams et al.. 1996). Conclusions reached in this work included the following three major results which, if valid, have very important implications for the adequacy of the treatment used in TCE:

1. The mitigation effects neglected by TCE are very important, except that the neglect of any failure to achieve complete equilibration between debris and gas may not be very important (the magnitude of this effect is quite uncertain). In particular, the mitigating effect of atmosphere-structure heat transfer combined with the effect of delayed or incomplete combustion of DCH-produced hydrogen is as important as the effect of de-entrainment of airborne debris in the subcompartments, in the CONTAIN calculations. The importance the CONTAIN analyses ascribe to these mitigation processes was supported by an independent "hand" calculation of the magnitude of the mitigation effects to be expected. This calculation is reproduced in Appendix C of this report.

2. Several convergent lines of reasoning, including but not limited to CONTAIN analyses of the Zion IET experiments, support the conclusion that DCH processes included in TCE and CLCH contribute only ~50% (possibly less) of the total containment pressurization and hydrogen production observed experimentally. This evidence is summarized in Section 4.2, especially Section 4.2.3, of SAND94-1174, with additional relevant information given in Section 6 of that report. Other processes not included in TCE clearly do contribute to DCH in the Zion IET experiments, and these other processes are fully as important as those that are treated in TCE. The contribution of these "other processes" in the experiments other than the Zion IET experiments appears to be less important, but it is still significant.

3. Although the evidence is strong that processes other than those allowed for by TCE do make large contributions to DCH in the IET (Zion) experiments, it is less clear what these other processes are. It is still less clear how these other processes can be modeled adequately to permit trustworthy extrapolations to scenarios not studied experimentally, including any NPP scenario (which necessarily requires a large extrapolation with respect to scale). Processes considered in the CONTAIN model (in a partially parametric manner) include debris interactions with co-dispersed water (Sections 3.2.8, 4.2, 6.4, and 6.5 of SAND94-1174) and interactions of so-called nonairborne debris with noncoherent blowdown steam (Sections 3.2.7, 4.2, 6.3, and Appendix B of SAND94-1174); see also Appendix C of the present report. Substantial uncertainties must be allowed for in treating these processes, no matter what model is used.

For the sake of convenience, we next summarize some of the main arguments that led to these conclusions here. Figure 3-1 gives comparisons between CONTAIN calculations and experimental results for ΔP and hydrogen produced. Hydrogen results are plotted after scaling up to plant scale by dividing by S^3, where S is the experimental linear scale factor, in order to facilitate comparison of experiments performed at different scales. Plot symbols distinguish experiments performed in open geometry, the limited flight path (LFP) experimental series other than LFP-8A, the SNL/IET Zion-geometry experiments with hydrogen combustion and without hydrogen combustion, the ANL/IET (Zion) experiments, and the SNL/IET (Surry) experiments; see Appendix D for summary descriptions of these experiments. In general, the CONTAIN ΔP and hydrogen production results reproduce the overall trends of the experimental data reasonably well, although scatter is somewhat greater for the hydrogen data. Williams et al. (1997) give additional details concerning these results, including some caveats that apply.

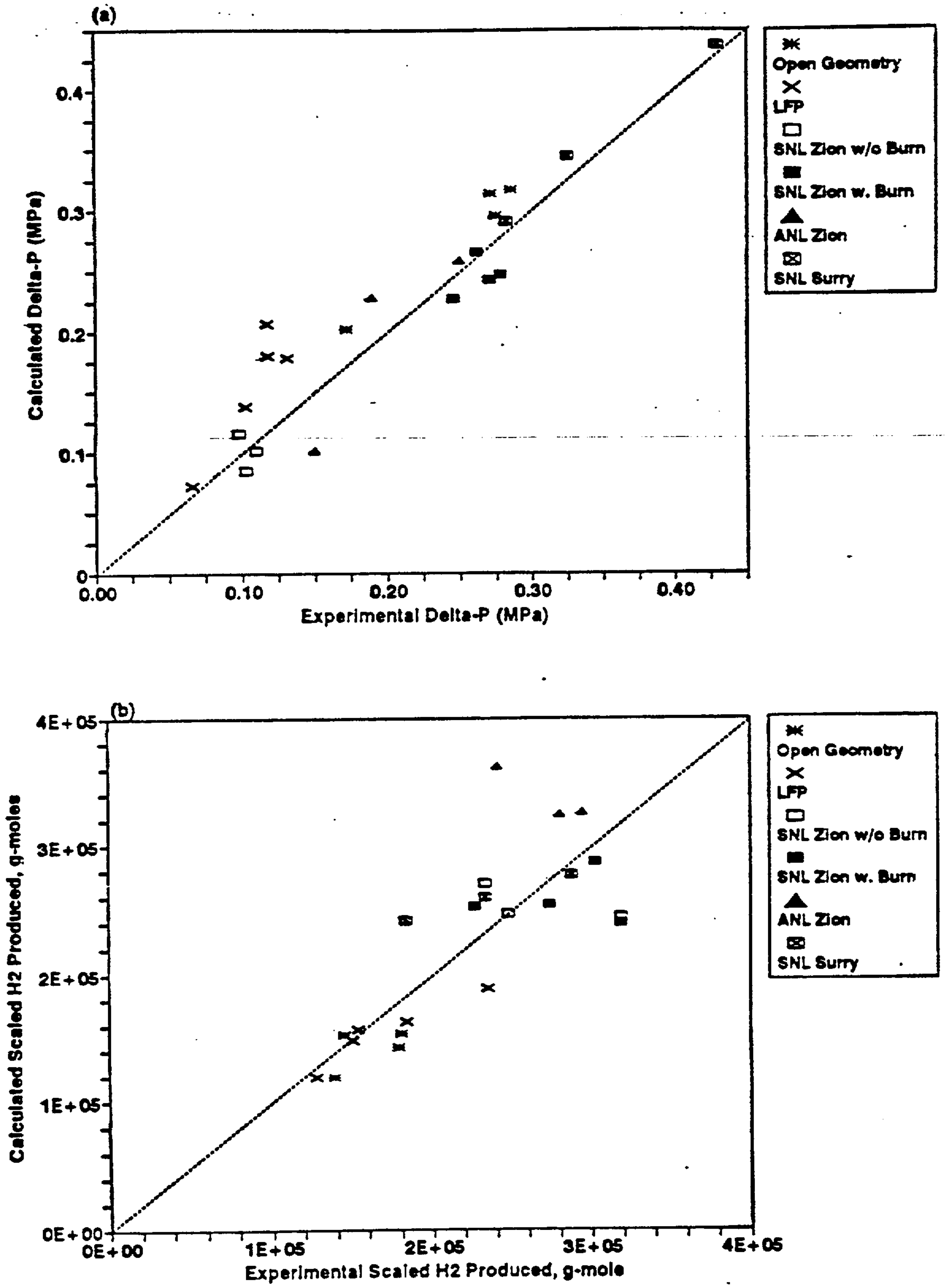

Figure 3-1. CONTAIN predictions versus experimental results for (a) ΔP and (b) scaled H_2 production for the standard input prescription.

CONTAIN modeling used to obtain the results summarized in Figure 3-1 were obtained using what was called the "standard input prescription" that was defined in SAND94-1174. This standard prescription included models for the mitigative effects that are neglected by TCE, and it also allows for the interaction of the noncoherent portion of the blowdown steam with nonairborne debris (NAD). Modeling of the NAD interactions was very important in the standard prescription analysis of the Zion-geometry IET experiments. Caution is required in interpreting these results, however, as there is some reason to believe that part of the effect attributed to NAD interactions in the standard prescription analysis of the Zion-geometry IET experiments actually result from debris interactions with co-dispersed cavity water; details are given in SAND94-1174 and a more limited discussion is provided in Appendix C of the present report. For present purposes, the difficulty in distinguishing the effect of NAD interactions versus debris-water interactions is of secondary importance, since neither are modeled in TCE.

In Figure 3-2, results are presented for CONTAIN calculations in which the processes contributing to DCH are restricted to those considered in TCE (the match is only approximate; an exact simulation of the TCE model assumptions is not possible using CONTAIN). In particular, neither NAD interactions nor debris-water interactions are included. The mitigation processes neglected by TCE are still included, however. It is seen that many of the ΔP results, and almost all the hydrogen production results, are significantly underpredicted when the CONTAIN model is restricted in this way. By a considerable margin, the largest underpredictions are for the Zion-geometry IET experiments (square and triangular plot symbols). The underprediction in hydrogen production is at least a factor of two for these cases, and the underprediction of ΔP is also about a factor of two for those SNL/IET (Zion) experiments in which the hydrogen produced could burn (solid square plot symbols).

The principal reason for this underprediction is that, with the mitigation processes included, calculations restricted to the DCH processes considered by TCE do not transfer sufficient energy to the containment atmosphere to account for the observed containment pressurization, nor can these processes generate sufficient hydrogen to account for the reported hydrogen production. Extensive sensitivity studies are cited in SAND94-1174 that support the conclusion that uncertainties in the processes that are modeled in obtaining the results given in Figure 3-2 are not nearly large enough to explain the deficiency in the calculated ΔP and hydrogen production, at least in the case of the Zion IET experiments. Processes not modeled in either the Figure 3-2 CONTAIN calculations or in TCE must be contributing.

Additional insight is provided by summarizing some CONTAIN sensitivity studies performed for the SNL/IET-3 and SNL/IET-4 Zion-geometry experiments. These experiments included oxygen in the containment atmosphere and thus DCH-produced hydrogen could burn. There was no pre-existing hydrogen, which eliminates uncertainties associated with the behavior of pre-existing hydrogen in the experiments.

Some results are summarized in Table 3-1. The first line (in bold) gives the experimental results for DCH-induced ΔP and hydrogen production. Case 1 in the table

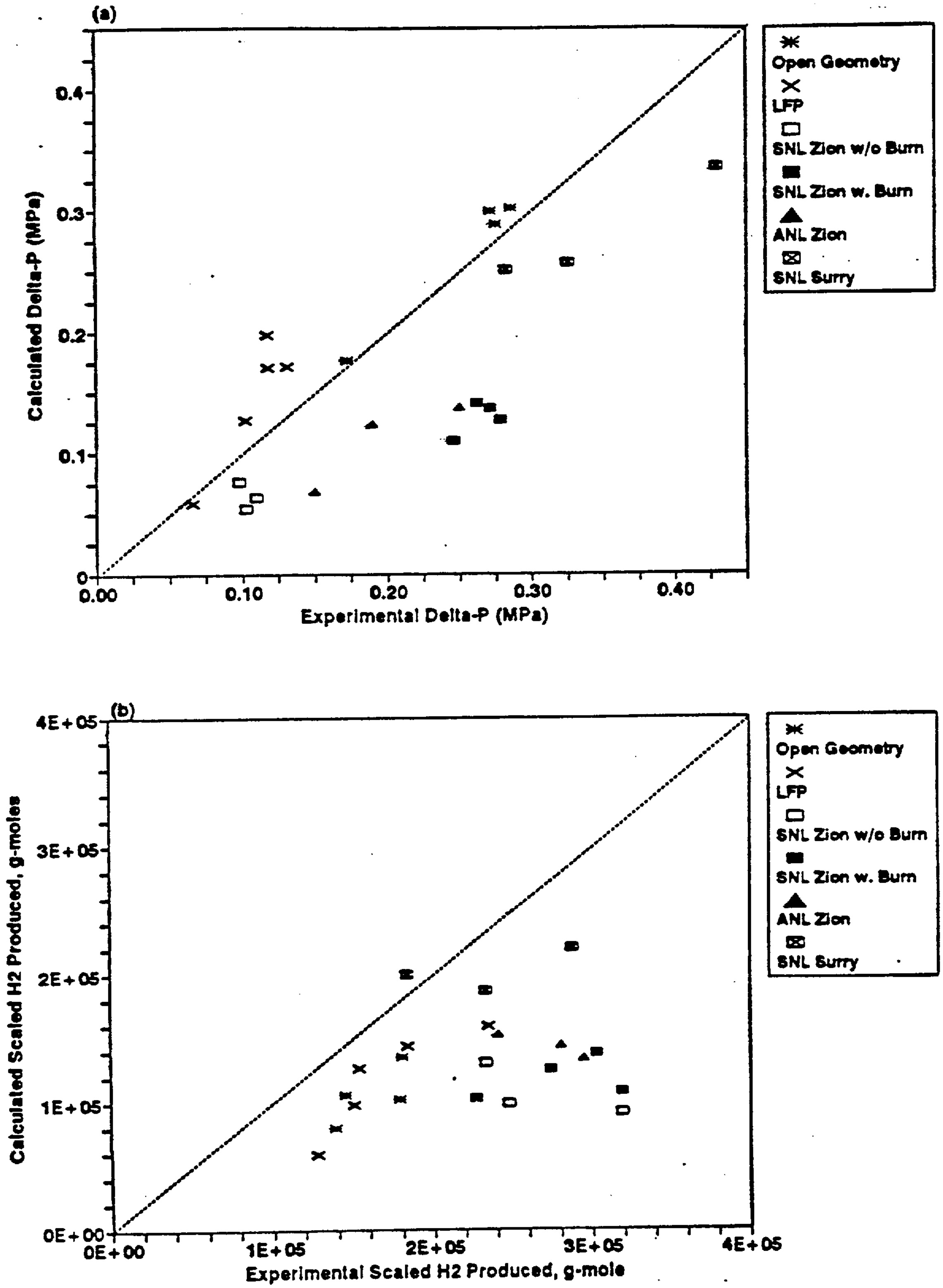

Figure 3-2. CONTAIN predictions versus experimental results for (a) ΔP and (b) scaled H_2 production with only processes considered in the DCH issue resolution models allowed to contribute to the DCH energy release.

gives the TCE results; it is seen there is a moderate underprediction of ΔP and a much larger underprediction in hydrogen production. Case 2 gives the results for the CONTAIN standard prescription, which shows reasonably good agreement for both ΔP and hydrogen production.* Case 3 gives the CONTAIN results with the NAD interactions deleted, as in Figure 3-2. Both ΔP and hydrogen production are underpredicted by about a factor of 2.

Table 3-1
Model Comparisons with Experiment

Case	Description	SNL/IET-3		SNL/IET-4	
		ΔP (MPa)	H_2 Prod. (g-moles)	ΔP (MPa)	H_2 Prod. (g-moles)
	Experimental Results	**0.246**	**227**	**0.262**	**303**
1	TCE	0.186	115	0.209	137
2	CONTAIN std. input prescription	0.228	253	0.266	288
3	No NAD	0.110	103	0.141	138
4	No NAD, no atm-struc hx; 100% burn DCH-produced H_2	0.183	104	0.235	140
5	No NAD, default atm-struc radiation	0.122	104	—	—
6	No NAD, no atm-struc radiation	0.130	104	—	—

Case 4 gives CONTAIN results calculated with no NAD or debris-water interactions modeled, with no atmosphere-structure heat transfer modeled, and with all DCH-produced hydrogen allowed to burn. Thus the processes considered are, to a reasonable approximation, restricted to those considered by TCE, and the results agree reasonably well with the TCE results for both ΔP and hydrogen production. This lends additional support to the belief that TCE achieves approximate agreement with experimental ΔP results (but not with hydrogen production results) only because the neglect of important mitigation processes is approximately balanced by the neglect of important processes that contribute to DCH.

Since CONTAIN Cases 3 and 4 include no debris-water interactions or NAD interactions, these conclusions are in no way sensitive to the assumptions that have been used to model NAD interactions and/or debris water interactions, phenomena which are admittedly quite uncertain and concerning which there has been some controversy. Instead, the conclusions are only dependent upon the mitigation processes that are modeled by CONTAIN but neglected by TCE, of which the two principal processes are:

*The fact that CONTAIN ΔP gives better agreement with experiment than TCE for these two cases is not in itself very significant because TCE sometimes does better than CONTAIN for other experiments; however, the fact that TCE did tend to underpredict ΔP for the SNL/IET (Zion) geometry experiments in which hydrogen could burn is considered significant (see Section 7.2).

1. Oxygen supply in the cavity and subcompartments is far too limited to permit complete combustion of all the DCH-produced hydrogen; hence oxygen starvation in the subcompartments delays combustion of much of the DCH-produced hydrogen until it is transported to the dome, and some hydrogen that remains in the subcompartments may not burn at all.

2 Significant atmosphere-structure heat transfer occurs during the event, which reduces the pressure rise that would otherwise occur. The delay in hydrogen combustion noted in (1) increases the time available for atmosphere-structure heat transfer to mitigate the event.

Concerning the first process, there can be little debate over the fact that hydrogen cannot burn until it is transported to an oxygen-bearing environment. Concerning the second process, the CONTAIN heat transfer models are, with one exception, among the most mature models in the code. The recent CONTAIN peer review (Boyack et al., 1995) assigned them to Category 1, which is the most favorable of the seven categories the peer review used to categorize the technical adequacy of the models in the CONTAIN code.

The one exception noted above involves the calculation of atmosphere-structure radiant energy transfer under DCH conditions. The CONTAIN default radiation model includes only the optically active gases and neglects aerosol effects. In the DCH standard input prescription, it is assumed that dense, highly luminous clouds of aerosols (as observed in many experiments) enhance atmospheric emissivity. Hence, in the DCH standard prescription, the default model is overridden by a user-specified value of 0.8 for the atmospheric emissivity. As Boyack et al. (1995) noted, this treatment is nonmechanistic and sensitivity studies were recommended to assess the impact of uncertainties in this treatment. A number of sensitivity calculations for this purpose are reported in SAND94-1174, two of which are included in Table 3-1. Case 5 was run using the default radiation model, with no credit given for luminous aerosols; comparison with Case 3 shows only a modest increase in ΔP. Even if atmosphere-structure radiant heat transfer is totally deleted (Case 6), which is surely very unrealistic, a substantial degree of mitigation is still calculated and the experimental ΔP is seriously underpredicted.

Other sensitivity studies reported in SAND94-1174 examined sensitivity to uncertainties in debris-gas interaction rates and uncertainties related to nonuniform gas distributions within the subcompartments. Neither gave any indication that heat transfer uncertainties were nearly large enough to account for much of the discrepancy between Case 3 and the experimental results; nor are they large enough to cast doubt upon the conclusion that the mitigation effects neglected by TCE are actually quite important, and that TCE must also be neglecting other important effects that augment DCH.

As an additional check, a hand calculation was performed for estimating the amount of mitigation that might be expected from atmosphere-structure heat transfer and incomplete hydrogen production. Results, summarized in Appendix C of this report, are in reasonable agreement with the extent of mitigation implied by the differences between Cases 3 and 4 in Table 3-1.

Figures 3-1 and 3-2, and also the cases given in Table 3-1, illustrate another important point concerning the CONTAIN calculations presented in SAND94-1174. Except for the cases in which atmosphere-structure heat transfer was artificially turned off, the code generally obtained good results for the ΔP data in the IET experiments if and only if modeling assumptions were used which also permitted it to obtain reasonable agreement for the hydrogen data. Obtaining this result depends upon the balance between several processes: debris-gas heat transfer, debris-gas chemical reaction, hydrogen combustion energy release, and atmosphere-structure heat transfer. The balance between these processes cannot be changed by the parametric features of the nonairborne debris modeling and/or the debris-water interaction modeling because these models still use the same basic heat/mass transfer analogy as is used elsewhere in CONTAIN. Hydrogen production is controlled by gas-phase mass transfer rates in the model and, because of the heat-mass transfer analogy, heat and mass transfer cannot be tuned separately. In addition, changing the input to the nonairborne and debris-water models has no effect upon the atmosphere-structure heat transfer model or the combustion models. Hence the fact that either ΔP and hydrogen results are both in reasonable agreement with experiment or else neither are in agreement provides support for the heat/mass transfer analogy and the atmosphere-structure heat transfer modeling in CONTAIN, despite the uncertainties in the modeling of nonairborne debris and debris-water interactions.

As noted previously, it is my belief that the major processes contributing to DCH that TCE (and CLCH) neglect are debris-water interactions and the interactions of nonairborne debris with the noncoherent portion of the blowdown steam. Some arguments as to why these hypotheses are physically reasonable are summarized in Appendix C of this report. The uncertainties in models for these effects are admittedly large and the hypothesis that these effects matter at all is controversial, as not all knowledgeable investigators have accepted it. However, the key point here is that the arguments for believing that TCE neglects important DCH contributors do not depend upon the validity of the nonairborne debris and/or debris-water interaction hypotheses, nor do they depend upon the CONTAIN treatment of these processes. Instead, they depend principally upon the arguments for believing that the *mitigation effects* neglected by TCE and CLCH are important. There is much less uncertainty concerning these mitigation effects than there is concerning debris-water interactions and nonairborne debris interactions. Indeed, if the latter effects could be shown to be completely negligible, it would simply mean that the augmenting effects that compensate for the mitigation effects neglected by TCE have not even been identified, and the DCH "issue" would be even further from "resolution" than I would argue.

The combined effects of neglecting important contributing processes and also neglecting important mitigators, together with a certain amount of tuning of the coherence ratio (see Section 5 and Appendix B of this report), do permit TCE (and CLCH) to obtain an approximate match to the experimental ΔP data. However, the DCH data base samples only a limited subset of the relevant parameter space; it is not likely that this fortuitous cancellation of opposing errors will apply to all scenarios of interest to DCH analysis at NPP scale. TCE as applied in the DCH issue resolution work includes <u>no allowance</u> for any of these effects, and <u>no allowance</u> has been made for any <u>uncertainty</u> resulting from the neglect of these effects. Until these uncertainties have been evaluated, the claim that DCH has been "resolved" in the existing DCH issue resolution studies is seriously compromised.

4 Limitations to the Validation Claimed for TCE

A limitation of the presentations of TCE (and CLCH) given in the issue resolution documents [principally in Appendices D and E of Pilch et al. (1994a)] is that there is relatively little "bottom-up" support offered for several of the basic modeling assumptions that were used in these models. That is, there is neither detailed analysis nor separate-effects data cited to support the assumptions that debris-gas equilibrium is achieved for airborne debris or that atmosphere-structure heat transfer, incomplete hydrogen combustion, debris-water interactions, and nonairborne debris interactions are all negligible. Hence the defense for the use of TCE rests principally upon the integral validation results claimed for it. In Section 4.1, we consider comparisons between TCE and experiment, and note reasons why there are severe limitations in the degree to which DCH models can be validated by comparisons with the ΔP results alone. In Section 4.2, we show that the resolving power of the integral data base is increased if one also includes comparisons between DCH model predictions and experimental results for hydrogen production; however, TCE fails almost completely to correlate the hydrogen production data except for a limited subset of the data and the reasons offered to explain this failure are far from convincing. Section 4.3 provides some additional discussion of the limitations of the existing data base for DCH model validation.

4.1 TCE Validation Claimed for ΔP

In Figure 4-1a, predicted and experimental values of ΔP are compared for the TCE model. The significance of Figure 4-1b is discussed below. Plot symbols distinguish cases in which hydrogen could burn versus cases in which an inert atmosphere prevented combustion; cases performed with a linear scale factor, S, of 0.1 versus smaller-scale experiments; and the 1/6- scale Surry IET experiments performed in the CTTF facility (labeled SNL/CTTF/S in the legend). TCE predictions are taken from Appendix E of Pilch et al. (1994a). This reference gives ΔP results only for experiments performed in compartmentalized geometries and, hence, only these cases are plotted in Figure 4-1a. In addition, only data for steam-driven tests are included in the figure.*

It is apparent from Figure 4-1a that, with some qualifications, TCE gives a reasonable correlation of the DCH ΔP data base; indeed, global agreement between the model and experiment is comparable to that obtained with CONTAIN in Figure 3-1a. However, this result is not as significant as one might suppose because it turns out that the DCH data base exhibits a relatively simple systematics that can be fit by DCH "models" that are demonstrably very inadequate. We can illustrate this point using what will be called the total steam correlation (TSC). This correlation is based upon the simple assumption that, in

*ANL/IET-8 is not included here because TCE substantially overpredicted ΔP for this experiment owing to incorrectly predicting the threshold for combustion of DCH-produced hydrogen and the well-known difficulties associated with predicting combustion thresholds is not at issue here; SNL/IET-12 is omitted because this experiment exhibited anomalous behavior in several respects (Blanchat et al., 1994a) and it has not been used for model validation purposes.

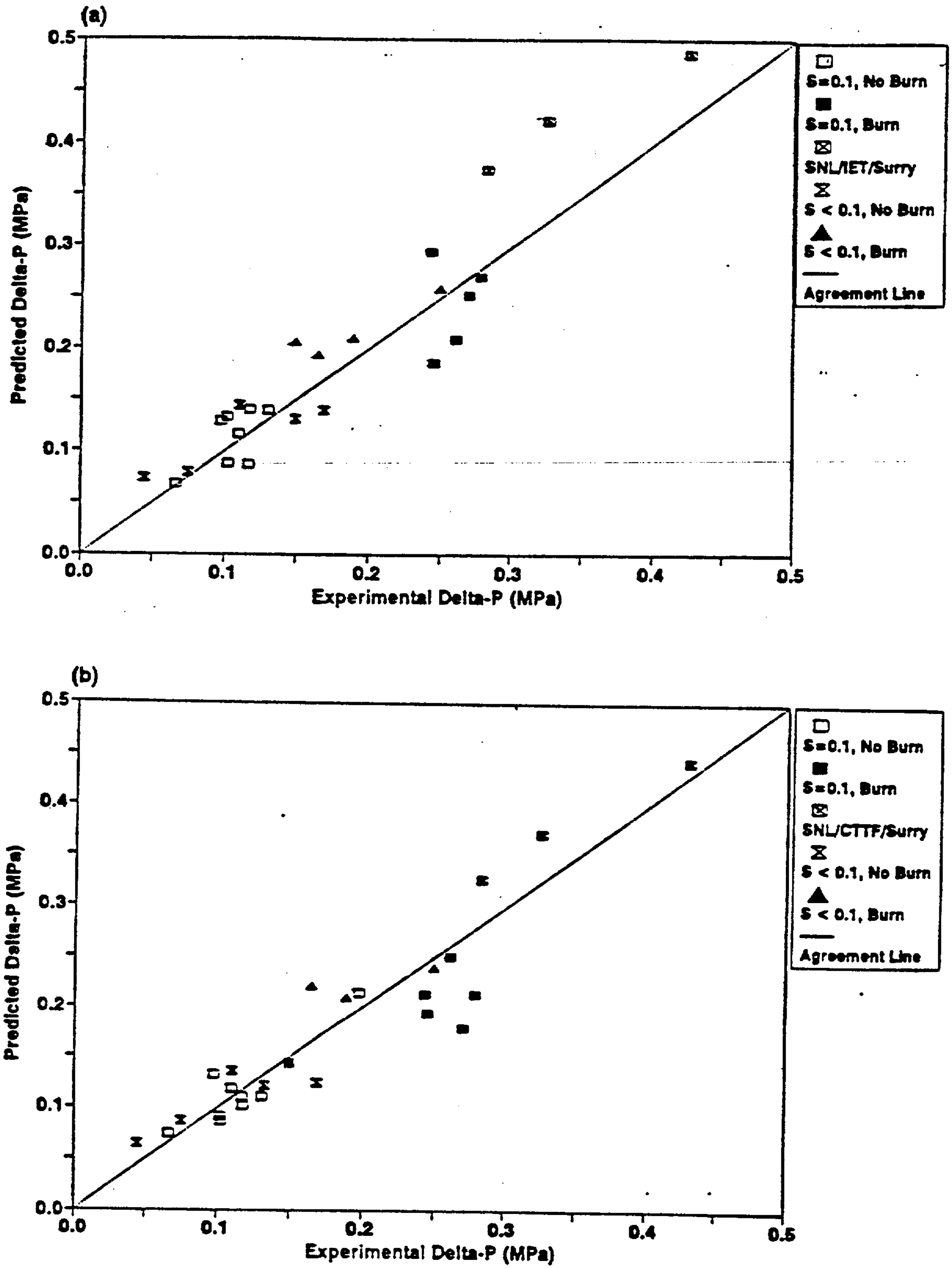

Figure 4-1. Predicted versus experimental ΔP results for (a) the two-cell equilibrium (TCE) model and (b) the total steam correlation (TSC).

compartmentalized geometries, the total net energy addition (thermal and chemical) to the containment atmosphere is proportional to the total steam supply in the accumulator that simulates the RPV. One motivation for seeking such a correlation is provided by the importance of the role that the steam supply was found to play in early CONTAIN analyses of DCH in controlling rates of transport of thermal energy and hydrogen to the containment dome (Williams et al., 1987). However, no detailed theoretical justification for this approach is offered here (none could be offered as it is clearly a gross oversimplification at best); instead, we simply consider the degree to which some dominant trends of the DCH data base can be fit by this assumption.

We represent the assumed relationship between energy added to the containment (ΔU) and the accumulator steam supply by $\Delta U = C_1 N_{0,acc}$, where $N_{0,acc}$ is the number of moles of steam initially present in the accumulator and C_1 is the proportionality constant. Using the ideal gas law, the corresponding pressure rise in the containment can be shown to be approximately

$$\Delta P \approx \frac{N_{con} R \Delta T}{V_{con}} = \frac{R \Delta U}{V_{con} C_v} = C_1 \frac{R N_{0,acc}}{V_{con} C_v}. \qquad (4\text{-}1)$$

Here, N_{con} is the total number of moles of gas and steam in the containment vessel, R is the universal gas constant, ΔT is the containment temperature rise, V_{con} is the containment volume, C_v is the constant-volume molar heat capacity of the containment atmosphere, and we have used the relationship $\Delta T = \Delta U / N_{con} C_v$ to obtain the second form of Eq. (4-1). The constant C_1 is estimated by fitting to the data; since hydrogen combustion is very important to the chemical energy contribution, different values of C_1 are allowed for cases in which DCH-produced hydrogen did or did not burn. Other than this distinction, the same value of C_1 is used in all cases, independently of all other parameters of the experiment. Only experiments performed in compartmentalized geometries are included in the fitting.

Note that C_1 is not dimensionless, and it is not to be expected that Eq. (4-1) could be of use in estimating DCH loads generally. For example, Eq. (4-1) does not even include such obviously important parameters as melt mass and composition. Here we are only examining its ability to correlate the existing data base.

In Figure 4-1b, ΔP values given by Eq. (4-1) are plotted against the experimental values for all DCH experiments that have been performed in which the containment was compartmentalized and steam was the driving gas. Data required for evaluating Eq. (4-1) were taken from the compilation of DCH experimental parameters and results given by Pilch et al. (1994a), and the experiments included are the same as those included for TCE in Figure 4-1a. It is evident that the ΔP values are strongly correlated by the accumulator steam supplies and hydrogen combustion behavior, with about 86% of the variance in the ΔP values being explained by these two factors (i.e., $R^2 = 0.86$). Furthermore, the ability of Eq. (4-1) to correlate the data is about as good as is the case for TCE in Figure 4-1a, for which $R^2 = 0.88$.

Lest there be any confusion, TSC is not offered as a predictive model for DCH loads. Quite the contrary, the principal purpose of introducing TSC in the present context is to illustrate how a demonstrably *inadequate* model can fit the ΔP data reasonably well. TSC cannot possibly provide an adequate model for predicting DCH loads in general: it includes no dependence upon most of the potentially important DCH parameters such as melt characteristics (mass, composition, temperature), vessel failure size, coherence ratio, fraction of debris dispersed from the cavity, presence or absence of pre-existing hydrogen in the containment, etc. The fact that TSC correlates the ΔP data as well as does TCE means that one cannot claim to have validated the dependencies of the TCE model upon these parameters simply by presenting plots such as Figure 4-1a. However, this type of plot is the only validation for TCE that is offered in the entire issue resolution effort. For example, there are no attempts to identify cases in which a single parameter is varied and to determine whether TCE reproduces the observed variations in the experimental results.

Some reasons for the limited utility of the DCH ΔP data base for model validation are discussed in Section 4.3.

4.2 TCE Validation Claimed for Hydrogen Production

Figure 4-2a compares TCE predictions with the experimental results for hydrogen production, and Figure 4-2b presents the comparison for TSC.* As in Figures 3-1b and 3-2b, results are expressed in terms of g-moles of hydrogen produced after scaling up to plant scale by dividing by S^3 in order to facilitate comparison of results obtained at different scales. Data for TCE are taken from Appendix E of Pilch et al. (1994a), and include results for both open-geometry and compartmentalized-geometry experiments. In the legend, "dry & inert" means there was no water in the cavity and the containment atmosphere was inert, "wet" means there was at least some water in the cavity, "Ox" indicates oxygen was present in the containment atmosphere, and "SNL/IET/S" refers to the 1/6-scale Surry-geometry IET experiments. The latter experiments had oxygen in the containment atmosphere, as well as steam.

When the complete hydrogen production data base is considered, it is evident from the data plotted in Figure 4-2a *that there is no statistically significant correlation at all between TCE model predictions for hydrogen production and the experimental results ($R^2 \approx 0.01$).* These results may be contrasted with the CONTAIN predictions of hydrogen production, which reproduced the dominant experimental trends reasonably well (Figure 3-1b). Note also the contrast with respect to the ΔP results, for which TCE and CONTAIN demonstrate comparable abilities to reproduce the experimental data. Even the simplistic TSC reproduces the experimental trends for hydrogen production better than does TCE; although Figure 4-2b shows much scatter in the data, there is still a significant correlation ($R^2 \approx 0.5$).

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*For hydrogen, TSC consists simply of the assumption that hydrogen production is proportional to the accumulator steam supply: $N_{H2} = \epsilon N_{0,Acc}$, where ϵ is the steam-to-hydrogen conversion efficiency. Again, ϵ is to be determined by fitting to the data. Here a single value was used for both the burn and no-burn cases. (The value of ϵ obtained is about 0.5).

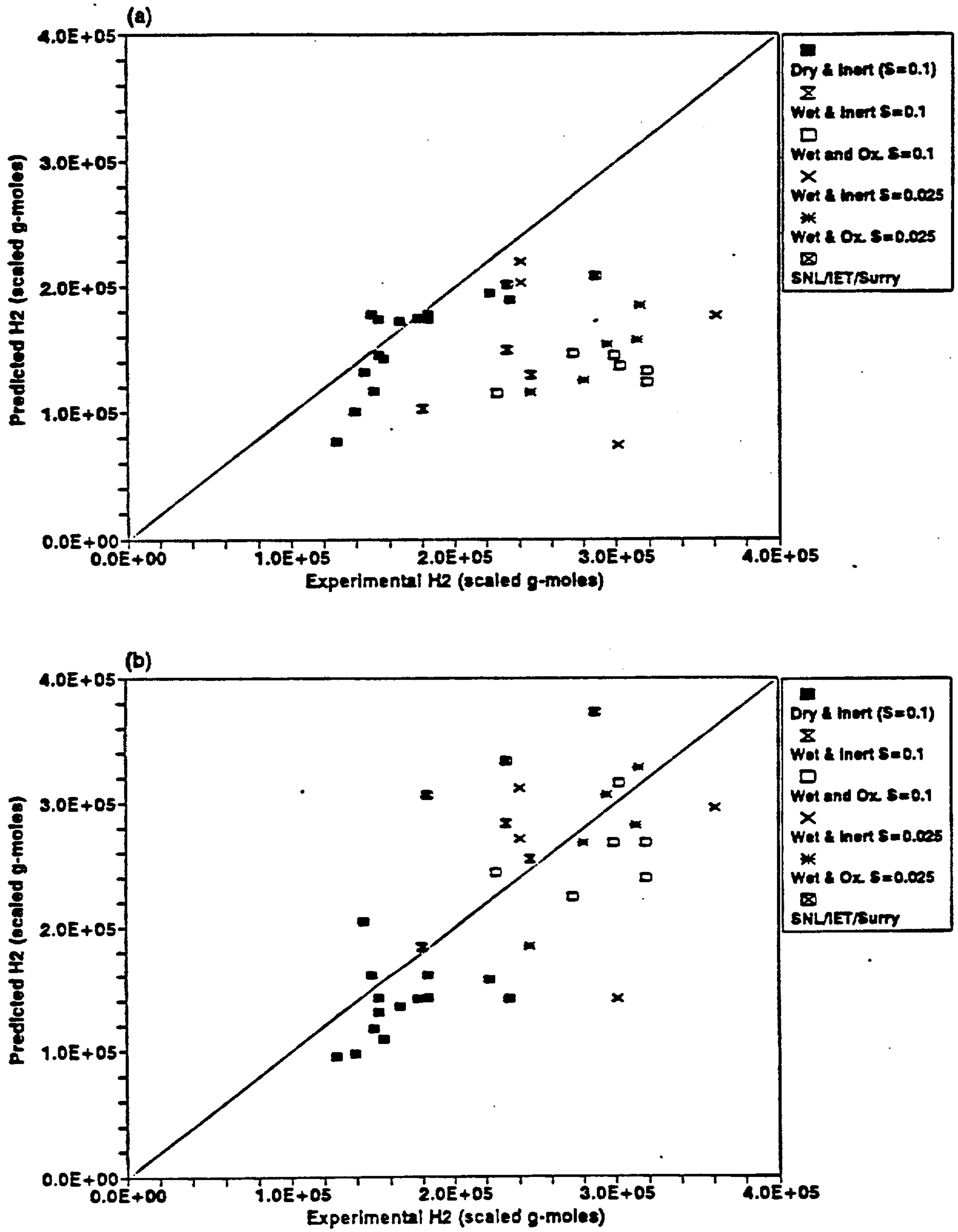

Figure 4-2. Predicted versus experimental scaled hydrogen production results for (a) the two-cell equilibrium (TCE) model and (b) the total steam correlation (TSC).

Pilch et al. (1994a) acknowledge that TCE substantially underpredicts the hydrogen production in many of the experiments for which there was either water in the cavity or oxygen in the containment atmosphere, or both.* However, it is argued there that only the experiments with no water in the cavity (or elsewhere in the containment) *and* with inert atmosphere should be included in validating model predictions for hydrogen production on DCH time scales. Here, "DCH time scales" may be taken to be approximately the time required to complete the blowdown of the steam accumulator. This blowdown time was typically about equal to, or slightly greater than, the time at which the containment vessel pressure reached its maximum value.

The only cases accepted for TCE validation by Pilch et al. (1994a) are the "dry & inert" cases in Figure 4-2, and these cases do show an approximate correlation between TCE predictions and experimental results. Note that restricting validation to these cases limits the data base for model validation to experiments that have very nonprototypic atmospheric compositions. It also limits the validation base to experiments with relatively low driving pressure (accumulator pressures $\leq$ 4.6 MPa) and with nonprototypic containment geometries, because all the experiments with higher driving pressures and/or prototypic containment geometries (that is, the IET experiments) had either water in the cavity, oxygen in the containment atmosphere, or both.

The argument offered for restricting comparisons to the "dry & inert" cases was that, if either water or oxygen were present within the containment, the apparent production of hydrogen would be increased by slow reactions of metal with water and/or oxygen that occur too late to contribute to DCH, but which would still be reflected in the results of the gas analyses used to infer hydrogen production. Arguments that have been advanced in favor of this "late reaction" hypothesis are reviewed in Appendix A of this report, where it is concluded that the arguments are unconvincing in all cases and, in some cases, clearly involve misinterpretations of the available data. Hence it is concluded in Appendix A that the "late reaction" hypothesis is essentially *ad hoc*, with no evidence to support it other than the fact that the experimental results do not agree with TCE.

Here again there appears to be an irreconcilable conflict with the CONTAIN analyses of the DCH experiments, especially the Zion-geometry IET experiments. In Section 3.2, it was noted that CONTAIN could reproduce the ΔP results reasonably well *only* if one also included processes that permitted the code to reproduce the hydrogen production reasonably well. If there was insufficient hydrogen production in the calculation, ΔP was also too low, especially in the cases in which combustion of the DCH-produced hydrogen is an important contributor to ΔP. (Only hydrogen production on DCH time scales was modeled in the CONTAIN analyses; no "late reactions" of metal were modeled.) Hence, if it were to be established that 50% or more of the hydrogen production reported for these experiments

*The fact that there is no correlation between the model predictions and the experimental results is less apparent in Pilch et al. (1994a) because the data are presented in four-cycle log-log plots without factoring out the effects of experiment scale. Hence the plots are dominated by effects of the ~200-fold variation in melt mass in going from the 1/40-scale ANL/IET experiments to the 1/6-scale SNL/IET (Surry) experiments.

actually is produced too late to contribute to DCH, it would be very difficult to reconcile the CONTAIN model with the experimental results.

For TCE, the situation is the reverse. For the experiments in which DCH-produced hydrogen can burn, one could not bring both hydrogen production and ΔP into agreement with experiment without making major alterations to the fundamental assumptions of the model. Both the extent of debris-gas heat transfer and the extent of hydrogen production are limited by the amount of coherent steam in the TCE analyses of the Zion IET experiments. If one made changes that increased the hydrogen production sufficiently so as to agree with experiment (e.g., by increasing the estimates of the coherent steam), then ΔP would be substantially overpredicted. Thus, either ΔP will be considerably overpredicted or else hydrogen production will be substantially underpredicted in TCE; no simple tuning of the model or its input could bring them both into agreement. Hence invoking the "late reaction" hypothesis to explain away the failure of the model to predict the hydrogen data is essential for accepting the model, and it would appear that the validity of the model must largely stand or fall with the validity of the "late reaction" hypothesis.

It should also be noted that the "late reaction" hypothesis as offered by Pilch et al. (1994a) was purely qualitative. That is, there was no attempt to develop a quantitative model for late reactions that would predict the amount of hydrogen that is actually inferred from the experiments. No explanation has been offered as to why the amount of "late reaction" occurring should just happen to correspond to the amount of hydrogen that the CONTAIN model indicates is required in order to explain the ΔP results once the mitigating effects neglected by TCE are taken into account.

If the basic assumptions of TCE are as deficient as is argued here, it is of some interest to inquire as to why the model does approximately reproduce the trends for hydrogen production in the "dry and inert" cases. This question is also discussed in Appendix A. Very briefly, it is concluded there that these experiments happen to be insensitive to the basic assumption of TCE that debris-steam interactions are limited to the interaction of airborne debris with the coherent portion of the steam blowdown, and it is the failure of this assumption that is responsible for many of TCE's shortcomings. The reasons for this insensitivity to the coherence assumption are related to parameters of these particular experiments that have nothing to do with the postulated occurrence of late reactions when water and/or oxygen are present; see Appendix A for details.

4.3 Some Limitations to the DCH Data Base for Model Validation

The DCH issue resolution documents repeatedly emphasize that the DCH models have been validated against the "extensive database" (Pilch et al., 1996) but present little discussion of possible limitations in this data base for model validation purposes. In Section 4.1, it was shown that even demonstrably inadequate models can do a surprisingly good job of reproducing the major trends in the data base, at least insofar as the ΔP results are concerned. Here we consider some of the reasons why there are important limitations to the data base for model validation purposes.

Before continuing, I wish to acknowledge that the DCH data base represents a remarkable technical achievement in many ways. A large number of experiments have been performed using highly energetic materials that are difficult and potentially even dangerous to work with. The experimentalists, especially, are to be commended in their successful execution of these experiments, and nothing herein is intended to imply criticism of their efforts.

That said, it needs to be noted that the requirements for model validation have not been the principal guide for design of the overall experimental program. In the design of the experimental program, the NRC and its guiding review groups adopted a strategy emphasizing study of specific accident scenarios identified as being important by the SASM Technical Program Group (Zuber et al., 1991) and other NRC peer review groups; it has not been designed as a general model validation exercise. There are a number of potentially important parameter sensitivities that have not been systematically studied experimentally and for which DCH models are therefore not fully validated. Uncertainties associated with this limitation require careful consideration when the need arises to apply these models outside the range of the supporting data base. As will be noted later in this subsection, the existing DCH issue resolution applications do involve a number of extrapolations outside the data base in several regards; considerably larger extrapolations could be required if future work indicates a need to consider wider uncertainty ranges in the initial conditions than have been acknowledged in the issue resolution work.

Limited Parameter Variations. One limitation of the data base is that there are a number of potentially important parameters that have not been varied, or have not been varied under conditions for which DCH models would predict that the variations would make a difference. It is partly for this reason that the almost-trivial TSC can provide about as a good a fit to the ΔP data for compartmentalized containment geometries as do more sophisticated DCH models. Some examples of this limitation of the data base include the following:

- The scaled melt mass, metallic content, and temperature were essentially the same in all the Zion and Surry IET experiments. There were some variations in the melt mass in earlier, less prototypic experiments, but driving pressure (and hence steam supply) was low ($\leq$ 4.6 MPa, mostly $<$ 4 MPa) in these experiments and therefore the extent of debris-steam interactions was limited by the steam supply. Hence there are no data for testing model predictions as to how DCH loads depend upon melt mass except for conditions under which little sensitivity to melt mass would be expected. (This is especially true for experiments performed in compartmentalized geometries.)

  Three experiments, designated the ANL/U series, were performed at ANL using prototypic core materials (UO_2, ZrO_2, Zr, Cr, Fe) in the 1/40-scale Zion IET geometry. Although there were some differences with respect to the results of experiments using aluminum/iron oxide thermites, the results of the ANL/U experiments generally supported the expectation that the thermite experiments do provide useful simulations of DCH events. Total melt mass and metallic content of the ANL/U experiments were scaled to the thermite experiments and the results therefore do not provide a test of how model predictions depend upon melt mass and metallic content.

- DCH models generally indicate that DCH loads in compartmentalized geometries will increase as the vessel failure size increases when the driving pressure is high but the effect is small when the driving pressure is low. There is, however, no test of this prediction because hole size has not been varied significantly except in experiments performed at low pressures, ≤ 4 MPa.

- The CONTAIN code indicates that small to moderate amounts of cavity water co-dispersed with the debris may have the potential to enhance DCH loads in compartmentalized geometries, but there are no wet/dry counterpart experiments adequate to provide a direct experimental test of this possibility. Likewise, CONTAIN predicts moderate amounts of co-ejected RPV water have the potential to enhance loads, but there are no experimental tests of this possibility. The possible effects of water in DCH are discussed further in Appendix C of this report.

- Although some experiments have been performed with pre-existing hydrogen in the containment atmosphere, none have been performed under conditions for which the CONTAIN model predicts that its combustion would have a substantial effect (Williams et al., 1997).

Extrapolations Required. There are several applications of TCE in the DCH issue resolution work that require extrapolations beyond the existing data base. Examples include:

- All the scenarios involved in the issue resolution work include RPV water co-ejected with the debris. CONTAIN calculations indicate that, like cavity water, moderate amounts of co-ejected RPV water have the potential to enhance DCH loads in compartmentalized geometries. Scenario VI (see Section 2), at least, falls in the regime for which enhancement is possible. In the DCH issue resolution work, however, it is assumed water will either have no effect or will mitigate DCH loads. There are no experimental data adequate to test any of these assumptions concerning co-ejected water.

- Pre-existing hydrogen concentrations in many of the DCH issue resolution analyses are considerably higher than in the experiments used to justify the TCE modeling assumptions that predict the pre-existing hydrogen will not contribute to DCH in station blackout accidents (see Section 6.2 for additional discussion).

- As was noted in Section 2, the melts assumed in the DCH issue resolution work have a much lower metallic content than the melts used in the experiments. While there is little doubt that reduced metallic content is a mitigative factor, it remains true that there is no validation for the extent of mitigation that TCE (or CONTAIN for that matter) predicts. If, for example, nonstoichiometric uranium oxide effects can enhance hydrogen production from metal-poor melts, it would not be revealed in the existing data base.

- The RPV is surrounded by a stainless steel foil thermal insulation which has been simulated in only one experiment (SNL/IET-11, Surry geometry). This one experiment indicated that the insulation was melted and ablated by debris and may have contributed to hydrogen production (Blanchat et al., 1994); the DCH issue resolution analyses make no allowance for any enhanced hydrogen production from the insulation (see Section 7.5).

- Obviously, application of any DCH model to NPP analysis requires large extrapolations with respect to scale. The TCE modeling assumptions and supporting scaling analyses include only scale-invariant processes and hence the model predicts that DCH loads will not depend upon scale. The fact that plots such as Figure 4-1a yield no gross scale dependence in the ability of the model to correlate the integral ΔP data was interpreted as validating these modeling assumptions (Pilch et al., 1994a). Other analyses (Williams et al., 1997; Kmetyk, 1993) have cited evidence that there is substantial scale dependence in specific DCH phenomena including the coherence ratio and hydrogen combustion efficiency; Sections 5 and 6 give some additional details. The issue resolution analyses have not allowed for these possible scale dependencies in extrapolations to NPP scale.

It is inevitable that there will be a need for substantial extrapolations beyond the available data base in any comprehensive analysis of an important NPP severe accident issue. What is of concern here is that no allowance has been made for the uncertainties involved in making these extrapolations. The claim is repeatedly made that the applications made of TCE primarily involve only "interpolation rather than extrapolation" with respect to the existing data base (Pilch et al., 1994a; Pilch et al., 1994b; Pilch et al., 1995; Pilch et al., 1996). When the modeling uncertainties are discussed at all, it is either argued that the DCH issue resolution models are conservative or that the uncertainties involved are minor. Some sensitivity studies are presented involving uncertain inputs to the TCE model (although these are quite limited); however, no allowance for modeling uncertainties in the TCE model itself are factored into the probability distributions calculated for containment loads. This failure to include an adequate allowance for the cumulative impact of the uncertainties considered here is an important failing of the DCH issue resolution work.

5 Role of the Coherence Ratio in TCE and CLCH

The modeling used in the DCH issue resolution work assigns great importance to mitigation of DCH loads that results from the limited temporal coherence between debris dispersal and blowdown steam from the primary system. In Section 5.1, some evidence is presented that coherence may not be as important as is claimed in the issue resolution work. Section 5.2 summarizes some problems with the methods used to estimate coherence from the experimental data and notes some implications of these problems, which include an unacknowledged scale dependence of the coherence and a tendency to yield a spurious improvement in the agreement between TCE ΔP predictions and the experimental results.

5.1 Importance of Coherence to DCH Loads

In TCE, coherence is parameterized in terms of the coherence ratio, $R_\tau = \tau_e/\tau_b$, where τ_e is the time required to entrain and disperse debris from the cavity and τ_b is the characteristic blowdown time (Pilch et al., 1994a). A slightly different definition is used for CLCH but the essential concept is the same. The importance ascribed to coherence is illustrated by the following passage (p. 45, Pilch et al., 1994a):

> The *key modeling parameter* in both [the TCE and CLCH] models is the melt-to-steam coherence ratio. Because the entrainment time is short compared to the blowdown time, molten debris is exposed to a small fraction of the primary system steam during the dispersal process. Since this steam is the medium for carrying the melt energy and the hydrogen produced by steam/metal interactions to the main containment volume, this incoherence is a *crucial mitigating factor*. (Emphasis supplied.)

The high importance assigned to coherence necessarily follows if one accepts *the assumptions of the models* because it is *assumed* that debris which is not transported beyond the subcompartments can only interact with steam while the debris is airborne and that it remains airborne only during the time interval over which debris is dispersed from the cavity. Implicit in the argument are assumptions that a number of other processes that might contribute to the extent of debris-steam interactions may be neglected; e.g.:

- It is assumed that debris does not significantly interact with other sources of steam that may be present; e.g., steam generated by the vaporization of co-dispersed cavity water and/or co-ejected RPV water.
- It is assumed that the time interval over which airborne debris can interact with blowdown steam cannot be significantly extended by finite de-entrainment times in the subcompartments; that is, the time required to de-entrain debris once it enters the subcompartments is assumed to be negligible compared with the time required to disperse debris from the cavity.
- It is assumed that RPV blowdown steam does not interact with nonairborne debris in either the cavity or the subcompartments.

No analytical support is given for any of these assumptions; that is, there is no detailed analysis offered to support the assumption that these processes are negligible. Pilch et al. (1996) conclude that the results of DCH experiments in which water was present in the cavity are consistent with the hypothesis that cavity water does not enhance DCH loads. However, a review of the data base shows that there have been no clean experimental tests of the hypothesis that water can enhance containment loads; e.g., there are no wet/dry comparison cases available for conditions such that enhancement is potentially possible (Pilch et al., 1997; Williams et al., 1997).

Experimental Validation for the Importance of Coherence. In view of the importance assigned to coherence in the DCH issue resolution work, it seems surprising that the DCH issue resolution documents *cite no experimental data supporting the claim that coherence is important in determining DCH loads*; it is simply a conclusion drawn from the *model*. Admittedly, it is not straight-forward to define an experimental test from the existing data base. However, this difficulty does not reduce the potential importance of the fact that the coherence hypothesis lacks experimental support, a lack that is never acknowledged in the DCH issue resolution work.

One experimental test of the coherence hypothesis that does not depend upon detailed modeling assumptions is suggested by the approach used in developing the total steam correlation (TSC) of Section 4.1. If it is actually *coherent* blowdown steam, rather than *total* blowdown steam, that controls DCH loads, one would expect to obtain an improved correlation by replacing $N_{0,acc}$ by $f_{coh}N_{0,acc}$:

$$\Delta P \approx C_1 \frac{R f_{coh} N_{0,acc}}{V_{con} C_v}. \tag{5-1a}$$

Here, f_{coh} is the fraction of the total blowdown that is coherent with the debris dispersal period, and is related to the coherence ratio R_τ by

$$f_{coh} = 1 - \left[\frac{\gamma - 1}{2} R_\tau + 1\right]^{-\frac{2}{\gamma - 1}}, \tag{5-1b}$$

where γ is the ratio of specific heats (Appendix E, Pilch et al., 1994a).

Using data on coherence from Table E-8, Appendix E of Pilch et al. (1994a), Eq. (5-1) was fit to the data in the same manner as was Eq. (4-1) for the TSC. Results for the total steam and coherent steam correlations applied to the experiments in compartmentalized geometries are displayed in Figures 5-1a and 5-1b, respectively. It is apparent that the correlation with coherent steam is actually considerably *poorer*, with an R^2 value of only 0.58 compared with 0.86 for the total steam correlation. Note also that it is the Zion SNL/IET experiments with hydrogen combustion (solid square plot symbols) that are the most conspicuously underpredicted by the coherent steam correlation, just as they are in the CONTAIN results obtained when only interactions of airborne debris with coherent steam are considered (Figure 3-2). These results support the belief that DCH loads *cannot* be understood in terms of the interactions of debris with the coherent portion of the blowdown alone. Furthermore, only a relatively large effect would be readily apparent in such a simplistic analysis, and the very simplicity of the analysis renders it essentially independent of any specific uncertainties related to the detailed CONTAIN models.

Role of Coherence in CONTAIN Analyses. Some CONTAIN sensitivity studies reported by Williams et al. (1997) for the SNL/IET-6 experiment (Zion geometry) are of interest in evaluating the importance of coherence to DCH loads. This experiment was selected for analysis because the experimental coherence estimated by Williams et al. (1997) was especially low for this case, $R_\tau \approx 0.21$, which would be expected to enhance sensitivity to increases in R_τ. However, increases in R_τ by factors of two to three were found to increase the calculated ΔP by only ~10%. Early CONTAIN calculations for the Surry plant (Williams and Louie, 1988) also showed an approximately 10% increase in ΔP when the

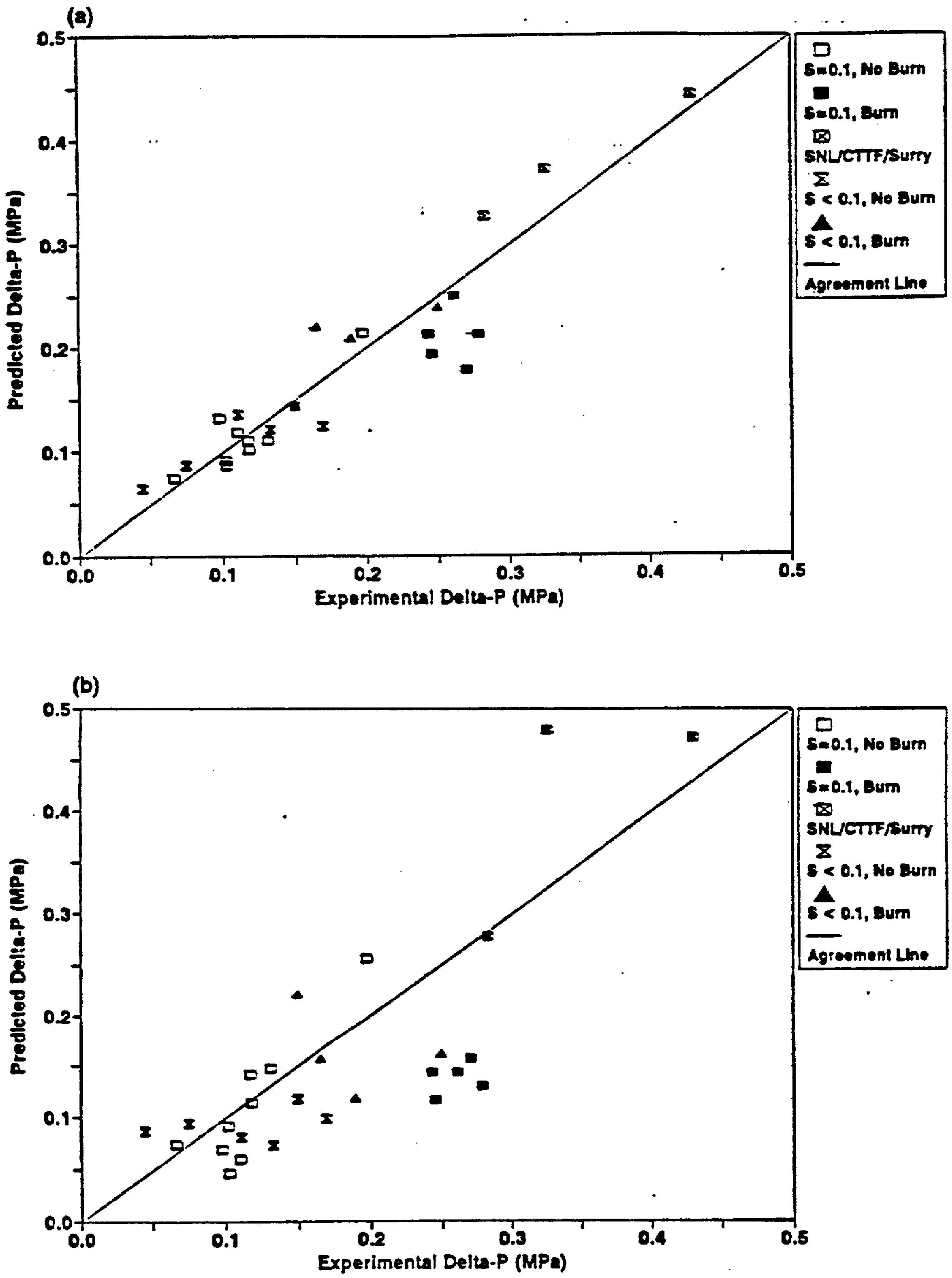

Figure 5-1. Predicted versus experimental ΔP values for (a) the total steam correlation [Eq. (4-1)] and (b) the coherent steam correlation [Eq. (5-1)].

coherence was increased by about a factor of two. These results suggest that coherence is not irrelevant to DCH loads but that it is not a dominant factor. One should not overgeneralize from the limited number of cases considered, however; even the TCE model is insensitive to coherence under some conditions (Pilch et al., 1996). In the case of the SNL/IET-6 experiment, it would be expected that TCE would show considerably higher sensitivity than did CONTAIN, but comparable sensitivity studies with TCE have not been reported.

There are several reasons why CONTAIN shows less sensitivity to coherence than TCE. One is that the CONTAIN model can include other debris-steam interactions (nonairborne debris, vaporized water) not included in TCE. Another is that protracting the debris dispersal interval, while increasing coherence, also increases the opportunity for heat transfer to structures to mitigate DCH loads.

5.2 Problems with the Experimental Determination of R_τ

Pilch et al. (1994a) estimated an experimental value for the coherence ratio for each of the experiments used in the TCE validation data base. These estimates required a determination of the time required to disperse debris from the cavity, which was derived primarily from the cavity pressurization histories. In all DCH experiments using molten thermite, there is an interval during which pressures in the cavity are significantly higher than in the main containment vessel. This time interval is plausibly interpreted as being the interval during which debris is dispersed, and pyrometers focussed on the cavity exit provide qualitative support for this interpretation.

The procedure used and the difficulties with it are discussed in detail in Appendix B of this report. Briefly, the procedure was as follows:

1. From the cavity pressurization curves, the time at which dispersal of debris was complete, t_e, was estimated. This time is taken to be the time at which the net pressurization of the cavity relative to the main containment vessel becomes negligible.

2. From the accumulator depressurization curves, the pressure in the accumulator at time t_e was determined; this pressure is designated P_e.

3. The coherence ratio, R_τ, is then calculated from the relationship

$$R_\tau = \frac{\tau_e}{\tau_b} = \frac{2}{\gamma - 1}\left[\left(\frac{P_0}{P_e}\right)^{\frac{\gamma - 1}{2\gamma}} - 1\right]. \tag{5-3}$$

There is considerable subjectivity in estimating t_e from the cavity pressurization curves and this has resulted in considerable inconsistency in the way t_e has been defined for different experiments. Pilch et al. (1994a) acknowledge a degree of subjectivity, but the extent of inconsistency seems to be greater than what one might reasonably expect. This problem is illustrated in Figure 5-2, in which the cavity pressurization histories are compared for the SNL/IET-6 and ANL/IET-6 experiments, which were scaled counterparts of one another.

It is immediately apparent from the curves that the net cavity pressurization does not abruptly decline to zero at a well-defined time; instead, pressurization tails off gradually which poses a problem in defining the "correct" value of t_e for use in TCE. It is also clear that the shapes of the pressurization curves are quite different, which poses a problem in defining t_e in a manner that is consistent in going from one experiment to the next.

No specific methodology for determining the appropriate values of t_e from the cavity pressurization curves is discussed by Pilch et al. (1994a); apparently, this was done by simple inspection of the curves ("eyeballing"). The vertical arrows labeled t_e in Figure 5-2 indicate the values that were assumed by Pilch et al. (1994a) in calculating R_t for these two experiments. For SNL/IET-6, t_e was taken to be at the extreme right end of the tail in the cavity pressurization curve, while the pickoff point for ANL/IET-6 leaves much more of the tail outside the dispersal interval.

In Appendix B of this report, an alternate method is proposed for obtaining coherence ratios in a way that is thought to yield more consistent comparisons between different experiments. This method is based upon identifying the time, t_{95}, at which the area between the cavity and the containment pressure-time histories reaches 95% of its final value. Vertical arrows labeled "t_{95}" in Figure 5-2 indicate the values of the debris dispersal time obtained using this method for the two experiments.

The accumulator is depressurizing rapidly at the time that debris dispersal ends, which makes the value of R_t quite sensitive to uncertainties in the value of t_e. The values of R_t based upon t_e cited by Pilch et al. (1994a) are 0.31 and 0.35 for SNL/IET-6 and ANL/IET-6, respectively. These values suggest that R_t is reasonably scale-invariant as is claimed by Pilch et al. (1994a). However, when R_t values are calculated using the t_{95} method, the corresponding values are 0.185 and 0.56. The differences between the values of R_t obtained by the two methods would result in significant differences in the loads calculated by TCE for these two experiments. Furthermore, the t_{95} method implies there is a large difference in R_t for the two experiments. If this difference is interpreted as representing a scale effect, it would imply that R_t exhibits a substantial dependence upon facility scale.

The IET-6 counterpart pair provides the most extreme example of a possible scale effect but it is not unique. In Appendix B of this report, the t_{95} method is applied to all the ANL/IET and SNL/IET experiments that can be considered scaled counterparts of one another. The ANL/IET R_t are substantially greater than their SNL/IET counterparts in all cases, with the average difference being somewhat greater than a factor of two.

If it is accepted that there are substantial inconsistencies in the estimation of experimental coherence ratios by Pilch et al. (1994a), there are two important consequences:

1. Uncertainties in R_t are probably greater than has been acknowledged in the DCH issue resolution work, especially when extrapolating to NPP scale.

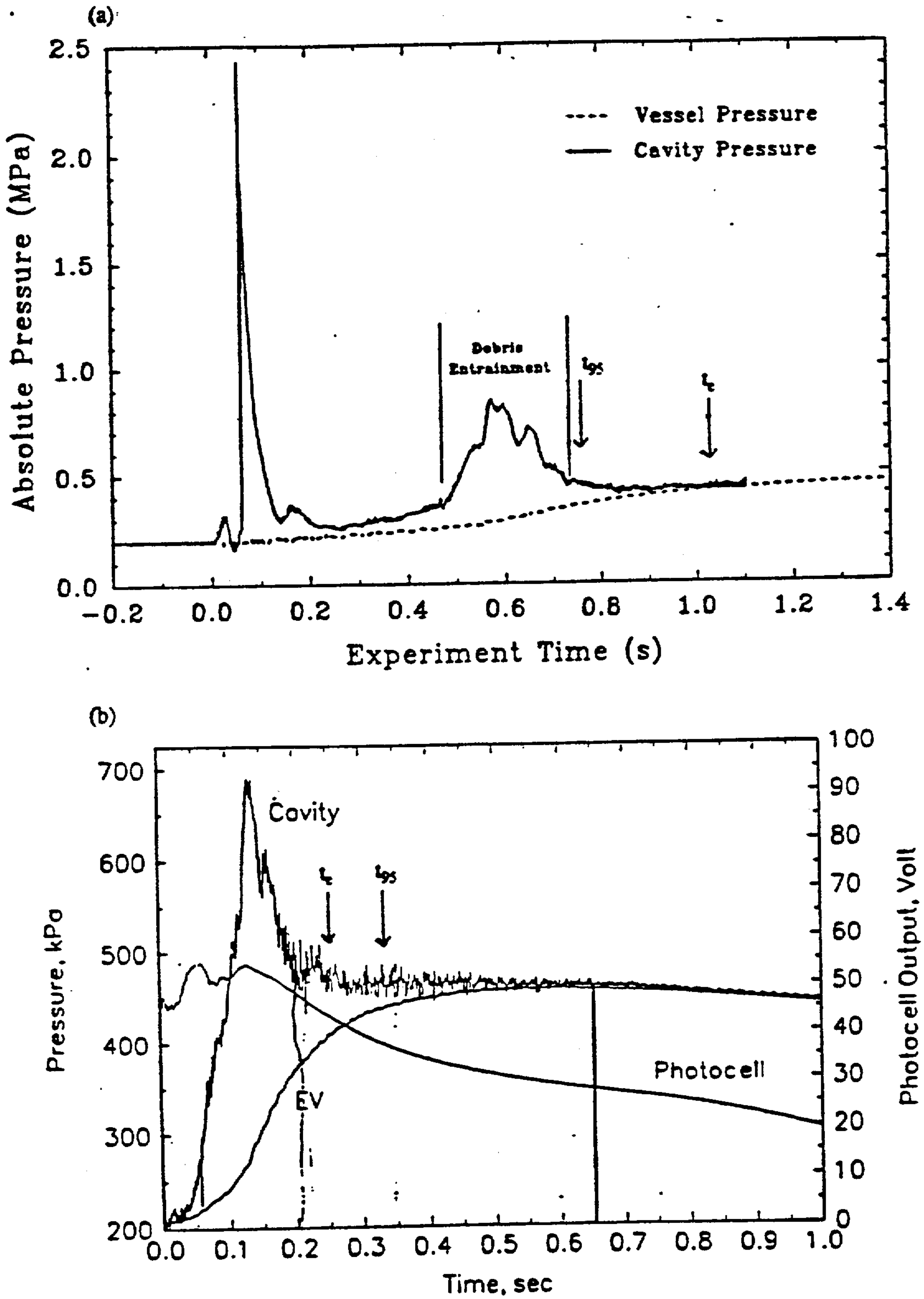

Figure 5-2. Cavity pressurization histories for (a) the SNL/IET-6 experiment and (b) the ANL/IET-6 experiment.

2. Since the validation of TCE is based upon loads calculated using the experimental value of R_γ estimated for each experiment individually, rather than using the correlation for coherence, inconsistency in estimating R_γ values affects the validation claims. In general, it appears that correcting the inconsistencies would worsen the agreement between predicted and observed ΔP values in a number of cases.

In the application to the scenarios considered in the DCH issue resolution work, the first point may not be very important because margins to containment failure are large and sensitivity to coherence is reportedly small for the cases that were considered (Pilch et al., 1996). This uncertainty would be more important if the model were to be applied to other scenarios, including scenarios potentially capable of generating containment-threatening loads.

The second point is clearly important. In the Zion IET experiments, coherence ratios were relatively low. In the TCE analyses of these experiments, the extent of both debris-steam heat transfer and hydrogen generation were limited by the amount of coherent steam, not the amount of debris or available metal. If the R_γ values input to the model for the ANL/IET analyses were twice as large as for the SNL/IET analyses, as suggested here, TCE would predict substantially higher loads for the ANL/IET experiments than for the SNL/IET experiments. Thus a substantial negative scale effect would be predicted by the model. In reality, the scale effect appears to be positive for those experiments in which DCH-produced hydrogen can burn. With corrected coherence ratios, then, the model likely would be in serious error with respect to scale effects.

Even as it is, TCE tends to overpredict the ANL/IET experiments with oxygen-bearing atmospheres and underpredict the corresponding SNL/IET (Zion) cases (see Figure 4-1a). With more consistent coherence ratios, this trend would be enhanced. Other cases in which using more consistent coherence ratios would likely worsen agreement with experiment are noted in Appendix B.

6 Combustion of Pre-Existing Hydrogen

Hydrogen released to the containment prior to vessel breach (commonly called "pre-existing hydrogen") can make a substantial contribution to DCH loads if it can burn on DCH time scales. For station blackout accidents, dilution by steam in the containment atmosphere may mean that the standard hydrogen combustion correlations sometimes either predict that no burn will occur or predict that any burn will be slow and incomplete. However, these correlations are typically developed from experiments performed at temperatures close to saturation. In DCH scenarios, the containment atmosphere is heated to elevated temperatures, increasing the likelihood that the pre-existing hydrogen will also burn and further augment the heating and pressurization that would otherwise result from the DCH event. Analyzing this hydrogen combustion is very complex for two reasons:

- The seemingly-simple hydrogen-oxygen reaction is actually a complex chain reaction process involving many steps and a number of reactive intermediates including several free-radical species. Some of the controlling rate constants are not well known for the conditions of interest in DCH analysis.

- The DCH event involves transient heating and cooling effects combined with complex gas dynamics that result in gas compositions and temperatures that vary rapidly as a function of time and a function of location within containment. These variations impose very complicated initial and boundary conditions upon the basic chemical kinetics problem.

Like any model for complex containment phenomena, the TCE model necessarily makes a number of simplifying assumptions in evaluating the combustion of pre-existing hydrogen. The fact that approximations are made and uncertainties exist is itself no grounds for criticism, as the only alternative would be to attempt no analysis at all. What is of concern is that, although the discussions given acknowledge some uncertainties, no representations of these uncertainties are given in the results (e.g., there are no sensitivity studies on hydrogen combustion). Instead, it is claimed that the treatment given is conservative (apparently meaning bounding), thereby eliminating the need for uncertainty assessment.

In Section 6.1, some key features of the treatment of pre-existing hydrogen combustion in the DCH issue resolution work are reviewed, and some important unacknowledged uncertainties and nonconservative assumptions in the treatment are identified. In Section 6.2, the experimental validation claimed by Pilch et al. (1994a) and (1994b) for the hydrogen burn modeling is considered, and it is shown that at best the existing data base for hydrogen combustion in DCH provides a test of the modeling only in a very nonconservative regime, relative to the NPP applications. Section 6.3 presents a brief summary of the findings of the present review.

6.1 Pre-Existing Hydrogen Modeling in TCE

Modeling of hydrogen combustion in TCE was first described in Appendix F of NUREG/CR-6075 (Pilch et al., 1994a) and subsequently revised in Appendix E of the NUREG/CR-6075 Supplement (Pilch et al., 1994b). In this section, citations of these references will always refer to these specific appendices unless otherwise noted.

TCE includes three processes by which pre-existing hydrogen can burn (Pilch et al., 1994b):

1. Deflagrations propagating through the mixture;
2. Volumetric oxidation of hydrogen in the bulk mixture; and
3. Entrainment of pre-existing hydrogen into the jet of burning DCH-produced hydrogen

In addition, Pilch et al. (1994b) consider possible combustion in high-temperature mixing zones that might exist under certain circumstances, and concludes that these processes are too slow to require inclusion. The arguments given have not been examined in sufficient detail in the present review to permit comment.

Unlike the treatment of combustion of DCH-produced hydrogen, the TCE pre-existing hydrogen model attempts to credit mitigation by atmosphere-structure heat transfer and/or incomplete combustion of the hydrogen, if combustion occurs at all. This is done by estimating rates of energy generation by various combustion processes and comparing them with rates of atmosphere-structure heat transfer; combustion contributes to DCH only insofar as it occurs on the DCH time scale and only insofar as the energy generation rate exceeds the heat transfer rate. Though reasonable in principle, the approach appears to be applied to each combustion process individually with a contribution being allowed only if the process adds energy more rapidly than the energy loss rate. In reality, containment pressures will continue to rise so long as the total energy addition rate from all sources, including all combustion processes, exceeds the atmosphere-structure total heat transfer rate. An individual process may still contribute significantly to the net pressurization rate even if the process by itself does not add energy at rates exceeding the total energy loss rate.

The more serious problems, however, are related to the treatment of each of the three processes deflagration, volumetric oxidation, and entrainment individually. These problems are discussed in the next three subsections.

6.1.1 Deflagration Modeling

In the TCE model, the pre-existing hydrogen can burn in a deflagration if certain flammability criteria are met. Correlations are used to predict flammability limits, flame speed, and burn completeness as a function of the temperature and composition of the gas prior to the start of the deflagration. Unlike the correlations used in systems codes such as CONTAIN and MELCOR, the TCE correlations do include a treatment of the tendency of elevated initial temperatures to favor combustion, which is a positive feature of the treatment. Although the applicability of the data cited to justify the treatment of the temperature-dependence has not been assessed in detail here, the approach used seems reasonable in principle.

In the TCE treatment, a characteristic time for the deflagration is estimated and it is assumed to contribute to DCH loads only insofar as energy release rates exceed energy loss rates resulting from atmosphere-structure heat transfer. In evaluating the model, states considered are limited to the initial containment conditions and the end state obtained by mixing the plume gases, blowdown steam, and DCH-generated energy with the atmosphere. The possibility that intermediate states might be more reactive is neglected. However, it is not clear that this effect is very important.

Were it not for one serious oversight, the deflagration model is probably reasonable as a simple best estimate approximation, though not demonstrably conservative. The oversight is that the characteristic burn time is based upon a calculated flame speed and the time for combustion to propagate throughout the containment dome *from a single ignition point*. In a DCH event, however, one would expect hot debris flying through the containment to provide myriads of ignition points. Even a very small dome transport fraction corresponds to a very large number of debris particles. The effective "flame speed" would likely conform more closely to the particle velocities, typically 10-100 m/s (Allen et al., 1994; Blanchat et al., 1994).

Even in the absence of the hot-particle effect, the "ignition source" in a DCH event would consist of massive flaming jets or plumes of DCH-produced hydrogen burning as it entered the oxygen-bearing regions of the containment atmosphere. Such jets may be efficient initiators of hydrogen combustion and might yield burn rates and burn completeness greater than for burns initiated under milder conditions. In contrast with the DCH scenarios, typical experiments used to define flame speed and burn completeness correlations are initiated by small spark or glow-plug ignition sources. Krok (1993) and Ross (1996) have reported that hot steam/hydrogen jets entering an atmosphere containing pre-existing hydrogen result in more combustion than would be predicted by considering the expected jet behavior and pre-existing hydrogen behavior by themselves. Krok (1993) interpreted the data as indicating enhanced deflagration of the pre-existing hydrogen; however, Ross (1996) interpreted the data in terms of the pre-existing hydrogen enhancing the stability of the burning jet and also pre-existing hydrogen being entrained into the jet. The entrainment effect is treated in TCE (Section 6.1.3).

Burn times, therefore, probably will be much shorter than predicted by the model and mitigation by atmosphere-structure heat transfer correspondingly less. Burn completeness might also be increased by the presence of multiple ignition points and/or jet ignition sources. For example, the accelerated combustion might shift the balance between energy release rates versus energy loss rates in favor of energy release, allowing combustion to proceed to higher completion than for a flame front propagating from a single ignition source. This argument, however, may not be as clear as in the case of the characteristic burn time. Even if there is no enhancement of burn completeness, the effects of multiple ignition sources and large combusting jets upon the characteristic burn time are likely sufficient to introduce a substantial potential for nonconservatism into the deflagration model given by Pilch et al. (1994b).

6.1.2 Volumetric Combustion

In principle, any mixture containing hydrogen and oxygen will react at any temperature. The reaction rates are exceedingly slow at ordinary temperatures and accelerate rapidly with increasing temperature. If the DCH energy release heats the containment atmosphere sufficiently, the reaction of the pre-existing hydrogen may release energy sufficiently rapidly that it enhances the DCH load even though the criteria for a propagating deflagration are not satisfied. Pilch et al. (1994a) and (1994b) refer to this type of combustion as "volumetric combustion". It does not necessarily involve a propagating flame front or require an ignition source, although a DCH event will hardly lack for ignition sources. Pilch et al. (1994a) and (1994b) discuss this process in terms of an effective threshold temperature that is at least approximately related to the temperature at which the energy release rate exceeds rates of energy loss to structures. Since the release rate is proportional to volume while the energy loss rate is proportional to surface area, this effective threshold was predicted to decline with increasing scale. Other surface effects such as interactions of reactive intermediate species with surfaces may affect the threshold temperature; but the surface/volume argument concerning scaling was still expected to hold (Pilch et al., 1994a).

The hydrogen-oxygen reaction takes place as a complex system of chain reactions. In addition to showing a strong temperature dependence, reaction rates can be very sensitive to whether the chain-branching reactions exceed chain-terminating reactions, which depends upon the gas pressure, temperature, and composition. When there is net chain branching, reaction rates can accelerate abruptly even if the temperature were to be held constant. The boundaries of the regimes in parameter space governed by chain branching are often referred to as "explosion limits". Three explosion limits have been identified, with the first two being controlled by chain branching effects while thermal runaway effects are important in defining the third limit, although chain branching may also play a role (Dougherty and Rabitz, 1980). It is possible, but not proven, that DCH conditions primarily involve regimes where ignition is controlled by the thermal runaway effects, rather than the boundaries defined by regimes in which there is net chain branching.

The DCH issue resolution work does not consider the explosion limits as conventionally defined and implicitly treats the volumetric combustion as being governed by temperature alone. This approximation will be adopted in the present review also. It would obviously be desirable to consider the adequacy of this approximation further, but it was not undertaken as part of the present review.

For reasons that are not entirely clear, Pilch et al. (1994a) and (1994b) distinguish a "slow volumetric combustion" process from "sudden volumetric combustion (autoignition)". Other than the distinction between the regimes defined by the explosion limits, which were not considered, there is no fundamental basis for any such distinction. If a "slow" reaction is carried out at a constant temperature in an experimental apparatus that permits dissipation of the reaction energy as fast as it is generated, the temperature does not rise and no uncontrolled acceleration of reaction rates occurs unless the system is in the chain-branching regime. However, if the reaction generates energy more rapidly than heat is lost from the gas, the gas temperature begins to rise. Thanks to the strong temperature dependence of the reaction, a small temperature rise has a relatively large impact on the reaction rate, which quickly accelerates. The resulting positive feedback can produce a rapid, even explosive, runaway effect describable as "sudden" or "autoignition". This runaway effect is less abrupt, however, when hydrogen concentrations are relatively low; e.g., a few percent as in some DCH scenarios. Most experiments involving "autoignition" have been carried out at higher hydrogen concentrations.

<u>"Slow Volumetric Combustion"</u>. Pilch et al. (1994a) estimate the threshold temperature for the "slow" process using reaction times calculated by the SENKIN code (Lutz et al., 1991), which is a driver for the chemical kinetics code CHEMKIN. Results were reported in terms of an "induction time" and a "reaction time". The first represents the time at which the energy release is 5% complete and was interpreted in terms of the time required to build up reactive intermediate species. The reaction time reported was the time at which energy release was 95% complete. Some characteristic induction and reaction times reported by Pilch et al. (1994a) for two different steam-air-hydrogen mixtures are summarized in Table 6-1 as a function of the initial temperature. In this context, the "initial temperature" is the

temperature resulting after adding DCH energies other than pre-existing hydrogen combustion to the containment atmosphere. Pressures assumed were typical of DCH scenarios. The very strong temperature dependence of the reaction rate is evident. On the other hand, there does not appear to be a very strong dependence of reaction time upon composition in this model. Even for a stoichiometric air-hydrogen mixture, CHEMKIN reaction times of ~1000 s at 700 K and 0.1 MPa have been reported (Ciccarelli et al., 1994).

By comparing the reaction times for the 4.8% H_2 case with the estimated time constants for containment atmosphere cooling, and applying a correction for the time-dependent atmosphere temperature, Pilch et al. (1994a) estimated threshold temperatures of 782 K for the Zion plant. Estimates were also made by comparing the reaction time with the DCH time scale, which gave similar results, since one of the factors limiting the DCH time scale is the rate of energy loss from the gas. Owing to the scale effect discussed above, estimated thresholds were 848 K and 893 K for the 1/10 scale SNL/IET and 1/40-scale ANL/IET experiments, respectively.

Table 6-1
Induction and Reaction Times Calculated by SENKIN (CHEMKIN)
(Adapted from Pilch et al., 1994a)

T (K)	$X_{H2}=0.048$, $X_{O2}=0.12$, $X_{H2O}=0.38$		$X_{H2}=0.02$, $X_{O2}=0.059$, $X_{H2O}=0.7$	
	Induction Time (s)	Reaction Time (s)	Induction Time (s)	Reaction Time (s)
700	1008	1301	854	1720
800	16.6	22.2	13.7	30
900	0.61	0.81	0.55	1.2
1100	4.77×10^{-3}	5.81×10^{-3}	5.8×10^{-3}	0.012

Except for some concerns about the rates calculated by SENKIN that are noted below, this approach seems to be a reasonable means of obtaining a rough estimate of the temperature at which volumetric oxidation can begin to contribute to DCH loads. However, Pilch et al. (1994a) assert that this threshold corresponds to a "benign" combustion mode and that the threshold of "energetic" combustion of interest to DCH lies much higher, ~1000-1100. The origin of the latter number is unclear although stratification effects are cited as one justification for this assumption; these effects are discussed at the close of this subsection.

The allusion to a "benign" combustion mode refers back to an introductory discussion of volumetric combustion (p. F-2, Pilch et al., 1994a) that notes certain data on autoignition were obtained in experiments in which "... the autoignition threshold is demarcated by those mixtures that produce a slight pressure rise. These are relatively benign events (ΔP ~0.01 - 0.03 MPa), and similar pressurizations during a DCH event would be inconsequential." No reference is cited for this "benign" behavior. However, the experiments cited elsewhere in the discussion given by Pilch et al. (1994a) include those of Conti and Hertzberg (1988), which may be the source of the "benign" allusion. These investigators note that, in their experiments, the apparatus included a fiberglass diaphragm and that the criterion for ignition "... is the rupture of the diaphragm, at an overpressure of 0.1 to 0.3 bar [i.e., 0.01-0.03 MPa], with the simultaneous emission of flame from the top of the furnace." Obviously, an experimental pressure rise limited by failure of the diaphragm is completely irrelevant to the pressure rise to be expected in a DCH event. Without the pressure relief device, it is unlikely that these experiments would have yielded "benign" pressure rises.

Pilch et al. (1994b) revisit the question of "slow" volumetric combustion using comments provided by "Reviewer F" in the review of (Pilch et al., 1994a). These comments question the appropriateness of the reaction mechanisms normally used in CHEMKIN for application to the relatively low temperatures and low hydrogen concentrations involved in the DCH application. The comments (p. A-92, Appendix A, Pilch et al., 1994b) imply that CHEMKIN can underpredict reaction times by one to two orders of magnitude and also note that data obtained at Brookhaven National Laboratory (BNL) indicate significant reaction can occur on time scales of minutes at 650 K, which is actually considerably faster than the time scale of about 3 hours CHEMKIN calculates (Ciccarelli et al., 1994) at this temperature.

Despite this apparent inconsistency, Pilch et al. (1994b) use the first part of this comment to justify multiplying CHEMKIN reaction times by a factor of 100 and thereby obtain threshold temperatures of 1000-1100 K for volumetric combustion. In his subsequent review of this revision, "Reviewer F" warned that there was no justification for this treatment and states (p. A-249, Appendix A, Pilch et al., 1994b) that the reaction mechanisms assumed [by CHEMKIN] "In some cases ... *overpredict* reaction time - not underpredict as claimed on p. E-17" (emphasis original). Nonetheless, the factor of 100 is used in the published draft of Pilch et al. (1994b) and in the conclusions drawn from the analysis.

It turns out that this apparent inconsistency in the results cited by Reviewer F has a trivial explanation: it is the result of a *typographical error* in the original comment. The passage should have read that the reaction times predicted by CHEMKIN are one to two orders of magnitude greater than measured, not lower. If CHEMKIN reaction times were to be reduced by factors of 10 to 100, and threshold temperatures recalculated using the same approach as that employed by Pilch et al. (1994a) and (1994b), the threshold temperature for contribution to DCH would be ~700 K, not 1000-1100 K. This is a very large difference that would greatly increase the plausibility of pre-existing hydrogen contributing to DCH loads. Evidently, therefore, a rather significant piece of the DCH issue resolution argument turns out to rest on nothing more than a typographical error.

This high estimate of the threshold temperature is combined with the argument concerning stratification (discussed later in this subsection) to conclude that "slow volumetric combustion" cannot contribute to DCH.

<u>"Sudden Volumetric Combustion (Autoignition)"</u>. Pilch et al. (1994a) concluded that this process also cannot occur during DCH. Part of the argument is that pre-existing

hydrogen did not contribute to DCH in the SNL/IET Surry-geometry experiments even though average temperatures in the dome exceeded the threshold calculated using CHEMKIN. The claim that pre-existing hydrogen did not contribute in the experiments is examined further in Section 6.1.4 of the present report. Arguments concerning stratification are also invoked by Pilch et al. (1994a). It was, however, "conservatively" recommended that a threshold of 1100 K should be assumed, on the grounds that this is the highest value of the average dome temperature achieved in any of the experiments (the SNL/IET-11 experiment).

Pilch et al. (1994b) recommend using the bulk average dome temperature together with an assumed autoignition threshold to 950 K, "to ensure a conservative treatment". As is noted in the reference, the reduction from 1100 K makes no difference to the Zion analyses because calculated dome temperatures do not approach 950 K and thus autoignition of pre-existing hydrogen is never predicted to occur for either value of the threshold temperature. No TCE sensitivity studies exploring possible implications if the pre-existing hydrogen did burn are cited by Pilch et al. (1994b) or any of the subsequent DCH issue resolution documents.

The 950 K is based upon a reported autoignition temperature of 873 K for a 6% hydrogen-air mixture with no steam (Conti and Herzberg, 1988) and an observation attributed to Tamm et al. (1985) that the glow plug temperature required to ignite lean dry mixtures (5-20% H_2) increases 80 K when 30% steam is added ($873+80 \approx 950$ K). It is not explained why the steam effect measured for ignition by a hot surface (i.e., a glowplug) should be directly applicable to volumetric combustion. It is also not explained why Conti and Herzberg's results, which were obtained in a 0.0012 m^3 vessel, should be directly applicable to a 70000 m^3 containment dome with no allowance for scale effects. Elsewhere, scale effects in autoignition receive considerable discussion by Pilch et al. (1994a) and (1994b), and a model is even presented for estimating scale effects with validation being claimed based upon small-scale experiments (p. F-7, Pilch et al., 1994a). Evaluating this model predicts that, if the autoignition temperature is 950 K at 0.0012 m^3, it should be $\sim$760 K at 70000 m^3. The point is not, of course, that 760 K is the "correct" value; the point is only that the 950 K value is poorly justified, potentially nonconservative, and inconsistent with arguments given elsewhere by Pilch et al. (1994a) and (1994b).

Stratification Effects. Pilch et al. (1994a) and (1994b) argue that volumetric combustion will not occur in DCH scenarios because strong thermal stratification develops in the containment atmosphere during a DCH event. It is argued that most of the pre-existing hydrogen and containment oxygen supply remain in the lower part of the containment dome, where temperatures are considerably lower than the average temperature calculated by models that assume a well-mixed atmosphere (which includes TCE). Hence it was considered justified to use an artificially high threshold temperature in order to compensate for the effect of gas stratification.

One problem with this argument is that a chemistry parameter (i.e., an ignition temperature) is used as a surrogate for what is actually an uncertainty in a gas mixing problem. This representation is intrinsically unsatisfactory because the surrogate uncertainty parameter (temperature) does not respond to variations in the controlling initial and boundary conditions in the same way as do the actual physical processes involved (gas mixing dynamics). Hence no one threshold temperature is likely to give a good representation of the effect of the wide range of mixing behaviors expected for DCH scenarios, especially when the full range of plants analyzed by Pilch et al. (1996) is considered.

Another limitation is that the arguments for stratification consider only the Surry-geometry experimental results, which did show clear evidence of substantial stratification, especially in the SNL/IET-11 experiment. Gas mixing effects, however, are likely to be quite geometry-dependent. Based upon the temperature records reported by Allen et al. (1994), the Zion SNL/IET experiments showed little evidence for stratification effects except, apparently, in SNL/IET-7. The evidence therefore suggests that stratification is likely for at least some cases, but that it is questionable whether it is as universal a phenomenon as claimed in the DCH issue resolution work. Furthermore, stratification probably does not preclude combustion to the extent assumed by Pilch et al. (1994b). This will be discussed further in connection with the interpretation of the SNL/IET-11 experiment in Section 6.1.4.

Despite these caveats, the point made by Pilch et al. (1994a) and (1994b) that well-mixed conditions are unlikely to be fully achieved on DCH time scales is probably a good one. It does mean that use of the "true" threshold temperature (if one can be defined) in models that assume well-mixed volumes such as TCE (and CONTAIN) may yield conservative results in any case for which ignition is predicted to occur. If the mixing argument had been combined with the use of a conservative value of the "true" autoignition temperature, or even a best-estimate value, the case for conservatism in the overall treatment might have been defensible. What has been done, however, is to combine the unquantified conservatism of the well-mixed assumption with the unquantified (but probably large) nonconservatism of the inflated threshold temperatures, and claim that the net result is conservative. This claim cannot be defended and it is probably wrong; see Section 6.3 for a concluding discussion of the likely nonconservatism of the treatment of pre-existing hydrogen in the DCH issue resolution work.

6.1.3 Entrainment of Pre-Existing Hydrogen Into Burning Jets

In TCE, DCH-produced hydrogen is assumed to burn as a jet or plume upon entering oxygen-bearing regions of the containment. The amount of containment atmosphere that must be entrained into the jet is computed from the reaction stoichiometry and the amount of oxygen in the atmosphere. Pre-existing hydrogen in the containment atmosphere is assumed to enter the jet along with the oxygen and this hydrogen is assumed to burn, which is taken into account when calculating the amount of atmosphere that must be entrained. All combustion is assumed to be complete and no mitigation by atmosphere-structure heat transfer is credited; hence, this stage of the treatment is bounding as claimed.

Problems arise in the analysis of the possible reaction of oxygen and hydrogen entrained into the still-hot jet after the DCH-produced hydrogen is completely consumed. It was argued (Pilch et al., 1994b) that this process could be significant only if the energy released by burning the entrained hydrogen is sufficient to maintain the temperature of the jet. The condition specified for continued combustion is

$$X_{H_2} \Delta e_{H_2} \geq C_p(T_j - T_c), \quad (6\text{-}1)$$

where X_{H2} is the hydrogen mole fraction, Δe_{H2} is the hydrogen heat of combustion (2.4×10^5 J/g-mole), T_j is the jet temperature, and T_c is the temperature of the entrained gas from the containment. Eq. (6-1) was evaluated for $X_{H2} = 0.06$ [the highest value Pilch et al. (1994b) considered possible] and it was concluded that the energy release is only ~40% what would be required to maintain the temperature of the jet. Hence it was concluded that this process is negligible. The treatment was stated to be conservative because it neglects radiative heat losses from the jet.

Pilch et al. (1994b) evaluated Eq. (6-1) assuming $T_j = 1500$ K and $T_c = 400$ K. These values are difficult to understand. The jet temperature does not have to be maintained nearly as high as 1500 K in order for the reaction to continue. One might expect entrained hydrogen and oxygen to react so long as $\tau_{rx} \ll \tau_{mix}$, where τ_{rx} is the characteristic time for reaction and τ_{mix} is the characteristic time for the jet material to mix with entrained gas. Because openings between the subcompartments and the dome are large, jet entrance velocities are only of the order of tens of meters per second, and decay further by the time incoming hydrogen is consumed. Hence, at plant scale, τ_{mix} is likely to be of the order of seconds. Based upon the arguments of Section 6.1.2 concerning reaction times, maintaining $T_j \approx 800$-900 K might be adequate to sustain reaction of the entrained gas. Furthermore, $T_c = 400$ K corresponds to the pre-DCH conditions, and containment temperatures will rise substantially during the event. If $T_c = 550$ K and $T_j = 850$ K, Eq. (6-1) then predicts that combustion can be sustained with $X_{H2} \geq 0.038$. In addition, even if the continuing energy release were not sufficiently great to maintain T_j indefinitely at levels permitting combustion, substantial amounts of the containment atmosphere might be entrained and its hydrogen burned before combustion was snuffed out by the falling temperatures.

It is quite possible that this modeling approach is too simple to permit very useful conclusions to be drawn, whatever values are assumed for T_j and T_c. Once again we have some conservative modeling assumptions (complete combustion, neglect of energy losses) combined with unacknowledged nonconservatisms (values assumed for T_j and T_c, etc). The net result is difficult to evaluate except to note that uncertainties are likely to be substantial, but these uncertainties are not assessed. Instead, unqualified conservatism is claimed.

6.1.4 Comparison with the IET Experiments

Pilch et al. (1994a) and (1994b) cite the failure of pre-existing hydrogen to contribute to DCH loads in the IET experiments as an argument in favor of the modeling assumptions used in that work. In this section, we examine the experimental behavior of the pre-existing hydrogen in a little more detail and compare it with what might be expected from the preceding discussions. There is no claim that the following arguments are totally conclusive. It is possible that alternative interpretations that explain the data equally well might be found. The purpose is to show that there are quite plausible interpretations of the experimental hydrogen data that differ substantially from what is assumed in the DCH issue resolution work; it is not to prove beyond all doubt that the alternative interpretations are correct.

SNL/IET Zion-Geometry Experiments. In the Zion experiments, there is strong evidence that pre-existing hydrogen did not contribute substantially to DCH loads. Direct comparisons between counterpart experiments with and without pre-existing hydrogen are available and show at most very limited enhancement resulting from the hydrogen. In addition, CONTAIN calculations in which the hydrogen was forced to burn by artificially lowering the combustion thresholds substantially overpredicted containment pressurization; i.e., by ~0.09 MPa for SNL/IET-6 and ~0.12 MPa for SNL/IET-7 (Williams et al., 1997).

These results do not mean that no combustion of pre-existing hydrogen at all took place. Some hydrogen data for the Zion-geometry IET experiments in which hydrogen could burn are summarized in Table 6-2. The first column gives the experiment number and the next column the experimental ΔP. The remaining columns give various data for hydrogen production and consumption. The ANL/IET results have been multiplied by the cube of the SNL/ANL scale factor ratio, $(1/0.255)^3 = 60.3$, in order to facilitate comparisons between experiments of different scale. The hydrogen data summarized are the moles initially present, the moles produced, the moles burned, the moles remaining at the end of the experiment, and the net change in hydrogen moles after the experiment.

Table 6-2
Hydrogen Combustion Data from IET Zion-Geometry Experiments

Exp.	ΔP (MPA)	Hydrogen Data, g-moles*				
		Initial	Produced	Burned	Final	Net Change
SNL/IET-3	0.246	0	227	190	37	+37
SNL/IET-4	0.262	0	303	240	63	+63
SNL/IET-6	0.279	180	319	345	154	-26
SNL/IET-7	0.271	283	274	323	234	-49
SNL/IET-8B	0.244	288	299	281	306	+18
ANL/IET-3*	0.190	0	280	211	69	+69
ANL/IET-6*	0.250	139	295	255	178	+39

*ANL/IET hydrogen data are reported scaled up to SNL scale by multiplying by $(1/0.255)^3 = 60.3$ in order to facilitate comparison of experiments performed at different scales.

Considering first the SNL/IET data, we see the experiments with pre-existing hydrogen (SNL/IET-6 and SNL/IET-7) yielded only slightly higher values of ΔP than their counterparts with no pre-existing hydrogen (SNL/IET-3 and SNL/IET-4). However, the experiments with pre-existing hydrogen did yield ~100 moles more hydrogen combustion than did the experiments without pre-existing hydrogen. There is a net decline in the amount of hydrogen in containment in these experiments, while there was net production in SNL/IET-3 and SNL/IET-4, indicating that not all the DCH-produced hydrogen burned. By comparing SNL/IET-3 and SNL/IET-4 ΔP values with the results of the experiments in inert atmospheres, for which ΔP was only 0.1-0.11 MPa, we can estimate that combustion of hydrogen in SNL/IET-3 and SNL/IET-4 resulted in a pressure increase of about 0.0007 MPa per g-mole burned. Had the additional hydrogen combustion in SNL/IET-6 and SNL/IET-7 been equally efficient, one would expect ΔP values for these experiments to be ~0.07 higher than for SNL/IET-3 and -4, which evidently was not the case.

The SNL/IET hydrogen results in Table 6-2 are based upon analysis of gas grab samples taken 30 minutes after the event and thus provide little information concerning the time scale on which the reaction of pre-existing hydrogen in SNL/IET-6 and SNL/IET-7 did take place. However, the maximum dome temperature (average over the volume) in SNL/IET-7 was ~700 K (Allen et al., 1994) and this temperature fell to ~600 K after about 10 seconds. Hence it is plausible to infer that this combustion took place within ~10 s of the event. Temperature data are less complete for the other IET experiments and average temperature estimates less accurate, but the values that are available are consistent with maximum values close to 700 K or somewhat less (except in SNL/IET-8B). Some local temperatures are higher, as would be expected.

The maximum temperature of ~700 K is considerably less than the threshold value of ~850 K estimated from CHEMKIN (Pilch et al., 1994a). However, if CHEMKIN underestimates the reaction rates substantially as discussed in Section 6.1.2, 700 K is close to, or only slightly below, the temperature at which significant reaction might be expected to occur on time scales of ~10 s. In addition, some parts of the containment vessel were hotter than average prior to complete mixing, favoring reaction at those locations. Furthermore, it has also been proposed that the oxidic aerosol particles generated by a DCH event could provide catalytic effects that might favor reaction, although the present author is aware of no applicable data supporting this hypothesis. It seems plausible, therefore, that processes approximating those discussed as "volumetric combustion" took place in the SNL/IET Zion experiments, but on time scales somewhat too long to contribute substantially to the DCH load. This argument suggests the experimental conditions could have been close to the threshold for significant contribution of the pre-existing hydrogen.

In the SNL/IET-8B experiment, there were 62 kg of water in the cavity and much of this water was vaporized on DCH time scales. Over 40% of the total ΔP in this experiment represented addition of steam to the atmosphere and the containment temperatures were considerably lower than in the other experiments, about 460 K (Allen et al., 1994). As would be expected from the above arguments, the hydrogen data in Table 6-2 indicate that there was considerably less combustion of the pre-existing hydrogen than in SNL/IET-6 or SNL/IET-7. There was a small net production of hydrogen instead of net consumption as in the other two experiments.

<u>ANL/IET Zion-Geometry Experiments</u>. One might be tempted to conclude from the ΔP values for the ANL/IET-3 and ANL/IET-6 experiments that the pre-existing hydrogen did contribute significantly in ANL/IET-6. However, the difference in the amount of hydrogen burned in IET-6 versus IET-3 is considerably smaller for the ANL experiments than for the SNL counterparts. Furthermore, comparison of the ΔP values for the ANL and SNL counterparts shows that the SNL/ANL discrepancy reflects a low ΔP value for the ANL/IET-3 experiment, not a high ΔP value for the ANL/IET-6 experiment. It seems likely,

therefore, that the ANL/IET results reflect a tendency for DCH-produced hydrogen combustion to be less consistently effective in contributing to ΔP in the smaller-scale facility, not an increased contribution from pre-existing hydrogen. This trend is consistent with theoretical expectations and other data relevant to the scale-dependence of the combustion of DCH-produced hydrogen (Kmetyk, 1993; Williams et al., 1997).

If these arguments are accepted, the data in Table 6-2 imply that considerably less pre-existing hydrogen burned in the ANL/IET-6 experiment than in SNL/IET-6 and SNL/IET-7. This scale dependence is what one would expect if the experimental conditions for the SNL experiments were close to the threshold for the pre-existing hydrogen as suggested above. Less reaction would be expected at the scale of the ANL experiments, which is what is observed. On the other hand, at full plant scale, there might be a contribution to ΔP for conditions analogous to the SNL experiments. Likewise, the pre-existing hydrogen might have contributed in the SNL experiments if the temperatures had been somewhat higher.

SNL/IET Surry Geometry Experiments. Pilch et al. (1994a) and (1994b) claim that pre-existing hydrogen did not contribute in the Surry-geometry experiments even though the average temperatures in the dome did exceed the threshold temperature estimated using SENKIN. However, the claim that pre-existing hydrogen did not contribute apparently rests on nothing more than comparisons of experimental ΔP values with TCE predictions, which substantially overpredict ΔP if the pre-existing hydrogen is assumed to burn in these experiments (Pilch et al., 1994a). Since a major theme of the present report is that TCE is not always a reliable predictor of DCH loads, basing conclusions concerning hydrogen phenomenology upon comparisons of TCE with experiment is not considered to be a convincing argument.

No experiments were performed in the Surry geometry without pre-existing hydrogen. Hence the contribution of pre-existing hydrogen cannot be assessed by direct comparisons of counterpart experiments with and without the hydrogen as could be done for the Zion experiments. When the CONTAIN standard input prescription was used to analyze these experiments, the pre-existing hydrogen did contribute; however, pre-existing hydrogen contributed only 5-15% of the total ΔP in the calculation owing to the small amounts of pre-existing hydrogen used in these experiments. Other analysis uncertainties were comparable to the pre-existing hydrogen contribution. Hence no conclusions were drawn as to whether the pre-existing hydrogen actually did contribute (Williams et al., 1997). Obviously, if hydrogen concentrations had been more nearly prototypic, the hydrogen could have made a much larger contribution to ΔP and it would have been more likely to contribute.

Pilch et al. (1994a) and (1994b) emphasize the SNL/IET-11 experiment in their analysis because it had the highest average dome temperatures (stated to be 1100 K) and thermocouple measurements showed very strong stratification effects, considerably stronger than in any other experiments. Maximum temperatures measured ranged from ~1500 K near the top of the dome to ~650 K low in the dome (Blanchat et al., 1994). It was argued this stratification prevented a contribution from pre-existing hydrogen despite the very high average temperature because both the pre-existing hydrogen and the oxygen would be concentrated in the lower, cooler stratum, while the high-temperature upper stratum consists principally of spent gases from combustion of DCH-produced hydrogen.

Gas composition data for SNL/IET-11 taken at 15 s after the event were also cited as showing evidence of stratification. The data taken at the two locations cited by Pilch et al (1994b) are reproduced in Table 6-3. One location is near the top of the dome while the other location is at the elevation of the seal table room (STR) but on the opposite side of the containment. The table gives the mole fractions of N_2, H_2, and O_2 and also includes the H_2/N_2 and O_2/N_2 ratios. The nitrogen ratios are given because no processes add or remove significant amounts of nitrogen during the event, and the noncondensible ratios are insensitive to uncertainties in estimating the steam mole fraction. Thus these ratios are good indicators for the extent of change resulting from chemical reactions. Also given in the table are the initial values of the gas composition data and the values at 15 minutes, when mixing was largely complete.

Table 6-3
Selected Gas Data for SNL/IET-11

	15 s Data		Average Values	
	STR Level	Dome Top	Initial	Final
X_{H2}	0.0068	0.0	0.0239	0.0049
X_{O2}	0.0805	0.0482	0.1366	0.0684
X_{N2}	0.43	0.465	0.5098	0.386
X_{H2}/X_{N2}	0.0158	0.0	0.0469	0.0127
X_{O2}/X_{N2}	0.1872	0.104	0.268	0.177

The data for the low (STR) location show that the H_2/N_2 ratio at 15 s is about 1/3 the initial value, indicating that much of the pre-existing hydrogen has burned even if none of what remains represents DCH-produced hydrogen. The closest thermocouple to this location was the lowest thermocouple of the B array, about 1 m away; it was on the same level as the gas sample intake and recorded a maximum temperature of ~650 K. The next thermocouple on the B array, 1.22 m higher, recorded a maximum temperature of ~850 K. These results indicate that significant hydrogen reaction can occur even in the "cool" lower stratum. Although it cannot be determined whether this reaction occurred on the DCH time scale for the experiment, even 15 s is sufficiently rapid to contribute to containment pressurization at plant scale. These results are also consistent with the supposition that even temperatures as low as 700 K may be adequate to produce significant reaction, although there is obviously considerable uncertainty as to the thermal history experienced by the gas collected at this location.

At the dome top, there is no hydrogen detected at 15 s. However, there is considerable oxygen; in fact the O_2/N_2 ratio is almost 60% of the containment-wide average after the event. Hence the gas at the dome top does not consist solely of spent gases produced by burning the plume of DCH-produced hydrogen. Considerable containment atmosphere has been mixed into the gas even at the dome top, and the pre-existing hydrogen associated with this part of the containment atmosphere has burned. While it cannot be proven this mixing and combustion occurred on the time scale of the DCH event in this experiment, it is reasonable to assume that much of the mixing did occur during the time that the turbulence of the DCH event and the accumulator blowdown would have provided a strong driving force for mixing.

These results indicate that the containment atmosphere cannot be divided into a sharply defined cool lower layer that contains the pre-existing hydrogen and a hot upper layer consisting only of spent plume gases from burning DCH-produced hydrogen. Even in an event as strongly stratified as the SNL/IET-11 experiment, there may be considerable combustion in the lower layer, and considerable pre-existing hydrogen can be mixed into the upper layer and burned. Stratification may well inhibit *complete* combustion but it is not reasonable to assume it will prevent *all* combustion of the pre-existing hydrogen. Most of the pre-existing hydrogen in the SNL/IET-11 event did burn (Blanchat et al., 1994), and there is no evidence for believing this occurred primarily after the event.

6.2 Nonconservative Nonprototypicalities in the DCH Hydrogen Data Base

In defending the treatment of pre-existing hydrogen, the DCH issue resolution documents emphasize that experiments were performed in both Zion and Surry geometries that included pre-existing hydrogen in the atmosphere, and it is claimed that this hydrogen failed to contribute to DCH pressurization. Section 6.1.4 cited reasons for questioning the assertion that the hydrogen did not contribute in the Surry-geometry experiments, and for believing that the experimental results are consistent with the hypothesis that combustion is much more likely to occur than implied by the modeling assumptions of Pilch et al. (1994b). In the present subsection, we compare the conditions of the experiments with those of DCH scenarios in NPP and conclude that the conditions of the experiments do not provide a conservative test of the relevant modeling assumptions; in fact they are at least somewhat nonconservative relative to the full-scale NPP scenarios for the Zion experiments and they are strongly nonconservative for the Surry experiments. Thus validation is limited to a nonconservative regime and the model is then applied to conditions that might be considerably more favorable to combustion in the NPP applications. We consider first the application of the Zion and Surry experimental results to the respective NPP, and then consider implications for the extrapolations to other Westinghouse plants with dry containments analyzed by Pilch et al. (1996).

6.2.1 Zion Experiments

In considering whether low concentrations of pre-existing hydrogen might be expected to burn in a DCH event, the two most important parameters are probably the hydrogen concentration and the temperature to which the other DCH energy releases heat the atmosphere (assuming sufficient oxygen is available). The temperature is controlled by the DCH energy release, the number of moles in the atmosphere and the atmospheric composition, and the initial temperature of the atmosphere.

In the analysis of DCH in atmospheric large dry containments under station blackout conditions, Pilch et al. (1996) assume an initial containment pressure of 0.25 MPa and a temperature of 400 K. For these conditions, oxidation of 100% of the clad in Zion would yield a hydrogen concentration of about 7.3% on a molar basis. The experimental hydrogen concentrations in the SNL/IET Zion experiments were 2.76-3.97%, corresponding to about 35%-55% clad oxidation. This provides a reasonable match to what is assumed in the DCH issue resolution work (40% median zirconium oxidation, 65% upper bound; see Pilch et al., 1996). It is, however, more of a best-estimate value than a conservative value, especially in comparison with prior work. For example, the NRC hydrogen rule for PWRs with ice condenser containments postulated 75% clad oxidation for degraded-core accidents arrested in-vessel (10 CFR 50.44). For accidents proceeding through vessel breach, the NUREG-1150 study allowed for an upper-bound hydrogen generation equivalent to 80-140% zirconium oxidation, depending upon the scenario; values could exceed 100% because some of the NUREG-1150 experts included some steel oxidation in their estimates of the upper bound (Harper et al., 1990).

In the Zion experiments, the containment initial pressures were 0.2 MPa, the temperature was ~300 K, and the containment volume was overscaled by about 11% with respect to Zion. Taken together, these conditions imply atmospheric moles were overscaled by about 18% in the experiments. This reduces the temperature rise expected for a given energy input. However, this effect is at least partially compensated by the use of nitrogen rather than steam as a diluent gas in the experiments, since steam has a higher heat capacity and is a more effective inertant than nitrogen. What is more important is that the initial temperature was lower than prototypic by ~100 K, and the peak containment dome temperatures reached during DCH will therefore be almost 100 K lower than prototypic for an equivalent energy release.

In Section 6.1.4, it was noted that partial combustion of pre-existing hydrogen did occur in the SNL/IET Zion experiments, and it was suggested that reaction kinetics at the relatively low temperatures involved may have been one factor preventing the reaction from being fast enough to contribute effectively to DCH pressurization. If this suggestion is correct, the 100 K higher temperatures associated with the NPP application could suffice to produce a more complete and more rapid combustion that could contribute to DCH loads, especially when the effect of scale is also considered.

6.2.2 Surry Experiments

Pilch et al. (1996) assume an initial containment pressure of 0.15 MPa and temperature of 360 K in the analysis of DCH in subatmospheric dry containments under station blackout conditions. Since steam was used in the Surry-geometry IET experiments, the initial containment temperatures were closer to prototypic values than in the Zion experiments. There was some variation in initial pressure and steam concentration from prototypic values, but this is not the most serious concern. The principal issue for the Surry experiments is the very low hydrogen concentrations used.

Oxidation of 100% of the zirconium clad in Surry corresponds to a hydrogen concentration of 14.2% for the containment conditions assumed by Pilch et al. (1996).

However, the actual hydrogen concentrations in the Surry experiments were 1.98-2.39%, corresponding to only 14-18% zirconium oxidation.* These concentrations are a factor of three or more below the prototypic range even as defined by Pilch et al. (1996), and by still larger factors with respect to the more conservative bounding estimates of in-vessel zirconium oxidation that were cited above. In view of the strong dependence of hydrogen behavior upon hydrogen concentration under the conditions of interest, the Surry results cannot be used to infer the validity of the TCE treatment under prototypic conditions, even if it were established that the TCE treatment was correct for the experiments.

6.2.3 Extrapolation to Other Plants and Accident Scenarios

Since the experimental data base was developed for Zion and Surry, it is of interest to consider how these plants compare with the other Westinghouse plants with dry containments analyzed by Pilch et al. (1996), insofar as pre-existing hydrogen behavior is concerned. As noted previously, we assume that the two parameters of greatest interest are the hydrogen concentration and the temperature rise as a result of the addition of other DCH energies to the atmosphere, since the higher the temperature the more likely the hydrogen is to burn.

For a given fraction of zirconium oxidation, hydrogen concentrations in the containment will be proportional to m_{Zr}/n_c, where m_{Zr} is the mass of zirconium clad in the core and n_c is the number of moles of gas in the containment atmosphere. Using the ideal gas law, $n_c = P_c^0 V_c / R T_c^0$, where P_c^0 and T_c^0 are the containment pressure and temperature prior to vessel breach, V_c is the containment volume, and R is the ideal gas constant. The atmospheric temperature rise will be proportional $\Delta U/n_c$, where ΔU is the DCH energy added to the atmosphere from processes other than pre-existing hydrogen combustion. For a given DCH efficiency, ΔU will be approximately proportional to the UO_2 mass in the core, since other potential energy sources also tend to scale with core size.

Using Zion as a standard of comparison, we can define global scaling parameters ϕ_{H2} for hydrogen concentration and ϕ_T for temperature rise as follows:

$$\phi_{H_2} = \frac{m_{Zr} T_c^0 / P_c^0 V_c}{\left(m_{Zr} T_c^0 / P_c^0 V_c\right)_{Zion}}, \quad \phi_T = \frac{m_{UO_2} T_c^0 / P_c^0 V_c}{\left(m_{UO_2} T_c^0 / P_c^0 V_c\right)_{Zion}} \qquad (6\text{-}2)$$

Obviously there can be additional plant-specific effects that these scaling parameters cannot capture.

As part of the present review, the global scaling parameters were evaluated using data for plant parameters and containment initial conditions from NUREG/CR-6338 (Table 4.3, Pilch et al., 1996). In Figure 6-1, values of ϕ_{H2} are plotted against ϕ_T for the plants of interest. Values greater than unity represent a potential for nonconservatism when Zion results are extrapolated to other plants. It is apparent that ϕ_{H2} and ϕ_T are strongly

*The SNL/IET-12 experiment had 5.66% hydrogen. However, this experiment behaved anomalously in several respects, and it has not been used for model validation purposes.

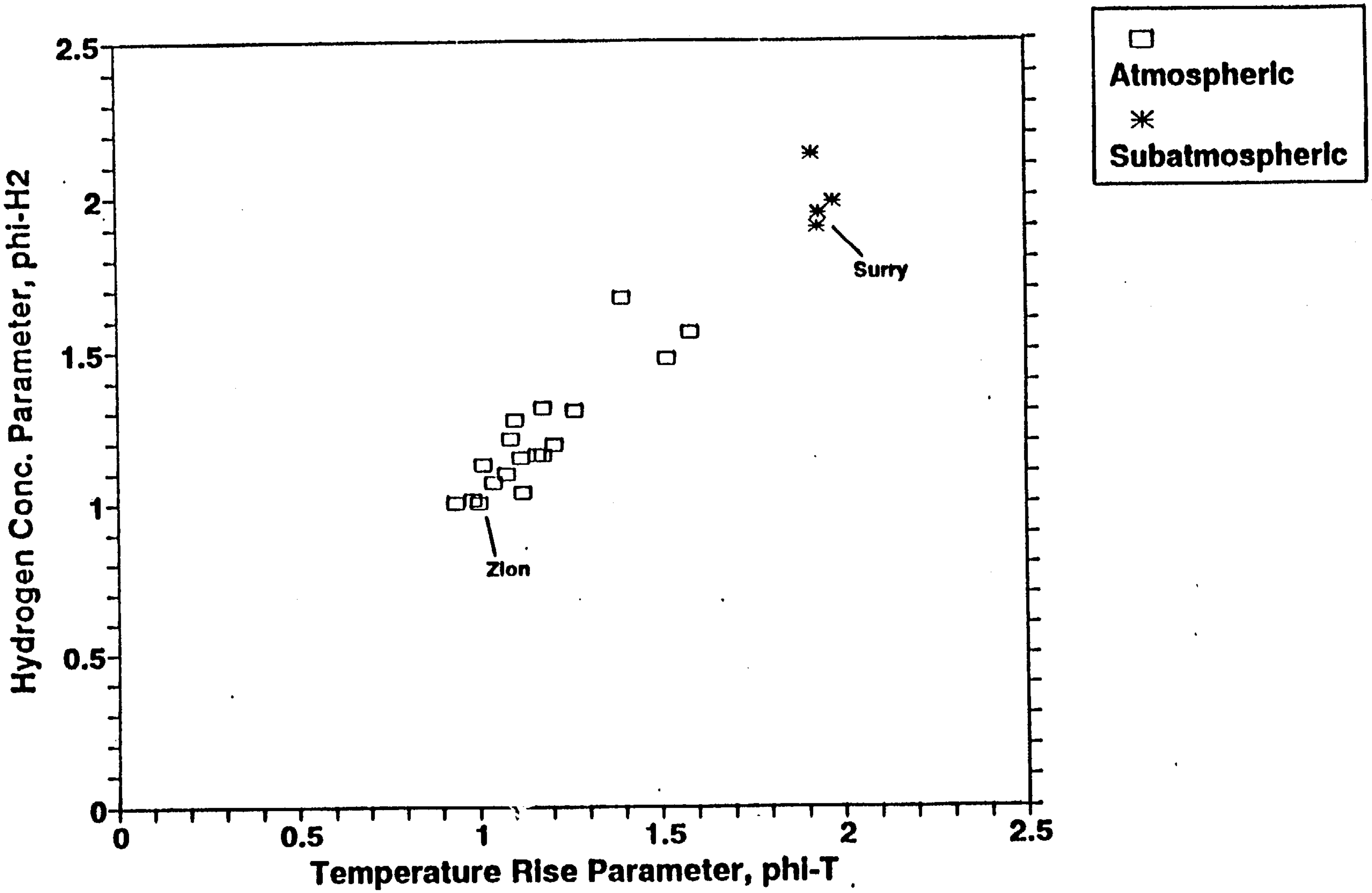

Figure 6-1. Hydrogen concentration and temperature rise scaling parameters, ϕ_{H2} and ϕ_T, for the Westinghouse plants with dry containments considered in NUREG/CR-6338 (Pilch et al., 1996).

correlated, which is only to be expected since both scaling parameters depend upon the same plant parameters except for m_{Zr} in ϕ_{H2} versus m_{UO2} in ϕ_T, and Zr/UO_2 ratios do not vary greatly among the plants of interest.

Figure 6-1 shows that Zion lies at the very bottom of the range for ϕ_{H2} and close to the bottom of the range for ϕ_T. This means that, for most plants, a given fraction of in-vessel zirconium oxidation yields higher hydrogen concentrations than in Zion. Likewise, a given DCH efficiency results in greater temperature rises than in Zion. For the atmospheric plants, the values of ϕ_{H2} and ϕ_T range up to about 60% greater than for Zion, and they are about a factor of two greater for the subatmospheric plants. For both parameters, larger values are expected to increase the tendency of pre-existing hydrogen to burn during a DCH event, and the experiments included somewhat nonconservative features even for Zion. Hence it seems clear that validating any DCH combustion model against the Zion experiments provides insufficient basis for using the model to extrapolate to the other plants analyzed unless uncertainties associated with these trends are assessed. No such assessment of these uncertainties has been carried out in the DCH issue resolution work, and the subject was never even mentioned.

For the subatmospheric plants, values of ϕ_{H2} and ϕ_T do not vary greatly. Surry is a good representative for these plants, and would be a conservative representative for the atmospheric containments. However, the fact that hydrogen concentrations in the Surry IET experiments were so much below the prototypic range renders it very difficult to use these data as a validation basis for application of DCH combustion models to prototypic conditions. Implications of the low hydrogen concentrations in the Surry experiments were never mentioned in the DCH issue resolution documents.

Note also that, if the pre-existing hydrogen does burn, the pressure rise will be proportional to $P_c^0 \phi_{H2}/T_c^0$, other things being equal. Thus combustion of this hydrogen is not only more likely for most plants than it is in Zion, but the potential pressure rises are also larger than for Zion.

Other Accident Scenarios. The DCH issue resolution work considered only two containment states. One corresponded to a station blackout accident with no containment heat removal. In the other, it was assumed ESFs were operating, keeping steam concentrations low and containment pressures and temperatures only slightly above normal operating conditions. For the latter scenario, pre-existing hydrogen was predicted to burn, and its contribution approximately compensated for the reduced initial pressure. A point of possible concern is that there are scenarios with intermediate containment conditions, and hydrogen might be more likely to contribute effectively in these scenarios than in station blackout accidents, while the initial pressure is still higher than in accidents with ESFs operating.

Pilch et al. (1996) do report a single sensitivity calculation for the Zion plant with intermediate containment conditions implying that the two cases considered in the standard treatment bound the results. Though details are not given, it appears that the pre-existing hydrogen did not contribute in this sensitivity calculation. This failure of the hydrogen to contribute is subject to all the limitations of the modeling discussed in Section 6.1, and

Figure 6-1 shows that the Zion plant is among the least sensitive to hydrogen issues. Hence results cited for this single sensitivity case are not conclusive.

6.3 Conclusions, Pre-Existing Hydrogen Combustion

The following conclusions are offered concerning the treatment of pre-existing hydrogen combustion in the DCH issue resolution work:

1. It is incorrect to eliminate a combustion process from consideration simply because the process by itself does not add energy at rates exceeding the total energy loss rate; the criterion should be that containment pressurization can continue so long as total energy input from all processes exceeds the total loss rate.

2. The treatment of deflagrations is likely quite nonconservative because of the neglect of multiple ignition points provided by hot debris and the neglect of jet ignition effects. These effects would be expected to substantially enhance burn rates and may enhance burn completeness.

3. The treatment of volumetric combustion is based in part upon misinterpretation of experimental behaviors and upon a typographical error. The treatment probably tends to be nonconservative and clearly underestimates the uncertainties in hydrogen behavior under DCH conditions. Effective threshold temperatures for substantial combustion of pre-existing hydrogen may be much lower than assumed in the DCH issue resolution work.

4. Failure to obtain complete containment mixing on DCH time scales may be a significant effect, as is emphasized by Pilch et al. (1994b). However, the claim that stratification will essentially prevent combustion of pre-existing hydrogen is very dubious and conflicts with experimental evidence provided by the SNL/IET-11 experiment.

5. The claims that the models are validated by comparison with hydrogen behavior in the IET experiments neglect the partial combustion that apparently did occur in the Zion SNL/IET experiments and also depend upon an unproven claim that pre-existing hydrogen did not burn on DCH timescales in the Surry IET experiments.

6. There is no consideration of the fact that the IET experiments provide a nonconservative test of pre-existing hydrogen behavior under DCH conditions, especially when extrapolation to plants other than Zion is considered.

Concerning the second point, there is some evidence that significant volumetric combustion of hydrogen might occur in DCH events at NPP scale at temperatures as low as 700 K. It should also be acknowledged that not all the available evidence supports such a low threshold, although the threshold appears almost certain to be lower than the values of 950-1100 K assumed in the DCH issue resolution work.

It seems clear that modeling of hydrogen combustion under DCH conditions should allow for more rapid (and perhaps more complete) deflagrations and for lower volumetric combustion temperature thresholds than is done in the DCH issue resolution work. An equally important point, however, is that the behavior of pre-existing hydrogen in DCH events is probably too complex to be well represented by simple models of the type included in TCE no matter what values are chosen for such parameters as deflagration rates and completeness, autoignition thresholds, etc. Instead of focussing exclusively on uncertainty ranges for the "correct" values of these parameters, uncertainty assessment might best be performed by viewing "hydrogen combustion" as the uncertainty parameter and varying the extent of combustion in sensitivity studies. This would permit evaluation of the degree to which the conclusions of interest are sensitive to uncertainties in the hydrogen behavior. This approach has been recommended for CONTAIN code applications to DCH (Williams et al., 1997), since the CONTAIN model includes similar oversimplifications of hydrogen behavior. Unfortunately, no such sensitivity studies are included in the DCH issue resolution work.

7 Other TCE Modeling Concerns

Sections 3 - 5 of this report presented reasons for believing that there are important deficiencies in the TCE (and CLCH) modeling assumptions at a sufficiently fundamental level that they could not be corrected without making major changes to the conceptual basis of the models. In this section, we consider some additional modeling concerns that are less fundamental in the sense that it might be possible to correct them without abandoning the basic premises of the model to the degree that would be required to correct the problems noted in Sections 3 - 5. These concerns could, however, be important in individual cases.

7.1 Nonconservative Approximations and Inconsistencies in the Implementation of TCE

Even if it were accepted that TCE gives an adequate representation of the basic physical processes governing DCH, and that TCE is therefore "bounding" in the sense claimed in NUREG/CR-6075 (Pilch et al., 1994a), there are a number of approximations and inconsistencies in the way that the model has been implemented, applied, and/or validated. The nature of some of these approximations and inconsistencies are such that they can yield nonconservative results.

The possible effects of these concerns is illustrated by comparing "Case 9" of the CONTAIN calculations for Surry reported in Appendix G of NUREG/CR-6109 (Pilch et al., 1995). This case was designed to simulate TCE in that only basic physical processes considered by TCE were included; i.e., no nonairborne debris interactions or debris-water interactions were included, atmosphere-structure heat transfer was eliminated, and the debris particle size specified (0.5 mm) was sufficiently small that local debris-gas thermal and chemical equilibrium (as assumed in TCE) should be reasonably well approximated. Debris transport to the open dome volume as modeled by CONTAIN was essentially the same as that assumed by TCE (21% in both cases), and the debris sources and blowdown were input so as to match the coherence ratio assumed in TCE. An attempt was made to set the hydrogen combustion model parameters so as to produce a similar amount of hydrogen combustion; however, this condition was achieved only for the Scenario V station blackout calculation and therefore only this case is considered here. Thus, all processes acknowledged by TCE as it has been described should be simulated reasonably well in the CONTAIN analysis, while processes excluded in TCE were also excluded in the CONTAIN calculation.

Results are compared with TCE in Table 7-1 for ΔP, hydrogen produced, and hydrogen burned. Both hydrogen produced and hydrogen burned agree well for the two calculations, and the energy potentially available to the containment is essentially the same for the two cases. Nonetheless, the CONTAIN ΔP results are over 60% higher than the TCE value, a very significant difference that clearly requires explanation. (It should be acknowledged here that CONTAIN "base case" results for this scenario agreed very well with the TCE results, apparently due to the cancellation of various opposing effects. However, the case for use of TCE in DCH issue resolution rests upon the claim that processes neglected by TCE are either negligible or conservatively bounded, not that they systematically cancel for some reason.)

Table 7-1
Comparison of TCE with the CONTAIN "TCE Simulation"
(Case 9, Surry Scenario V, Appendix G, Pilch et al., 1995)

Calculation	ΔP (MPa)	H_2 Produced (kg)	H_2 Burned (kg)
TCE	0.264	101	136
CONTAIN "TCE Simulation"	0.429	105	133

A number of reasons can be identified for this potential nonconservatism in TCE, but it is not entirely clear which reasons are dominant. Likely contributors will be discussed next.

Inconsistent Treatment of the Subcompartment Volume in the Surry Geometry. TCE allows debris transported to the dome to equilibrate with the dome atmosphere. This amount of debris is fairly small in both the experimental analysis and most of the NPP calculations and the finite heat capacity of the dome atmosphere inventory does not significantly limit the amount of energy transfer. The debris that is not transported to the dome is equilibrated with either the subcompartment atmosphere or the coherent blowdown steam (not both), whichever has the larger heat capacity.

A deficiency of the DCH issue resolution documentation is that it is never made clear how the subcompartment is defined in analyzing the experiments. It is my understanding that the subcompartment volume is defined to be sufficiently small that the debris interactions are governed by the amount of coherent steam, not the amount of atmosphere in the subcompartment. This may cause little difficulty in the Zion experiments, for which the dome volume includes over 90% of the total free volume of the containment and physical structures define a well-delimited subcompartment volume < 10% of the total containment volume. In the Surry-geometry experiments, however, the open dome volume was only about 70% of the total containment volume, and it is only about 50% in the Surry plant itself. Nonetheless, the subcompartment volume was still defined to be very small in both the experimental analysis and the Surry NPP analysis (1% of the total containment volume in the NPP analysis).

In analyzing the experiments, the distribution of debris between the subcompartment and the dome was taken directly from the experiments. In NPP analysis, the distribution of debris was also based largely upon the experimental results, although there is also a simple model for transport through the gap around the RPV (which was not present in most of the experiments). The difficulty is that in both the Surry geometry experimental analysis and in the CONTAIN plant analysis, relatively little debris is actually de-entrained in the small subcompartment volume as defined in TCE. Most of the debris is carried beyond the TCE subcompartment and de-entrained in other volumes such as the crane wall annulus and the basement volumes, which make up much of the containment volume not represented by the dome volume itself. In the TCE analysis, however, debris de-entrained in this "other volume" is counted as being retained in the subcompartment volume, while the atmosphere inventory of this "other volume" is counted as being part of the dome atmosphere, not the subcompartment atmosphere.

In the CONTAIN treatment (and presumably in reality), the large amount of debris carried beyond the TCE subcompartment into the "other volume" has some opportunity to interact with the atmosphere there, but this is not true of TCE. This difference may be a significant contributor to the difference in the ΔP results cited above.

In terms of the physical basis of TCE, there is no justification for this inconsistent treatment of the "other volume". Correcting the treatment would improve agreement with the CONTAIN result cited above but it would worsen agreement with the Surry-geometry experiments, for which TCE already overpredicts ΔP (see Section 7.2 below).

"Either-Or" Approximation in TCE. TCE interacts the debris not transported to the dome with either the subcompartment atmosphere or the coherent steam, but not both. In reality, if the interaction with coherent steam does proceed to equilibrium as assumed in TCE, it is likely that it will do so in the cavity and adjoining chute, before reaching the subcompartment. Once it enters the subcompartment, there will initially be fresh atmosphere with which it can interact, transferring additional energy. Since the subcompartment atmosphere may be rather rapidly expelled, this interaction may be limited, but it still does mean that TCE's "either-or" approach cannot be considered to be bounding as is claimed.

Use of Constant-Volume Heat Capacities. In equilibrating the debris in both the dome and the subcompartment, constant-volume heat capacities are used for the gas and steam. This choice is reasonable for the dome. However, in the subcompartments and the cavity, the use of the constant-volume assumption would be appropriate only if the gas and debris were equilibrated at constant volume with all flow to the dome prevented, then the gas allowed to flow to the dome with additional debris-gas heat transfer prevented. Obviously, this is not the actual process; as debris-gas energy transfer occurs, the pressure rise that would result from a constant-volume process is largely relieved by flow to the dome. Any actual pressure rise is much less than would be the case if the subcompartments or the cavity were closed off during equilibration. Hence, use of constant-pressure heat capacities would provide a better approximation.

The potential error involved can be estimated as follows. In TCE, the energy, $E_{d\text{-}g}$, transferred to the coherent steam (or subcompartment atmosphere) is given by

$$E_{d\text{-}g} = \frac{E_d^0 - E_d(T_g^0)}{1 + \psi_v}, \qquad \psi_v = \frac{N_d C_{vd}}{N_g C_{vg}}. \tag{7-1}$$

where E_d^0 is the thermal energy (including steam-metal reaction energy) initially available in debris dispersed to the subcompartment but not to the dome, $E_d^0(T_g^0)$ is the residual thermal energy the debris would have at the initial gas temperature T_g^0, N_d and N_g are the number of moles of debris and coherent steam respectively, and $C_{v,d}$ and $C_{v,g}$ are the respective molar constant-volume heat capacities. If the constant-pressure heat capacity approximation is used, a revised value of the debris-gas heat transfer, $E_{d\text{-}g}'$, can be calculated by replacing $C_{v,g}$ with $C_{p,g}$ in Eq. (7-1). It then follows that

$$\frac{E_{d\text{-}g}'}{E_{d\text{-}g}} = \frac{1 + \psi_v}{1 + \psi_v/\gamma}, \tag{7-2}$$

where γ is the ratio of specific heats ($\sim$1.33 for steam). For typical TCE applications, ψ_v ranges from about 2 to about 10. Hence Eq. (7-2) indicates that the constant-pressure approximation would result in about 20-30% greater energy transfer.

These arguments were checked by running a test problem simulating the TCE treatment on the CONTAIN code. Debris and steam were thermally equilibrated in a small closed subcompartment volume, the debris was removed from the atmosphere, and then the subcompartment was opened to the containment volume. The resulting containment ΔP was compared with that calculated when the same amounts of debris and steam were interacted in the cavity and subcompartment with the heated steam being free to expand into the containment volume, as is actually the case. No atmosphere-structure heat transfer was modeled. Parameters of the problem were approximately based upon those of the SNL/IET-1 experiment and the heat capacity ratio ψ_v was $\sim$8. The ΔP value calculated with the subcompartment open to the containment during debris-steam equilibration was 28% higher than in the constant-volume simulation, in good agreement with the prediction of Eq. (7-2).

In metal-rich scenarios (which include all the DCH experiments) the effect of using C_v may be compensated for to a considerable degree by the fact that much of the coherent steam is converted to hydrogen, which has a lower molar heat capacity. This effect also appears to be neglected in TCE. This compensation would be less important in the NPP analyses because the melts are assumed to be metal-poor in the DCH issue resolution scenarios. Since the model has been tuned to give agreement for the metal-rich experiments, it could yield nonconservative results when it is applied to the metal-poor NPP scenarios.

Use of Temperature-Independent Heat Capacities. In TCE, the heat capacities of both the gas and the debris are assumed to be temperature-independent (heats of fusion are lumped into the debris heat capacities). Since actual heat capacities for both debris and gas increase with increasing temperatures, the temperature-independent approximation can underestimate the extent of debris-gas heat transfer and containment pressurization. This effect may not be very large; nonetheless, its possible existence would be acknowledged and evaluated in a careful treatment.

Concluding Remarks. It is important to note that the effects considered in this subsection do not represent genuine phenomenological uncertainties such as nonairborne debris effects, debris-water interactions, coherence ratio uncertainties, hydrogen behavior, etc.; rather they represent errors due to certain approximations and inconsistencies in the treatment: errors that are avoidable in a more complete treatment. Even in the context of a simple model such as TCE, it would be possible to capture the dominant effects to a considerable degree. If these corrections were made, agreement with the experimental results would likely be worsened in some cases, including the Surry IET experiments. As in the case of the coherence ratio inconsistencies in analyzing the Zion experiments, the use of the inconsistent subcompartment treatment in analyzing the Surry experiments appears to be one way in which the model has been tuned to achieve improved agreement with experimental ΔP values.

7.2 Distortions in Inter-Plant Comparisons

Based upon the IET experimental results, there is considerable evidence that TCE overpredicts Surry relative to Zion by a significant amount even as it is currently implemented and validated; correcting the problems noted in Section 7.1 could increase this tendency. To demonstrate the overprediction of Surry relative to Zion, we consider here those SNL/IET experiments in which DCH-produced hydrogen could burn as these are the most nearly prototypic when all factors (including experimental scale) are considered.

Table 7-2 gives the ratio of the theoretical model prediction to the experimental value (T/E) for ΔP and H_2 production for TCE and for CONTAIN. SNL/IET-8B is not included in the tabulation because it had a half-flooded cavity that introduces a number of additional uncertainties concerning the effects of cavity water upon DCH. TCE data are taken from Table E.6 of Pilch et al. (1994a), CONTAIN data from Williams et al. (1997); experimental hydrogen numbers used for the Surry-geometry experiments are those used by Williams et al. (1997).

The TCE ΔP T/E ratios for Zion are all less than unity while they exceed unity for Surry, with the average for Surry being about 45% higher than for Zion; for CONTAIN, the average Surry T/E is only 11% higher than for Zion. The hydrogen data show more scatter, but the trends are qualitatively similar.

One reason for the tendency of TCE to overpredict the Surry/Zion ratio substantially may be that TCE is overly sensitive to the coherence ratio (second column of the table), and the Surry experiments yielded higher values of this coherence (the CONTAIN model exhibited considerably less sensitivity to coherence.) In addition, oxygen starvation in the subcompartments probably played a greater role in the CONTAIN analyses of Surry than in the Zion analyses. This effect is neglected in TCE.

Table 7-2
Dependence of Theory/Experiment Ratios upon Plant Geometry

		TCE T/E Values		CONTAIN T/E Values	
Experiment	R_7	ΔP	H_2	ΔP	H_2
SNL/IET-3	0.31	0.756	0.507	0.927	1.115
SNL/IET-4	0.29	0.798	0.452	1.015	0.950
SNL/IET-6	0.31	0.971	0.417	0.889	0.752
SNL/IET-7	0.5	0.930	0.536	0.900	0.931
SNL/IET-9	0.48	1.325	0.946	1.032	1.312
SNL/IET-10	0.86	1.294	0.945	1.058	1.116
SNL/IET-11	0.65	1.130	0.723	1.016	0.964
Zion ave.	0.353	0.864	0.478	0.933	0.937
Surry ave	0.663	1.250	0.871	1.035	1.131
Surry/Zion	1.882	1.446	1.822	1.110	1.207

The coherence ratios in the table are the NUREG/CR-6075 values, and thus subject to the inconsistencies described in Section 5.2 of this report. The likely effect of correcting those inconsistencies on the Surry/Zion T/E ratios has not been evaluated. However, it does seem clear that the inconsistencies concerning treatment of the subcompartment discussed in Section 7.1 would affect analysis of the Surry experiments more than the Zion experiments and that addressing these inconsistencies would be expected to increase the tendency of TCE to overpredict Surry relative to Zion.

Even as it is, the 45% effect found here is important and suggests that DCH loads may have substantial dependencies upon plant characteristics that the TCE model does not capture. This result indicates that there are additional uncertainties that should have been allowed for in the application of the model to other Westinghouse PWR dry containments in NUREG/CR-6338 (Pilch et al., 1996). As is so often the case in the DCH issue resolution work, the reports did not even acknowledge this evidence of uncertainty, let alone attempt to quantify it.

7.3 Inadequacy of the "Screening Criterion" Used for Other Westinghouse Plants

The basic criterion adopted for considering DCH to be "resolved" in the issue resolution work was to demonstrate that the conditional containment failure probability (CCFP) is less than 0.1. The methodology was applied in detail to Zion (Pilch et al., 1994a, 1994b) and Surry (Pilch et al., 1995), and was extended to all other Westinghouse plants with dry containments in NUREG/CR-6338 (Pilch et al., 1996). In the latter work it was acknowledged that the other plants were not studied at the level of detail that was devoted to Zion and Surry. Hence a "screening methodology" was adopted in which plants were analyzed taking into account a limited set of plant-specific parameters and testing against a CCFP success criterion of 0.01. Using the CCFP criterion of 0.01 rather than 0.1 was judged to provide sufficient margin to allow for both plant-specific details not included in the screening study and residual modeling uncertainties related to phenomena not included in TCE. The methodology called for more detailed study of any plants that failed the screening criterion; however, no plants did fail the screening criterion and hence no plants were subjected to the more detailed study.

A difficulty with this methodology is that the margin provided by this screening approach is inversely proportional to the steepness of the fragility curve for the containments. More precisely, the margin is proportional to $\delta P_{sm} = P_{0.1}-P_{0.01}$, where $P_{0.01}$ and $P_{0.1}$ are the pressures corresponding to CCFP values of 0.01 and 0.1, respectively. For some plants, δP_{sm} is considerably smaller than in Zion, and there is no reason for the magnitude of the phenomenological uncertainties affecting DCH loads to be particularly small for plants that have small values of δP_{sm}.

To examine this issue further, we define a scaling parameter ϕ_{sm} that reflects the robustness of the screening margin with respect to uncertainties in DCH efficiencies resulting from phenomenological uncertainties in the TCE model. The approach is similar to that used to define scaling parameters for sensitivity to pre-existing hydrogen issues in Section 6.2.3. For a DCH energy input ΔU, the pressure rise $\Delta P = R\Delta U/VC_v$, where R is the ideal gas constant, V is the containment volume and C_v is the constant-volume molar heat capacity. As in Section 6.2.3, we assume that, for a given DCH efficiency, ΔU is approximately proportional to the mass of UO_2 in the core, m_{UO2}. Hence the variation in DCH efficiency required to overcome the screening margin is approximately proportional to $\delta P_{sm}VC_v/Rm_{UO2}$. Again using Zion as a standard of comparison, we can define a measure of the relative robustness of the screening margin toward uncertainties in the DCH efficiency by

$$\phi_{sm} = \frac{m_{UO_2,Zion}}{m_{UO_2}} \frac{\delta P_{sm} V}{(\delta P_{sm} V)_{Zion}}, \tag{7-3}$$

where we neglect any variations in C_v among the plants.

Eq. (7-3) was evaluated for the plants considered by Pilch et al. (1996) using data on containment fragilities tabulated in Appendix D of that reference*. One of the phenomenological uncertainties affecting DCH efficiencies is combustion of pre-existing hydrogen, and a parameter ϕ_{H2} reflecting the relative sensitivity of various plants to uncertainties in the hydrogen behavior was defined in Section 6.2.3. In Figure 7-1, ϕ_{H2} is plotted against ϕ_{sm}. As expected, there is no tendency for ϕ_{H2} to be small when ϕ_{sm} is small. In fact, there is a weak inverse relationship because the dependence of ϕ_{sm} upon some plant parameters is the inverse of the dependence of ϕ_{H2} on these parameters.

From the figure it is evident that the robustness of the screening margins toward uncertainties in DCH efficiency varies by a factor of about 5 for the plants considered by Pilch et al. (1996) and that $\phi_{sm} < 1$ for all plants other than Zion, which by definition has $\phi_{sm} = 1$. This means that the protection against uncertainties in DCH efficiency provided by screening against a CCFP value of 0.01 is much less for some plants than for Zion. To provide some perspective, we note that in Zion, δP_{sm} is about 0.145 MPa (Appendix D, Pilch et al., 1996). This is comparable to the uncertainty in ΔP associated with pre-existing hydrogen combustion; note that the CONTAIN calculations for the SNL/IET (Zion) experiments yielded pressure increases of 0.09-0.12 MPa when the pre-existing hydrogen was assumed to burn (Williams et al., 1997). In contrast, for the plant having the smallest value of ϕ_{sm} in Figure 7-1, δP_{sm} is only 0.041 MPa, and ϕ_{H2} is relatively large (1.67) for this case. Although no experiments or code calculations are available for the potential effects of pre-existing hydrogen combustion in this plant, it was noted in Section 6.2.3 that the potential contribution of pre-existing hydrogen to ΔP will be approximately proportional to ϕ_m, other things being equal; scaling the CONTAIN results for the Zion IET experiments then yields an estimated contribution of 0.15-0.20 MPa for this plant. It seems clear that the margin provided by screening against a CCFP value of 0.01 is quite inadequate to protect against the potential impact of the uncertainties in pre-existing hydrogen behavior, to say nothing of all the other phenomenological uncertainties in the TCE prediction of DCH loads.

It is important that the significance of a small value of ϕ_{sm} not be misinterpreted. It does not necessarily mean that the plant has a containment that is particularly vulnerable to DCH loads. A very robust containment might still have a small value of ϕ_{sm} if the dependence of the CCFP on the pressure is very steep in the regime between $P_{0.01}$ and $P_{0.1}$.

*The fragility data used by Pilch et al. (1996a) were taken from the results of the individual plant evaluations (IPEs) performed by the utilities. There are, of course, uncertainties in these values and these uncertainties may be different for different plants, since the methodologies used in the IPEs were not the same in all cases. Some of the differences in δ_{sm} considered here may reflect differences in analysis techniques rather than actual differences in containment response. Since the principal focus of this critique is on the containment loads modeling, the question of uncertainties in the fragility data will not be considered further.

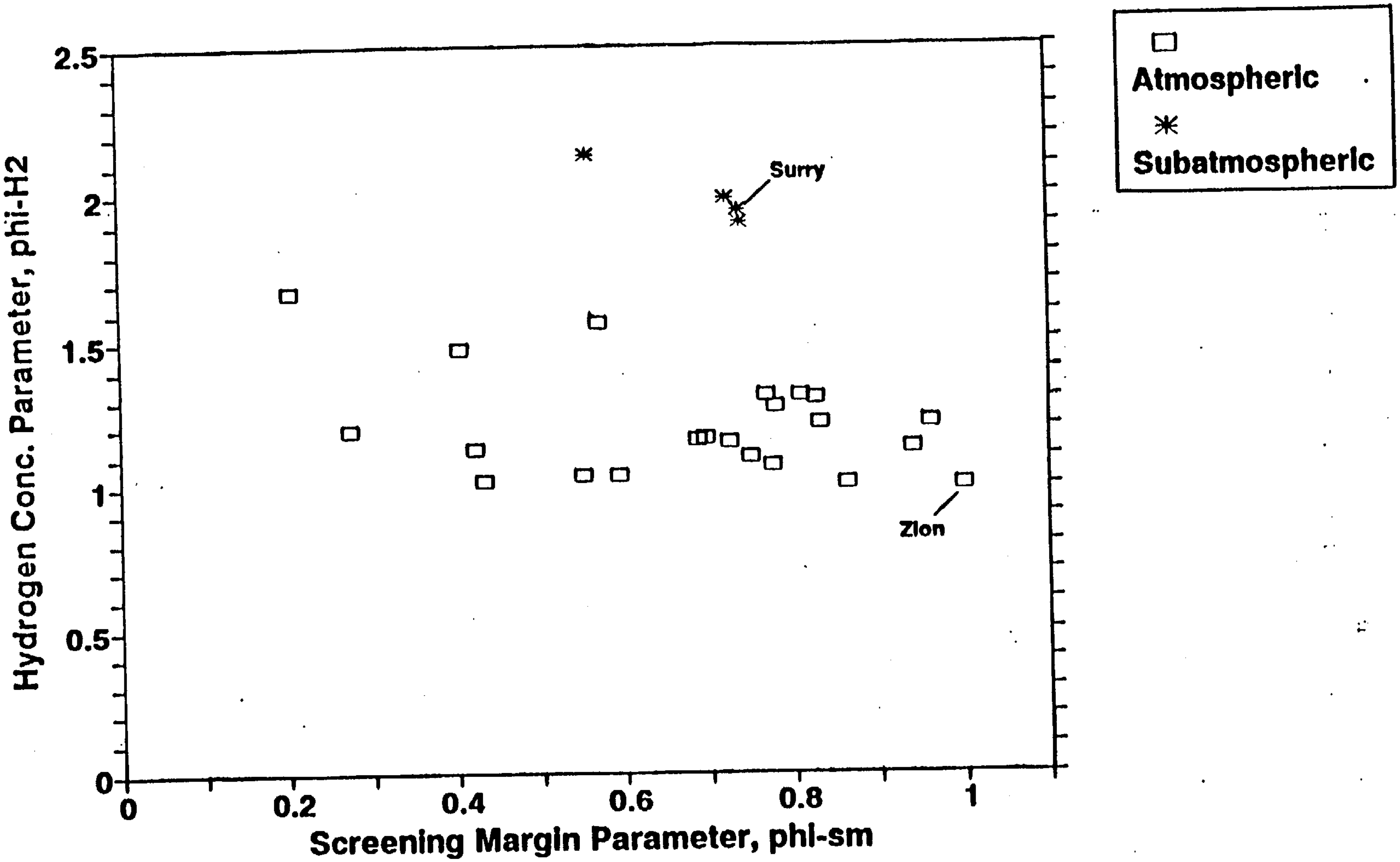

Figure 7-1. Hydrogen concentration and screening margin scaling parameters, ϕ_{H2} and ϕ_{sm}, for the Westinghouse plants with dry containments considered in NUREG/CR-6338 (Pilch et al., 1996).

For such a plant, the best estimate of DCH loads might be much less than $P_{0.01}$, in which case even a conservative allowance for phenomenological uncertainty in the loads modeling might not reverse the conclusion that DCH could be considered "resolved" for this plant. However, a small value of ϕ_{sm} does mean that simply demonstrating that the screening criterion of CCFP $\leq$ 0.01 is met in the TCE calculations provides very little protection against phenomenological uncertainties in the loads modeling. Hence the screening methodology used by Pilch et al. (1996) is inadequate without refinements to take into account the variations in ϕ_{sm}. No such refinements were presented; in fact none of these questions were considered at all.

7.4 Errors in the TCE Treatment of Iron Chemistry

Most DCH models (including CONTAIN and TCE) assume that metal-steam reactions can go to completion in the case of the reactive metals Zr, Al and Cr, but use at least a simple representation of chemical equilibrium effects in treating the iron-steam reaction. In the simplest approximation, we adopt the ideal solution assumption and equate the thermodynamic activity of the relevant species to their mole fractions, and this equilibrium may then be written

$$Fe + H_2O \rightleftharpoons FeO + H_2,$$
$$K_{eq} = \frac{X_{FeO} P_{H_2}}{X_{Fe} P_{H_2O}} = e^{-\frac{\Delta G_{rx}}{RT}}, \tag{7-4}$$

where the X's represent mole fractions of the species Fe and FeO in the metallic and the oxidic phases respectively, the P's represent the partial pressures of hydrogen and steam, and ΔG_{rx} is the standard Gibbs free energy change associated with the reaction.

For a rather wide range of conditions relevant to DCH, K_{eq} is about equal to 2. Iron metal and its oxide have only very limited miscibility and therefore form separate phases. If only Fe and FeO are present, both will have an activity close to unity in their respective phases and $P_{H2}/P_{H2O} \approx K_{eq} \approx 2$. This equilibrium ratio implies that, when steam supplies are limited, about a third of the steam will remain unreacted at equilibrium.

Metals more reactive than iron will be largely reacted before iron reacts to a large degree and only limited amounts of metals less reactive than iron will be present in reactor melts; hence, in the metallic phase, $X_{Fe} \approx 1$ is expected to be a reasonable approximation under conditions for which the iron-steam reaction is important. However, oxides other than FeO usually will be present in the oxide phase. Since molten oxides are generally miscible, $X_{FeO} < 1$ typically applies in the oxide phase, which permits the iron-steam reaction to proceed further to the right in Eq. (7-4) than is the case for a pure Fe/FeO system. The CONTAIN default model for iron-steam reactions includes this effect using a simple ideal solution model for FeO in the oxide mixture.

It should be acknowledged that the interactions of core debris constituents can be quite complex and there may be substantial uncertainties in the simple ideal solution model outlined here. However, the assumption that the metals are mutually soluble and oxides are mutually soluble, while metals and oxides are immiscible with each other, is the usual starting point for modeling molten core debris systems, even when nonideal behavior is taken into account.

TCE does not include the FeO dilution effect that is expected to exist when other oxides are present. More surprisingly, a study of Appendix E of Pilch et al. (1994a) indicates that TCE assumes that iron *metal* and iron *oxide* form an ideal solution with *each other*. Since these species actually are almost totally immiscible at any temperature achievable in a DCH event, this assumption of an ideal Fe/FeO solution seems very difficult to justify. Certainly no justification is given; in fact, the assumptions of the model are not explicitly stated at all and have to be inferred from the equations given.

When the extent of metal oxidation is severely limited by the amount of steam available, and Fe/FeO ratios therefore remain large, the X_{Fe}/X_{FeO} ratio will be high when Eq. (7-4) is evaluated assuming Fe and FeO are miscible, and TCE will therefore tend to favor a more complete reaction of the available steam than would be obtained assuming Fe and FeO reside in separate phases. On the other hand, when metal/steam ratios are low, and Eq. (7-4) would allow complete reaction with separate metal and oxide phases, the TCE model would be expected to predict that the iron reaction would remain incomplete because the ratio X_{Fe}/X_{FeO} becomes small as the reaction of iron approaches completion. The fact that TCE does not allow for dilution of FeO by other oxides enhances this effect. Since TCE has been tuned to give reasonable agreement in ΔP for the metal-rich experiments (in which it may tend to overestimate the extent to which the coherent steam can react), it may tend to be somewhat nonconservative for the metal-poor melts assumed in the DCH issue resolution work. At this point, no evidence has been identified that any such errors had a large impact upon the calculated results, but that is not a justification for adopting a treatment that is fundamentally indefensible.

7.5 Neglect of RPV Insulation

The RPV is typically covered with insulation consisting of thin stainless steel sheets and foils. This insulation was simulated in only one of the DCH experiments, SNL/IET-11. The insulation was largely stripped away from the RPV, opening up the annular gap between the RPV and the biological shield wall. The mechanism for insulation removal appeared to be melting ablation, and there is some evidence (not fully conclusive) that the ablated insulation contributed to hydrogen production (Blanchat et al., 1994; Williams et al., 1997). The insulation mass (~3000 kg for a 4-loop PWR) is comparable to the mass of metal in the melt compositions specified for the DCH issue resolution analyses and hence the potential for this additional metal to provide a significant relative contribution to hydrogen production and combustion is greater than in the SNL/IET-11 experiment, where the debris metal mass was much greater than the insulation mass. It seems plausible that insulation ablated from the vessel bottom would mix with the main mass of debris and interact with blowdown steam much as metal in the debris would, and this interaction would not be as steam-starved as it likely was in SNL/IET-11. Insulation ablated from the RPV sides may be largely carried up into the dome where it could react with steam and oxygen there. The longer flight paths and airborne residence times in the full scale plants might favor more complete reaction than in the SNL/IET-11 experiment. Hence the insulation could be considerably more effective in contributing to hydrogen production and combustion in the NPP scenarios than was the case in the SNL/IET-11 experiment.

The DCH issue resolution reports acknowledge that the insulation will likely be removed but the analyses do not include any possible effects of the insulation on hydrogen production. Pilch et al. (1996) briefly discuss the issue and cite a side calculation (not included in the main analyses) indicating that, in Surry, the chromium in the insulation could produce $\sim 1.45 \times 10^4$ additional g-moles of hydrogen, which could add ~ 0.023 MPa to ΔP if it all burned. Pilch et al. (1996) argue that the iron would not contribute because of "thermodynamic limitations" (presumably meaning the iron-steam equilibrium effect) and the limited coherence factor in the annulus surrounding the RPV.

The argument against the iron contributing seems difficult to defend. Thermodynamic limitations will not apply for that portion of the molten metal that is carried to the dome, where both free oxygen and large quantities of steam are present. For insulation ablated from the RPV bottom, which might mix with debris in the cavity, a simple calculation shows that the coherent steam supply in Scenario VI is adequate to oxidize all the metal in the dispersed core debris at the 99th percentile specified by Pilch et al. (1996), and it can then oxidize about 3300 kg of additional iron without the H_2/H_2O ratio exceeding the value of ~ 2 that corresponds to the iron-steam equilibrium, even neglecting the effect of dilution of FeO by other oxides present. This value equals or exceeds the total insulation mass, even if we neglect the fact that a considerable part of the insulation is probably carried to the dome instead of becoming mixed with the debris in the cavity. For Scenario V, the melt masses are smaller and the steam supply is larger. Hence in all cases there is enough steam available to oxidize all the metal in the core debris plus all the metal in the insulation without running into thermodynamic limitations in the iron-steam reaction.

For typical stainless steels, the Fe/Cr mass ratio is about 4. When the iron-steam reaction is included, a calculation analogous to that cited above would give an increment to ΔP of about 0.086 MPa, not 0.023 MPa as stated by Pilch et al. (1996). This is a bounding estimate since it assumes complete reaction of the metal, complete combustion of the hydrogen, and neglects mitigation by atmosphere-structure heat transfer. The actual contribution of the insulation likely would be significantly smaller. Its neglect does, however, represent one more nonconservative assumption made in the DCH issue resolution work and contributes to the cumulative impact of the many potentially nonconservative analysis assumptions that have been identified in the present report.

8 Summary and Conclusions

The present review of models used to predict DCH loads in the DCH issue resolution study has identified a substantial number of important deficiencies in the models and in the experimental validation claimed for these models. The major findings may be summarized as follows:

1. There is convincing evidence that mitigation effects neglected by the DCH issue resolution models actually are very important in both the Zion- and Surry- geometry IET experiments. It therefore necessarily follows that there are important contributors to DCH energy release that are not accounted for in the DCH issue resolution models, since the models do approximately reproduce the experimental ΔP values. No reasons have been offered for believing that this approximate cancellation of opposing effects will apply generally.

2. The degree of validation of TCE against the experimental data base is much less convincing than has been claimed; for example:

   - Alternative DCH models with a quite different physical basis (e.g., CONTAIN) fit the ΔP data base equally well and these models might give quite different results for some of the NPP scenarios analyzed in DCH issue resolution.

   - DCH models that are demonstrably *inadequate* (e.g., the total steam correlation, TSC) fit the ΔP data base as well as does TCE.

   - TCE is totally incapable of reproducing the hydrogen production database except for a subset of quite nonprototypic experiments. Arguments given for explaining away this failure are essentially *ad hoc*, lacking any independent support. Other DCH models [CONTAIN, MELCOR (Kmetyk, 1993)] provide reasonable predictions of hydrogen production if they also model processes that predict the ΔP results adequately.

   - The applications of TCE to NPP involve many extrapolations beyond the existing data base with respect to geometric scale, melt composition, co-ejected RPV water, pre-existing hydrogen, etc.

3. The concept of limited temporal coherence between debris dispersal and RPV blowdown is advanced as being a "crucial mitigating factor" for DCH but no experimental data supporting this hypothesis is presented. There is some experimental evidence (not entirely conclusive) that coherence is not as important as assumed, and the CONTAIN model predicts considerably less sensitivity to coherence. Furthermore, the methods used to extract coherence estimates from the experimental data are subjective and appear to have been applied inconsistently. Correcting the inconsistencies would probably reduce agreement between TCE and the ΔP data. It also appears that these inconsistencies have concealed a significant scale effect in coherence; the TCE treatment acknowledges no scale effect.

4. The treatment of pre-existing hydrogen combustion in DCH seriously underestimates the uncertainties involved and probably tends to be nonconservative. For example, rates and possibly completeness of deflagrations are substantially underestimated; the effective threshold temperature for the "volumetric combustion" process appears to be considerably too high; and excessive reliance is placed upon the assumption that stratification effects will prevent hydrogen combustion in DCH. The experimental data base used to defend the TCE treatment may have been misinterpreted in the DCH issue

resolution work; in any case, the data base falls in a quite nonconservative regime relative to some of the NPP applications.

5. There are a number of other nonconservative approximations and inconsistencies in the TCE formulation that are discussed in Section 7 of this report. These problems include inconsistent and nonconservative definitions of the subcompartment volume, use of nonconservative approximations for the gas heat capacity, and basing the iron chemistry model upon inappropriate assumptions concerning miscibility of the metal and the oxide phases. A CONTAIN calculation for the Surry plant indicated that correcting these deficiencies could increase the calculated ΔP by about 60% in the case considered. The model also neglects the possible enhancement of hydrogen production and combustion produced by ablated RPV insulation. In addition, comparison of the Zion-geometry and Surry-geometry IET results indicates that TCE does not capture the dependence upon containment geometry well, and it therefore distorts interplant comparisons substantially. Finally, the screening criterion used in the analysis of Westinghouse plants other than Zion and Surry provides very inadequate margin against modeling uncertainties for at least some of the plants considered.

The cumulative impact of all the limitations in the TCE model discussed here is sufficient that it is very difficult to know what conclusions, if any, can be safely drawn from the DCH issue resolution work as it stands. Furthermore, it seems doubtful whether one could correct these deficiencies within the basic approach that has been used in the DCH issue resolution work. This modeling approach was based upon making simple bounding analyses based upon thermodynamic limits for those processes that are treated, together with presenting arguments for believing that other processes are either mitigative or negligible in their impact, when the other processes are acknowledged at all. The problem with this approach is that many of the processes neglected actually are significant, and one would calculate that threatening DCH loads actually *can* arise, if one attempted to correct for some of the deficiencies in TCE by using simple bounding models to treat the effects that are currently neglected.

Consider, for example, the Surry TCE calculation for Scenario V cited in Appendix G of NUREG/CR-6109 (Pilch et al., 1995) that is used for comparison with CONTAIN calculations. The TCE calculation gave a peak containment pressure of 0.474 MPa. Containment fragility curve data provided in Appendix D of NUREG/CR-6338 (Pilch et al., 1996) indicate that the failure probability is zero for pressures below 0.61 MPa, and the CCFP is equal to 0.01 and 0.1 at pressures of about 0.66 and 0.80 MPa, respectively. A large margin therefore appears to exist between the TCE calculation and the pressures required to pose a significant threat.

However, Section 7.1 notes that a CONTAIN calculation restricted to consider only the physical processes modeled by TCE yielded a peak pressure of 0.64 MPa, not 0.474 MPa, suggesting that TCE would give a pressure of about 0.64 MPa if the various nonconservative approximations and inconsistencies in TCE that were discussed in Section 7.1 were to be corrected. Furthermore, neither the TCE calculation nor the CONTAIN calculation included combustion of pre-existing hydrogen, other than the small amount assumed to be entrained and burned along with the DCH-produced hydrogen. In the CONTAIN calculation, the maximum dome temperature calculated slightly exceeded 900 K, and in Section 6.1.2 it was argued that it is very difficult to defend the assumption that the pre-existing hydrogen cannot burn at temperatures this high. In the particular scenario considered here, 40% in-vessel zirconium oxidation was assumed, which corresponds to the median value assumed by Pilch et al. (1996), not a conservative or bounding value. Nonetheless, the adiabatic combustion of all this pre-existing hydrogen would increase ΔP by about 0.16 MPa. This increase would result in a calculated pressure of 0.80 MPa, about equal to the pressure for which the CCFP equals 0.1. Adding in the bounding estimate for the possible contribution of the RPV insulation (see Section 7.5) would increase this to about 0.88 MPa, well above the pressure for which the CCFP equals 0.1.

Even the treatment just outlined makes no allowance for several other potential contributors to DCH loads. For example, the treatment makes no allowance for whatever processes (nonairborne debris interactions, debris-water interactions, etc.) must be present in order to make up for the mitigation effects neglected by TCE as discussed in Section 3 of this report, and simple bounding estimates for these processes could result in substantial additional enhancements to the calculated loads, especially if mitigating effects are neglected as is done in TCE; see Appendix C for some additional details. In addition, Pilch et al. (1996) acknowledge that even the simple flashing of co-ejected RPV water in Scenario V, *without* considering any interaction between the debris and the water, could increase ΔP by about 0.07 MPa in Zion; however, the actual results presented by Pilch et al. (1996) do not include any contribution from the flashing of RPV water.

It is not, of course, argued that an approach based upon providing bounding estimates of the effects of all these processes could yield results that are at all realistic. The various processes considered in such an approach are treated making limiting assumptions and neglecting mitigation effects. It is well known that estimates based upon "stacking" a series of conservative allowances for uncertainties can be very unrealistic. However, simple thermodynamic limiting analyses of the sort adopted for DCH issue resolution have no way of treating the fact that the various processes involved may be unlikely to approach their theoretical limits, nor can they credit the reality that it is especially implausible that all these processes will closely approach their theoretical limits all at once in the same event.

The DCH issue resolution methodology for containment loads therefore left little choice but to either stack bounding estimates in a way that is clearly excessively conservative and thus fail to "resolve" DCH, or else ignore or argue away the processes that are not treated in the DCH issue resolution models. In most cases, the choice made was to omit these processes from the analysis, since to do otherwise would lead to the conclusion that DCH cannot be "resolved" using the approach that had been adopted. It may be for this reason that the DCH issue resolution documentation tends to be rather selective in favor of any evidence supporting the approaches used while downplaying or neglecting countervailing evidence. In the analysis of pre-existing hydrogen combustion, this selectivity reached the extreme of basing an important modeling assumption upon uncritically accepting a statement provided by a reviewer in which it turns out that a typographical error had reversed the meaning that was actually intended, even though other information *provided by the same source* was clearly inconsistent with the erroneous citation that was used as part of the basis for the DCH issue resolution modeling assumptions.

It is surprising that the NRC would have chosen to restrict its attempt to resolve DCH by relying almost exclusively upon a methodology that provides no clear means of addressing the uncertainties in loads modeling other than either making overly conservative bounding assumptions or else dismissing the uncertainties with unfounded claims that they are of no importance. What makes this approach especially puzzling is that, in the recent past, the NRC has developed and applied methodologies for assessing severe accident risks that are considerably more sophisticated than those applied in the DCH issue resolution work. For example:

- The NRC has developed the CONTAIN and MELCOR systems codes, which include models for DCH that are considerably more detailed than TCE and CLCH. The systems codes include two key capabilities that the simple DCH issue resolution models lack: modeling of important mitigation effects, and the flexibility required to assess uncertainties in the loads calculations resulting from the major uncertainties in DCH phenomenology. Taken together, these attributes should assist in making an assessment of DCH loads that is defensible as conservative and yet not so conservative that it precludes obtaining a resolution of the issue. The systems codes could have been applied to DCH issue resolution either alone or in conjunction with simple models such as TCE; e.g., to make a systematic assessment of the uncertainties associated with the use of TCE.

  Appendix G of NUREG/CR-6109 (Pilch et al., 1995) does give CONTAIN comparisons for a single TCE calculation for each of the issue resolution scenarios V, Va, and VI. However, the results were much too limited to systematically explore the phenomenological uncertainties as a function of the important DCH parameters. There was also insufficient evaluation of the results that were given; for example, there was no mention of the possible implications of the 60% higher values of ΔP calculated by CONTAIN when the code was nominally restricted to considering only the processes that are considered by TCE (see Section 7.1 of this report).

- Methods for formal elicitation of expert opinion have been developed that permit the application of expert judgment to the quantification of uncertainties in a way that is controlled, scrutable, and documented in detail. These methods can make use of expert panels selected from diverse institutional backgrounds and that represent diverse viewpoints on potentially controversial technical issues. Although subjectivity still cannot be avoided in assigning probabilities to uncertain phenomenological issues, the use of a diverse panel and a controlled elicitation process results in considerably higher credibility than does relying primarily on the opinion of a single lead investigator. One benefit of a more credible assignment of probabilities is that one can take credit for the especially low probability of scenarios that involve making limiting assumptions for all the uncertain phenomena involved. One can thereby avoid having the results being overly influenced by extreme cases obtained by "stacking" a large number of conservative assumptions.

As one example, the NUREG-1150 study (USNRC, 1990) assessing risks in U.S. nuclear power plants made use of both detailed systems code calculations (including CONTAIN and the industry's MAAP code) and expert elicitations in assessing DCH as well as many other severe accident threats. It could easily be argued that NUREG-1150 provides a more credible starting point for decision-making with respect to DCH than does the DCH issue resolution work as it currently stands. Since the NUREG-1150 study is not fully up to date, it would be necessary (or at least desirable) to re-evaluate its findings concerning DCH in the light of the extensive experimental results obtained since that time, new modeling capabilities developed for the systems codes, and results of the individual plant evaluations (IPEs) performed by the utilities.

Given the mild initial conditions, it could be credibly argued that a careful treatment of DCH loads would conclude that the CCFP for DCH is less than 0.1 for most if not all of the Westinghouse plants with dry containments. If this judgment were to be accepted, it could be argued that the concerns raised in this critique are somewhat academic. Doing so would, however, could be a mistake for several reasons:

- The DCH issue resolution findings do not simply conclude that the CCFP < 0.1; instead, they conclude that the CCFP is *zero*, often by a substantial margin, in all but a few plants (Pilch et al., 1996). There is also a flavor of high confidence expressed concerning this result, with little evidence of the many deficiencies and uncertainties in the analysis that have been considered in the present critique. In addition, the NRC has given the work high prominence; for example, the NRC arranged for the publication of a special issue of the journal *Nuclear Engineering and Design* devoted to the DCH issue resolution "success". In view of this highly visible conclusion that DCH cannot possibly pose a threat in this type of containment, the nuclear industry could hardly be blamed if it concluded that the precautions against DCH that it has currently taken or planned for the future are unnecessary. It is unclear how the NRC could oppose such a decision, since the industry would be able to provide justification for the decision in the NRC's own documentation for DCH issue resolution.

- There are substantial uncertainties in analyzing the in-vessel accident progression that determines the DCH initial conditions. It is possible that more severe scenarios (e.g., melts with a higher metallic content) may yet require consideration in the future. Given more severe scenarios, some of the uncertainties considered here would be larger, such as uncertainties associated with nonairborne debris interactions and debris-water interactions (Williams et al., 1997). In addition, the margins against containment failure would be less. Under these conditions, application of the DCH issue resolution methodology without fully assessing its limitations could easily result in erroneous conclusions concerning the threat to containment integrity.

- There are other containment types, such as ice condenser containments, that are considerably less robust than the dry containments and that do not possess the large margins against failure that the dry containments possess. Analysis of these plants would be much more sensitive to uncertainties in the loads modeling, even given the mild initial conditions. Again, application of the DCH issue resolution methodology to these plants without fully assessing the limitations of the methodology could easily result in erroneous conclusions concerning the threat to containment integrity.

- The NRC is moving toward the concept of risk-informed, performance-based regulation. In the past, DCH risks have been considered to be an important component of severe accident risks generally. Given the current NRC position on DCH issue resolution, it would not be surprising if the DCH issue resolution results and methodology were to play a role in evaluating the DCH component of severe accident risks in the future. Results presented here indicate that the methodology is insufficiently reliable for this purpose: it can be overly optimistic in some instances, overly conservative in others, and provides inadequate means for assessing the uncertainties involved in its use. It would be unwise and potentially dangerous to assume that "risk-informed" regulation could be based upon results obtained using this methodology as it stands.

- Perhaps most importantly, the defense-in-depth concept has been the traditional cornerstone of nuclear safety philosophy. In the case of DCH, this has meant both addressing the in-vessel accident progression that determines the DCH initial conditions and also understanding the phenomena controlling DCH containment loads. To dismiss as "academic" important deficiencies in the loads modeling methodology simply because the in-vessel accident progression is currently thought to be more favorable than was once believed, would be to accept a serious degradation of the defense-in-depth concept.

In concluding, I would stress that the burden of proof should properly lie with the DCH issue resolution work. The purpose of that work was not simply presentation of one more quasi-academic modeling study of DCH, to be considered by the technical community along with a number of other such studies that have been published. Instead, the purpose was to *resolve* the issue, so that the NRC and the industry could plan regulation and plant design relevant to DCH with reasonable confidence in the technical basis for decision-making. Furthermore, the NRC has greatly reduced or eliminated its experimental and analytical research programs studying DCH; one cannot count on future work to correct any deficiencies in the present DCH issue resolution study.

A "resolution" of a major nuclear safety issue that ignores important unresolved technical issues affecting the analysis is an oxymoron, and a claim to have proven that DCH cannot pose a threat in the face of so many unanswered questions is not honest. At a minimum, acceptance of the DCH issue resolution study as it stands, without appropriate qualifications exploring its limitations, compromises the technical integrity of the NRC and its contractors. At worst it could lead to overconfidence with respect to DCH and a degradation of safeguards against DCH that eventually could have deleterious effects upon plant safety.

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Appendix A
Use of Hydrogen Production Data for DCH Model Validation

A.1 Introduction

The ability to predict the extent of hydrogen production by metal-steam reactions during a DCH event is essential for any valid DCH model. Experimentally, comparison of experiments with inert versus noninert atmospheres indicates that combustion of DCH-produced hydrogen contributed over half the experimentally observed containment pressurization in the Zion-geometry SNL/IET experiments (Allen et al., 1994). Furthermore, the hydrogen produced during the DCH event is an integral measure of the extent of steam interactions with the debris and there is a close analogy between the mass transfer controlling hydrogen production and the debris-gas heat transfer that contributes to containment pressurization. For example, Williams (1992) analyzed the SNL/LFP and SNL/WC experiments using the heat/mass transfer analogy, and found that the extent of debris-steam energy transfer occurring in the cavity could be inferred from the experimentally measured hydrogen production, without invoking any particular modeling assumptions other than the heat/mass transfer analogy itself. Hence, if a model cannot predict the production of hydrogen during DCH, it is unlikely to predict the extent of debris-gas heat transfer reliably.

In this Appendix, we consider whether the data on hydrogen production obtained from the DCH experiments should be used for model validation purposes. In Section 4.2 of the main report, it was noted that TCE is unable to correlate the data for hydrogen production in DCH experiments except for a limited subset of the experiments in which the containment atmosphere was inert and there was no water in the cavity or elsewhere in the containment. Hydrogen production in the DCH experiments is inferred from analysis of gas grab samples taken at various times after the DCH event. Pilch et al. (1994a) have argued that only the "dry and inert" subset of experiments should be used for DCH model validation purposes, on the grounds that slow chemical reactions of metal with water, steam, and/or oxygen can enhance the apparent production of hydrogen as inferred from the gas sample analyses, but that these reactions occur too slowly to contribute to DCH.

This question is crucial to DCH model validation studies. If the "late reaction" hypothesis is not valid, it would be very difficult defend the TCE model because it underpredicts hydrogen production by a factor of two or more in a number of cases, including the important Zion-geometry integral effects tests (IET). On the other hand, validity of the late reaction hypothesis would pose important difficulties for the CONTAIN DCH model, because this model generally yields reasonably satisfactory results for ΔP *if and only if* processes are modeled that permit the code to provide a reasonable match to the hydrogen production data also (Williams et al., 1997). (Only hydrogen production occurring within the DCH time scale was modeled in the CONTAIN calculations.)

It should be noted that restricting model validation studies to the dry and inert cases would impose a serious limitation on hydrogen model validation efforts: it eliminates all experiments performed with prototypic atmospheres *and all experiments performed in prototypic geometries*, because all the IET experiments (among others) had either oxygen atmospheres, cavity water, or both. Much trouble and expense has been taken to obtain the hydrogen data in the more prototypic IET experiments, and the data are not likely to be supplemented with additional data obtained for these containment geometries and conditions in the future. The data represent an important technical resource that should not be discredited without good reason; the issue is broader than the conflict between the TCE and CONTAIN models.

This Appendix will present reasons for not accepting the "late reaction" hypothesis as it has been advanced by Pilch et al. (1994a). Before continuing, it should be acknowledged that it is at least possible that these late reaction effects may enhance apparent hydrogen production by small amounts, perhaps as much as 10-20%. For whatever reason, there have been variations in experimental hydrogen production numbers at least this large that no DCH model to date has consistently reproduced. What is of interest here is whether the late reaction effects could produce the much larger factor-of-two discrepancies between TCE hydrogen predictions and experimental results, as argued by Pilch et al. (1994a). These discrepancies are illustrated in Figure A-1, which compares predicted and experimental hydrogen production numbers for TCE. In order to facilitate comparisons involving experiments performed at different scales, all results are scaled up to plant scale by dividing by S^3, where S is the linear scale factor. TCE reproduces the trend for the dry and inert cases (closed symbols) reasonably well; however, when the complete data set is considered there is no significant correlation at all between the model predictions and the data ($R^2 \approx 0.01$).

The evidence that has been cited at various times for late reactions includes:

1. Hydrogen from late reactions in the CWTI experiments.

2. Late-time oxygen uptake allegedly observed in the early SNL/DCH experiments (e.g., DCH-3).

3. Evidence for late reactions was cited in the ANL/IET experimental report (Binder et al., 1994).

4. Comparisons between the inert-atmosphere and the noninert SNL/IET experiments that reportedly show apparent hydrogen production 25-30% greater in the noninert cases, with the difference attributed to direct reaction of metal with oxygen.

In what follows, each of the above is considered in more detail. An explanation is then provided for why TCE may give acceptable results for the dry and inert cases but not the other experiments.

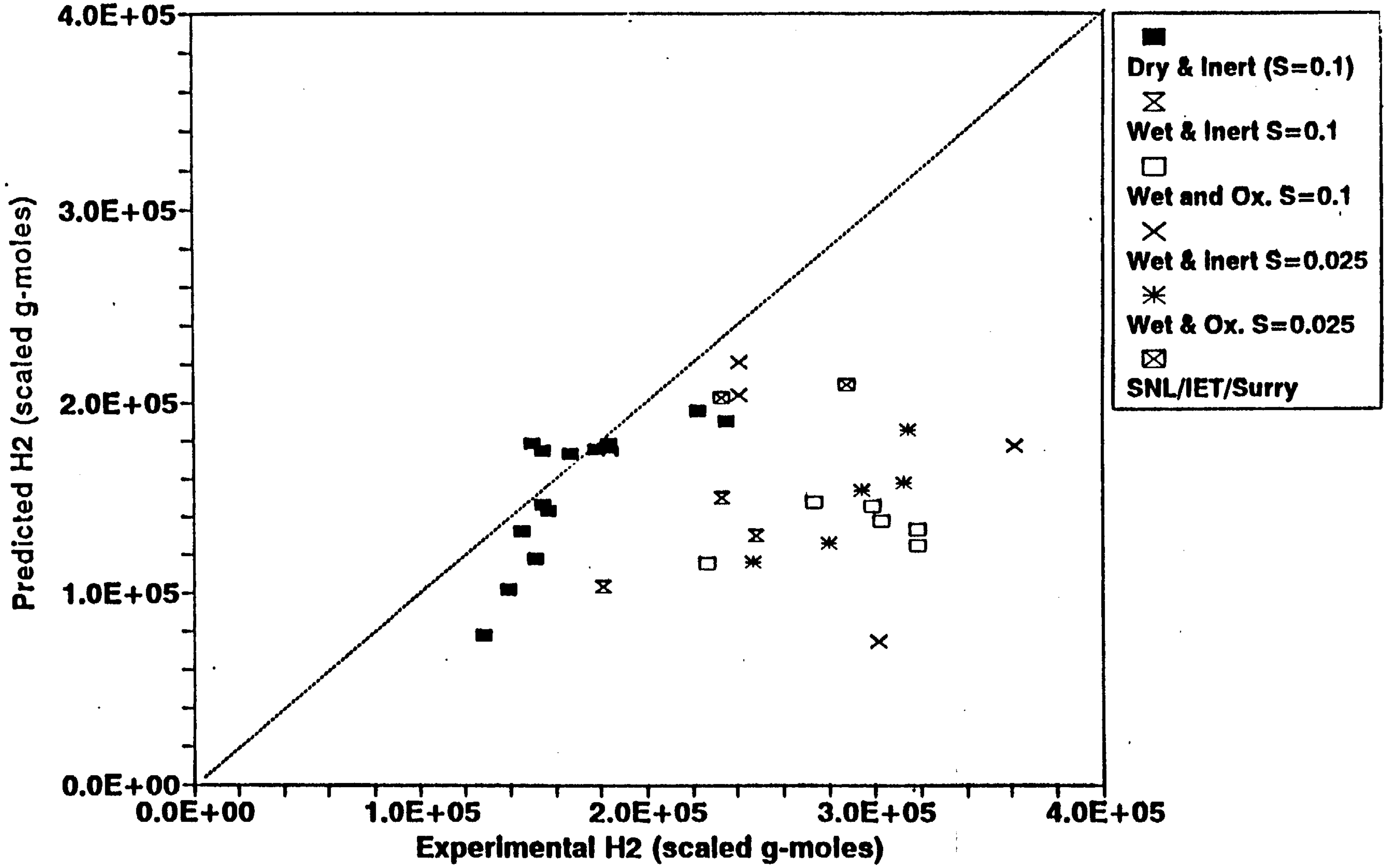

Figure A-1. Predicted versus experimental scaled hydrogen production for the two-cell equilibrium (TCE) model.

A.2 The CWTI Experiments

It has been argued that the CWTI experiments (Spencer et al., 1987) provide evidence of late reaction effects. However, a review of this reference did not identify any allusion to time-resolved hydrogen production data, nor is it apparent how any such data could have been obtained, since hydrogen production is stated to have been based upon gas samples taken 2-3 minutes after the melt ejection occurred. Some model results are presented that do show hydrogen production continuing somewhat longer than DCH time scales; i.e., for ~10 s. However, in all such cases, the model substantially underpredicted the rate of pressurization due to steam generation. When the model was modified to better match the pressurization rate, it also generated ≥85% of the total hydrogen within 1-3 s, in agreement with the interpretation that most hydrogen production does not occur over long times. While one should not put too much stock in this result (models can be fallible and the experiments modeled involved low pressure melt ejection, not HPME), there is no support here for the late hydrogen production hypothesis.

A.3 Early SNL/DCH Experiments: DCH-3

The argument for late reaction effects in the DCH-3 experiment was reproduced in the Surry IET experimental report (Blanchat et al., 1994), which cited results from DCH-3 apparently indicating late-time declines in oxygen. The data from the DCH-3 experiment are illustrated in Figure A-2 (taken from Blanchat et al., 1994), which seems to suggest that most of the oxygen consumption in DCH-3 occurred about 5 minutes after the DCH event. Such a result seems implausible on the face of it: it indicates that white-hot metal spewed through the Surtsey vessel without reacting, but that it abruptly reacted after five minutes, at which time it must have been quite cool.

It now appears that this was a gas mixing effect. The experimental configuration for DCH-3 is illustrated in Figure A-3, in which it is seen that the gas samples were withdrawn at the bottom of the Surtsey vessel, at an elevation well below that at which the hot, buoyant plume accompanying the HPME entered the vessel (Allen et al., 1991). Such a configuration is ideal for producing stratification effects that would have prevented the hot, oxygen-depleted atmosphere from reaching the sampling location at early times. It is, in fact, qualitatively similar to the configuration of recent CE experiments in which there was a cool subcompartment region below a hotter dome region, and in which stable stratification was observed to occur for periods of up to 30 minutes after the tests (Blanchat et al., 1996).

Aerosol measurements were considered important in the early DCH tests, and strong mixing fans were provided to assure representative aerosol samples. The fans were not on at the time of HPME. These fans were activated by a programmed controller that turned on the fans 20-30 seconds prior to opening the gate valve to start aerosol sampling*. The abrupt fan-induced mixing of the oxygen-depleted dome atmosphere with the atmosphere at the sampling location would cause an abrupt decrease in the apparent oxygen inventory. This explanation is consistent with other abrupt changes in gas composition noted at the same time

*Danny Lucero, Sandia National Laboratories, personal communication to the author.

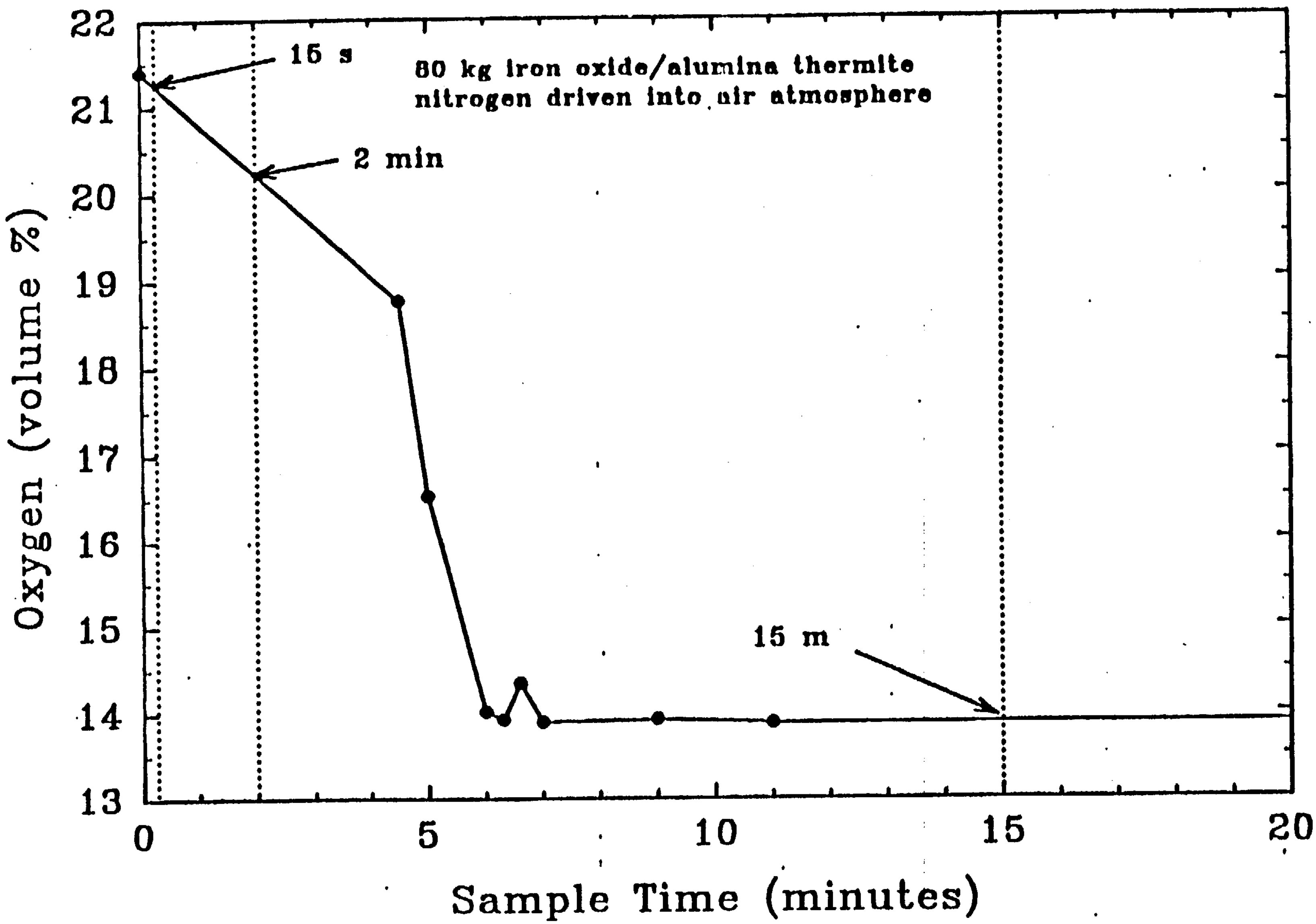

Figure A-2. Apparent oxygen consumption in the SNL/DCH-3 experiment (from Blanchat et al., 1994).

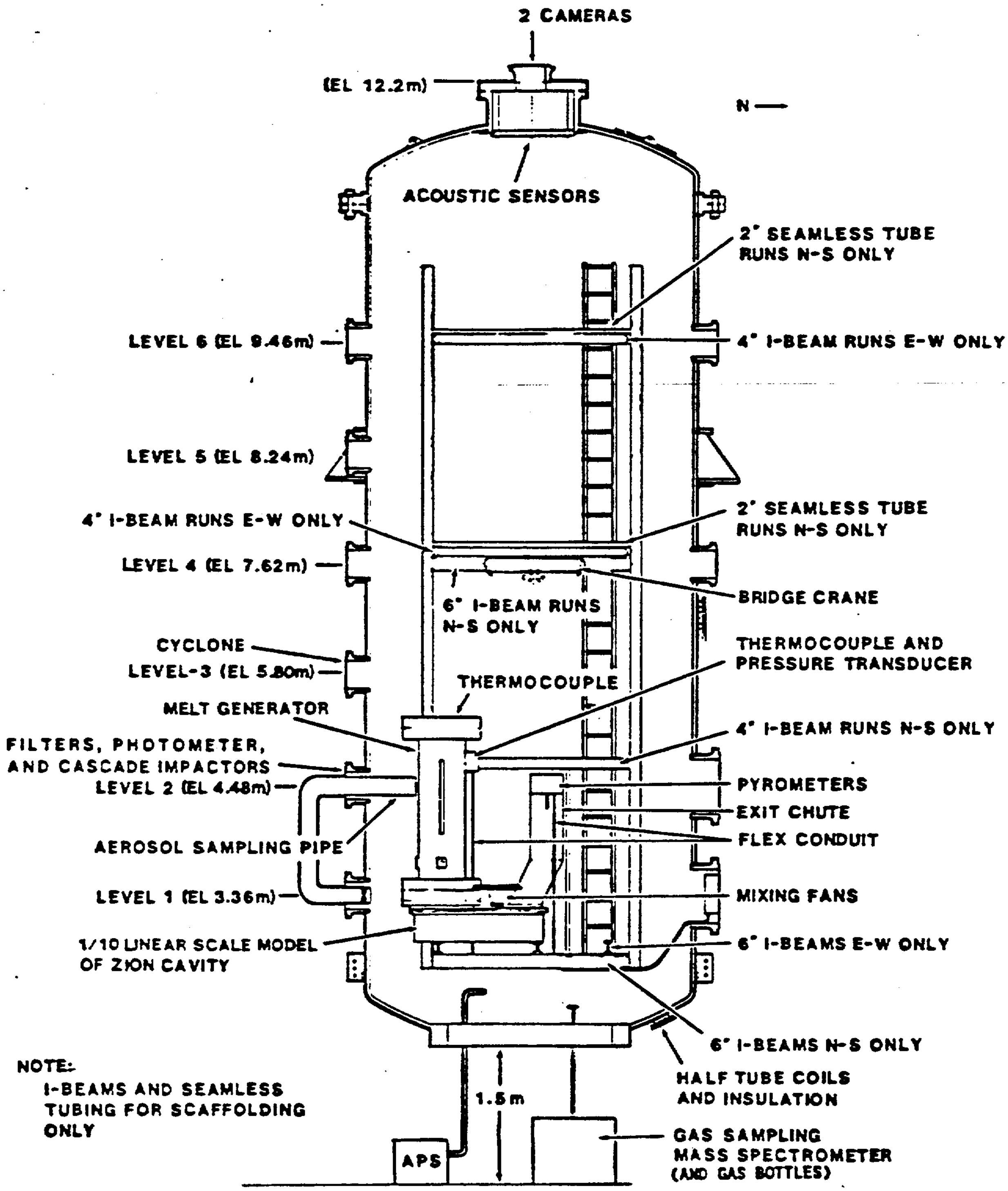

Figure A-3. Experimental configuration for the SNL/DCH-3 experiment (adapted from Allen et al., 1991).

(e.g., an increase in CO_2 concentration from 0.54% to 1.20%) that are inconsistent with the assumption that late oxidation of metal is the cause.

A difficulty is that the experimental report appears to indicate that the first aerosol samples was taken at 3 minutes, not 5 minutes, in DCH-3 (Allen et al., 1991). While it would be desirable to clear up this apparent discrepancy in timing, the evidence is strong that a gas mixing effect is the cause of the apparent decline in oxygen inventory at late times.

A.4 ANL/IET Experimental Report

Binder et al. (1994) discuss the possibility of late reactions perturbing hydrogen measurements and present Figure 4.4 (reproduced here as Figure A-4) in support of this hypothesis. The oxygen results supposedly show evidence of a continued decline after the DCH event; since oxygen depletion is interpreted as representing H_2 produced and then burned in calculating hydrogen production, this decline would increase the apparent hydrogen production.

Actually, the results of the ANL/IET-6 experiment, in which the melt was the usual iron-oxide/aluminum thermite reaction product, show only a very slight decline (the first data point plotted in Figure A-4 is the pretest value; hence the decline between it and the next point includes the decline that occurs during DCH). The ANL/U2 experiment, which used prototypic core materials, does appear to show evidence of a continuing decline in oxygen inventory. However, there were two manifolds for gas collection in this experiment, and only the data from one of the manifolds (which are the results plotted) show this decline. The data tabulations given by Binder et al. (1994) of the detailed gas analysis results indicate that the other data series shows no evidence of a decline. Furthermore, these data show better time resolution, with the first sample being taken at only 5-6 seconds, versus 30-31 seconds for the data series showing the apparent decline. On the other hand, the data series showing the apparent decline does include replicate samples.

There is no known reason to prefer the data series showing the decline in O_2 concentrations to the series that does not show the decline, and the discussion of this issue by Binder et al. (1994) represented, in part, an effort to be consistent with the assumptions made in the DCH issue resolution program. Thus it is questionable as to whether this should be considered independent evidence for late-time reactions even in the ANL/U2 experiment.* Even if it is accepted as such, these results still show no evidence of substantial late-time reactions for the iron oxide/aluminum thermite experiments. UO_2 is capable of being oxidized to higher oxidation states and any decline in atmospheric oxygen content at later times in the ANL/U2 experiment could reflect uranium oxide chemistry that has no analogue in the chemistry of Al_2O_3, which has no higher oxidation states. Since the

*The pressure and temperature data do show evidence of a delayed hydrogen burn occurring about 2 s after HPME. This is still much earlier than any of the gas data and is not the type of process being considered here. No other experiment showed similar evidence of a delayed hydrogen burn.

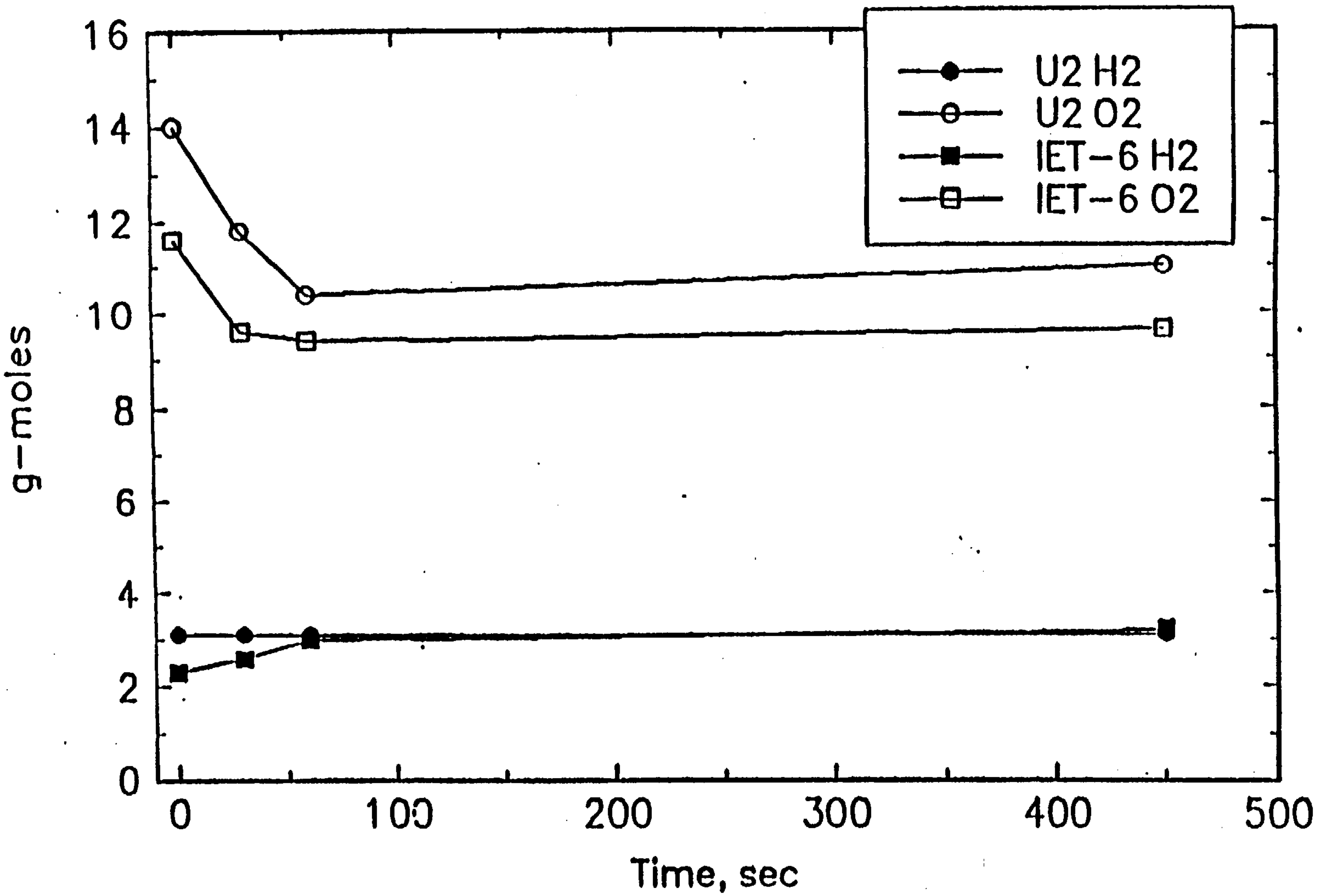

Figure A-4. **Oxygen and hydrogen moles in the ANL/IET-6 and ANL/U2 experiments (Binder et al., 1994).**

large majority of all DCH experiments involve iron oxide/aluminum thermite, including all the experiments that have been analyzed with the CONTAIN code, there is no support here for applying the late-reaction hypothesis generally.

A.5 Inert/Noninert Comparisons from the SNL/IET Experiments

It has been argued that examination of the SNL/IET tests with and without reactive atmospheres suggests that direct metal/oxygen reactions during or after the DCH event could increase the apparent amount of hydrogen produced and burned by ~25-30 percent. In considering this argument, it should first be noted that any direct metal-oxygen reaction occurring during the DCH event is part of what TCE or any other model should account for, since the energy release is equivalent to producing and then burning the equivalent amount of hydrogen; note also that even the fact that the oxygen reaction energy is initially deposited in the debris, not the gas, does not matter for an equilibrium model.

Second, it seems unlikely that this much direct oxygen uptake could take place in the SNL/IET Zion experiments, since the subcompartments surely became oxygen-starved very quickly and not much debris reached the dome.

Third and most important, it is unclear how this conclusion could be inferred from the data. Only the Zion IET experiments are considered here, since the Surry data included no inert-atmosphere cases to provide comparisons. Possible comparison cases include SNL/IET-1 and -1R for the inert cases and SNL/IET-3, -4, -6, and -7 for the noninert cases. (SNL/IET-5 is excluded from the comparisons, since it is not clear whether it should be classified as "inert" or "noninert"; if judged by the combustion behavior, it is "inert".) Experimental hydrogen production numbers for the inert cases are 233 and 248 g-moles, and are 227, 303, 319, and 274 g-moles for the noninert cases, respectively.

The only inert/noninert counterpart comparisons are provided by comparing SNL/IET-1 and -1R with SNL/IET-3, which obviously provides no support at all for the allegedly larger hydrogen production in the noninert cases. The other three noninert experiments have larger hydrogen production but these cases had other differences with respect to the inert cases and are not complete counterparts. Even if one ignores these differences, the noninert average is only 17% higher than the inert average, considerably less than the 25-30% claimed and much less than the factor-of-two effects of primary interest here. Furthermore, applying a simple rank ordering test indicates that the differences between the inert and noninert data are not statistically significant*, even if one ignores the other differences between these experiments.

A.6 Reasons for Inert/Noninert Differences in TCE Validation

It is concluded from these results that the only significant evidence for believing that only the dry/inert cases are suitable for model validation is that it is only these cases that

*R. Iman, Sandia National Laboratories, personal communication to the author.

agree with TCE. Since there are many other reasons discussed elsewhere in this report for questioning the validity of TCE, the fact that the noninert/wet hydrogen data disagree with TCE is not considered an adequate basis for rejecting these data. This belief is strengthened by the fact that other DCH models including MELCOR (Kmetyk, 1993) and CONTAIN (Williams et al., 1997) provide reasonable matches to the hydrogen data without rejecting the noninert/wet cases, and one of the models (CONTAIN) can consistently match the ΔP data *only* if phenomena are modeled that allow it to match the hydrogen data reasonably well. While it is true that none of the models provide a fully mechanistic "first principles" prediction of hydrogen production without any parametric features or ad hoc hypotheses, it also remains true that TCE is alone in its inability to predict the hydrogen results.

The present arguments would be supported further if an explanation could be found for why TCE behaves differently for the dry/inert cases versus the others. Such an explanation is suggested by the CONTAIN analyses of hydrogen production in these experiments. The latter results are shown in Figure A-5. The LFP experiments (crosses) and open geometry experiments (asterisks) include the dry/inert cases, and it is apparent that these do not differ significantly from the others in terms of CONTAIN's ability to reproduce the dominant trends. Sources of hydrogen production on DCH time scales that CONTAIN can consider that TCE does not are (a) debris-water interactions if cavity water is present, and (b) nonairborne debris interactions. [The results in the figure actually include only nonairborne debris; see Section 4, Williams et al. (1997) for discussion of the difficulty of distinguishing the nonairborne debris effects and water effects in the CONTAIN analyses.] If both these processes are eliminated, CONTAIN hydrogen predictions show qualitatively similar trends to the TCE predictions in Figure A-1 (see Figure 3-2b of the main report).

Restricting TCE comparisons to the dry/inert cases immediately eliminates any experiments (including all Zion IET experiments) in which debris-water interactions could have contributed hydrogen not accounted for in TCE. Nonairborne debris interactions might be supposed to still contribute in the dry/inert cases. However, the contribution of nonairborne debris is principally important by permitting the noncoherent portion of the blowdown steam to interact with nonairborne debris in the cavity and/or subcompartments; it is not expected that nonairborne debris interacting with the coherent steam can significantly add to the hydrogen generated from the airborne debris interacting with the coherent steam, since the latter interaction by itself appears to be quite efficient. Thus, nonairborne debris interactions are expected to be important only if a substantial fraction of the total blowdown steam is noncoherent; e.g., as in the Zion SNL/IET experiments, in which only 20-30% of the blowdown was coherent and the remainder noncoherent.

The dry/inert cases are the TDS experiments, LFP experiments, and two of the three WC experiments. The fraction of the total steam that is coherent, f_{coh}, can be estimated from

$$f_{coh} = 1 - \left(\frac{P_0}{P_e}\right)^{-1/\gamma}, \qquad \text{(A-1)}$$

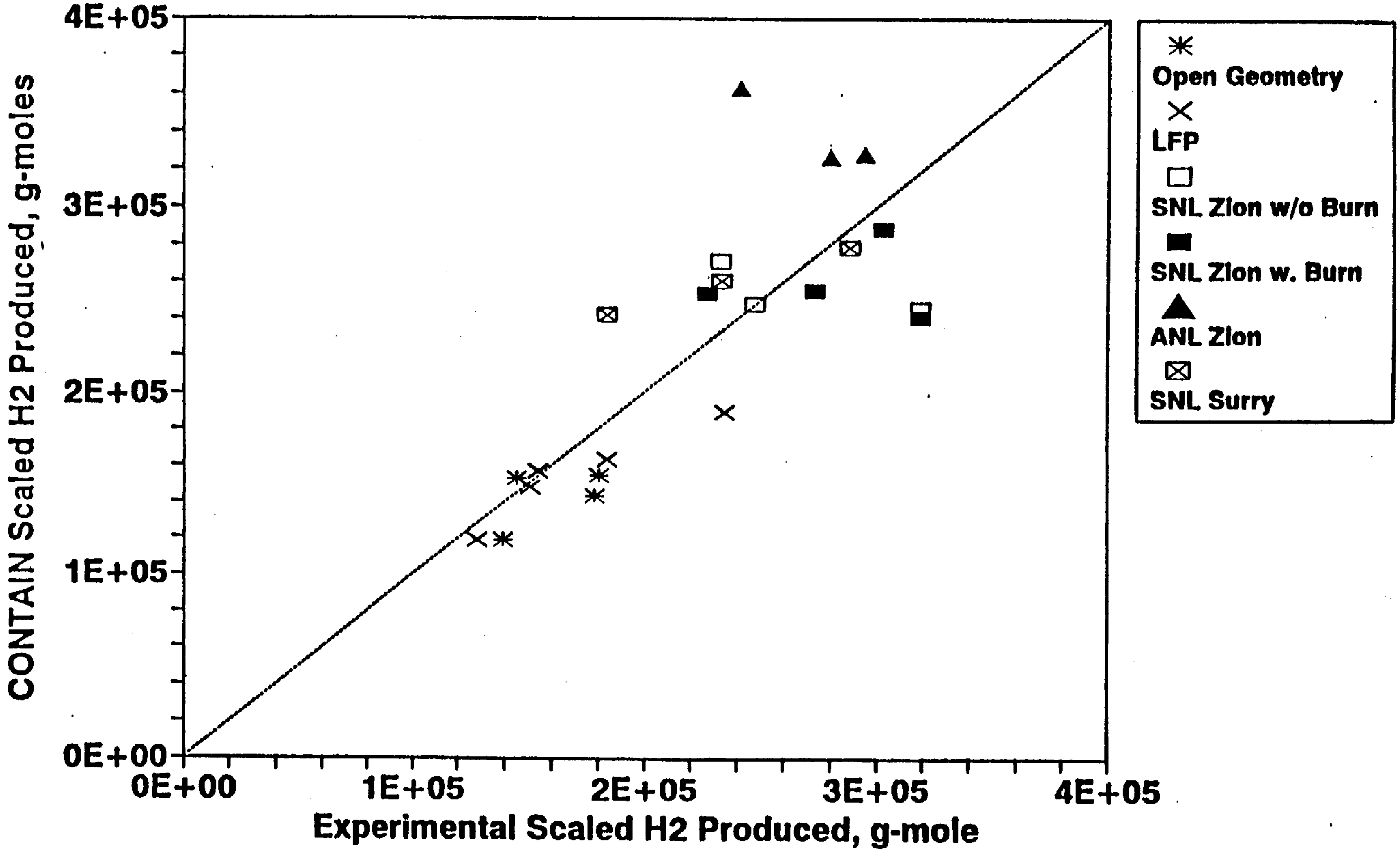

Figure A-5. Predicted versus experimental scaled hydrogen production for the CONTAIN code.

where P_0 is the accumulator pressure at the start of the blowdown, P_e is the pressure in the accumulator at the end of the debris dispersal interval, and γ is the ratio of specific heats for steam, taken to be 1.33. Coherence data including the ratio P_0/P_e are given for all the experiments in Table E-8, Appendix E, Pilch et al. (1994a). Based upon these data, all the dry/inert experiments except WC-1 had high coherence ratios, with the coherent steam as calculated from Eq. (A-1) varying from 55% to 74% of that initially present in the accumulator. Since driving pressures were low in these experiments, 15-20% of the initial steam remained in the accumulator at the end of the blowdown; taking this into account, only 10-33% of the total blowdown steam is noncoherent and therefore eligible to enhance hydrogen production by nonairborne debris interactions. Compared with the IET experiments, the potential for hydrogen production by nonairborne debris interactions is small.

For the WC-1 experiment, almost 60% of the total blowdown is noncoherent and the above argument does not apply. However, the debris dispersal was very high in this experiment, about 85%, meaning that there was relatively little metal left behind in the cavity to undergo nonairborne interactions. Furthermore, debris exiting the cavity immediately entered the large inerted volume of the Surtsey vessel in this open-geometry experiment, with essentially no opportunity for nonairborne debris interactions to occur following debris deposition. Again, nonairborne debris interactions would not be expected to make a large contribution. By contrast, most debris in the IET experiments (especially Zion) is trapped in a relatively small subcompartment volume that quickly develops a steam-rich atmosphere that could permit nonairborne debris interactions to continue.

It follows, therefore, that restricting validation to the dry/inert cases also restricts the validation to experiments in which the additional processes (water and/or nonairborne debris) considered to be significant by Williams et al. (1997) have at most a limited potential to contribute. Hence it is not surprising that TCE can reproduce hydrogen results reasonably well for these cases, but not for the others.

A.7 Summary and Conclusion

Evidence has been cited at various times that reportedly indicates that only DCH experiments with dry cavities and inert atmospheres should be used for validation of model predictions of hydrogen production on DCH time scales. A review of this evidence actually indicates that there is little support for the hypothesis that hydrogen results for other experiments should not be used. The only significant evidence for believing that experiments with wet cavities and/or oxygen atmospheres should not be used appears to be that these data do not agree with the TCE model, while data for the dry/inert cases do agree reasonably well. Since TCE validity is in question, and since other DCH models (MELCOR and CONTAIN) are not similarly restricted to the dry/inert cases in terms of their ability to reproduce the hydrogen data, this difficulty with the TCE predictions is not considered to be an adequate reason for rejecting the data. This conclusion is strengthened by the fact that other plausible explanations exist for the failure of TCE to reproduce the hydrogen data for experiments other than the dry/inert cases.

The existing database on hydrogen production is a valuable technical resource for DCH analysis that is unlikely to be supplemented by additional experiments in the future. It is therefore recommended that efforts to discredit the hydrogen data for experiments with water and/or oxygen atmospheres should not be continued, unless much stronger evidence for doing so can be presented than has been done to date.

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Appendix B
Experimental Determination of the Coherence Ratio

In the NUREG/CR-6075 Issue Resolution effort, the concept of limited coherence between the dispersal of debris and the blowdown steam plays a very important role as a mitigating effect. As is stated on p. 49 of the NUREG/CR-6075 Supplement (Pilch et al., 1994b):

> Most input parameters in the TCE model are related to initial conditions and material properties. The *key modeling parameter* in the TCE model is the melt-to-steam coherence ratio. Because the entrainment time is short compared with the blowdown time, molten debris is exposed to a small fraction of the primary system steam during the dispersal process. Since this steam is the medium for carrying the melt energy and the hydrogen produced by steam/metal interactions to the main containment volume, *this incoherence is a crucial mitigating factor.* With this understanding, it is possible to reduce most of the complexity of cavity phenomena to the coherence ratio ($R_\tau = \tau_c/\tau_b$ in the TCE model). [Emphasis supplied.]

Despite the importance ascribed to low coherence as a mitigating effect, no experimental evidence has ever been presented that coherence plays such a dominant role and evidence to the contrary has been not been considered; this issue is discussed in Section 5.1 of the main report and need not be revisited here. The present discussion considers the adequacy of the procedures used to estimate coherence from the experimental data. As will be seen, it is necessary to become rather intimate with certain details of the experimental results in order assess this issue.

The time required to disperse debris was estimated primarily from the cavity pressurization histories. In all DCH experiments using molten thermite, there is an interval in which cavity pressures are significantly higher than in the main containment vessel. This time interval is interpreted as being the interval during which debris is dispersed. Pyrometers focussed on the cavity exit provide at least qualitative support for this interpretation. In attempting to quantify coherence, Pilch et al. (1994a) reportedly made some use of pyrometer traces, in addition to cavity pressurization histories; however, no information was given as to how the rather qualitative pyrometer information was applied to extract quantitative estimates of the dispersal interval and the present discussion is limited to the cavity pressure histories.

Figures B-1 to B-5 illustrate the procedure, and some of the difficulties, for the experiments SNL/IET-1, SNL/IET-1R, SNL/IET-6, and ANL/IET-6. (The meaning of the vertical arrows in these figures is discussed below.) These figures give the cavity pressurization histories and Figure B-2 also gives the blowdown history for SNL/IET-1. In the cavity pressurization curves, the irregular peaks at early times (< 0.5 s) in the SNL cases are thought to represent FCIs, while the dispersal interval is thought to be represented by the later, broader peak that is typically on the interval 0.4-1.0 s. In extracting coherence

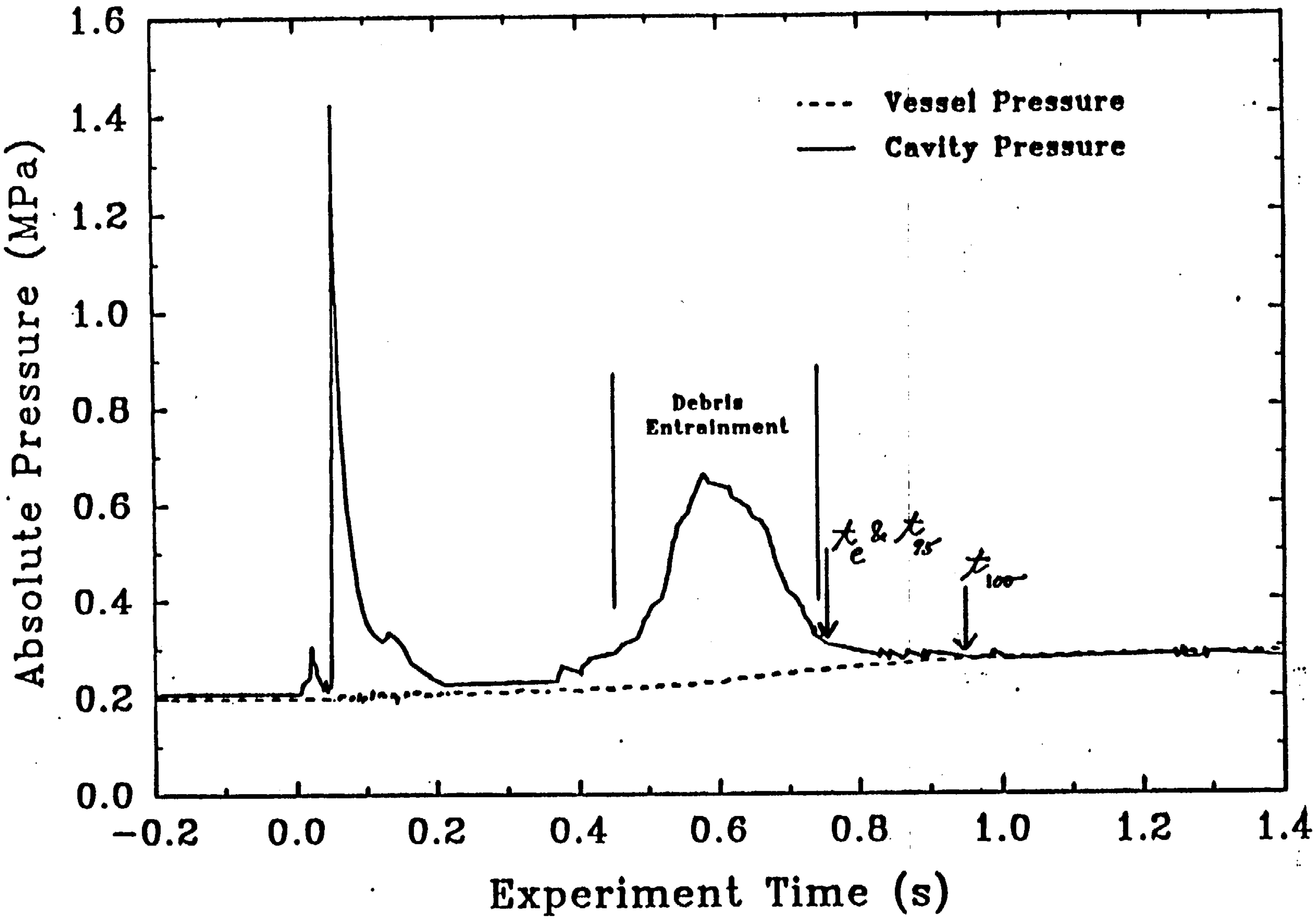

Figure B-1. Cavity pressurization history for the SNL/IET-1 experiment.

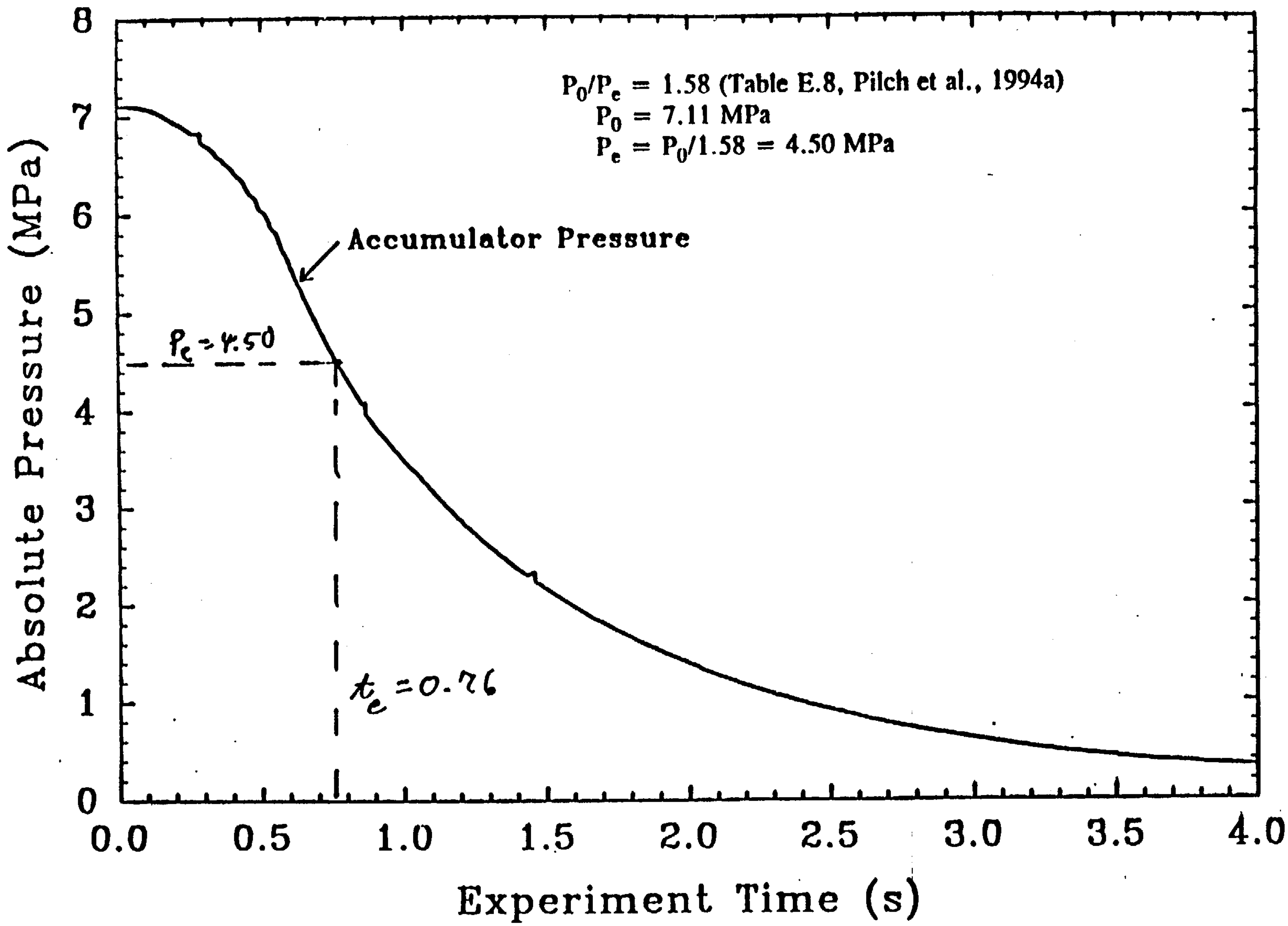

Figure B-2. Accumulator depressurization history for the SNL/IET-1 experiment, illustrating the method for determining the end of the entrainment interval, t_e, corresponding to the analysis of Pilch et al. (1994a).

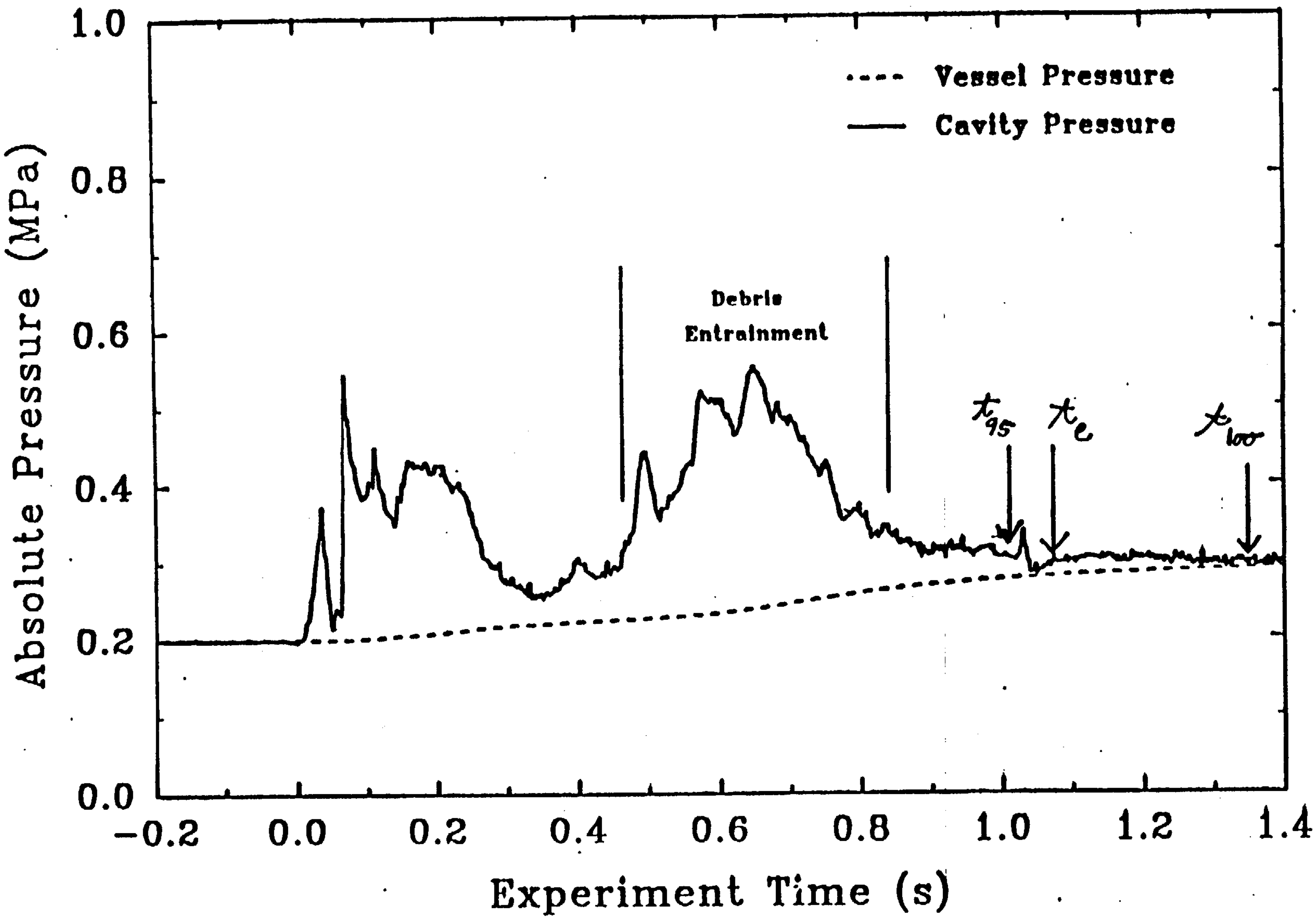

Figure B-3. Cavity pressurization history for the SNL/IET-1R experiment.

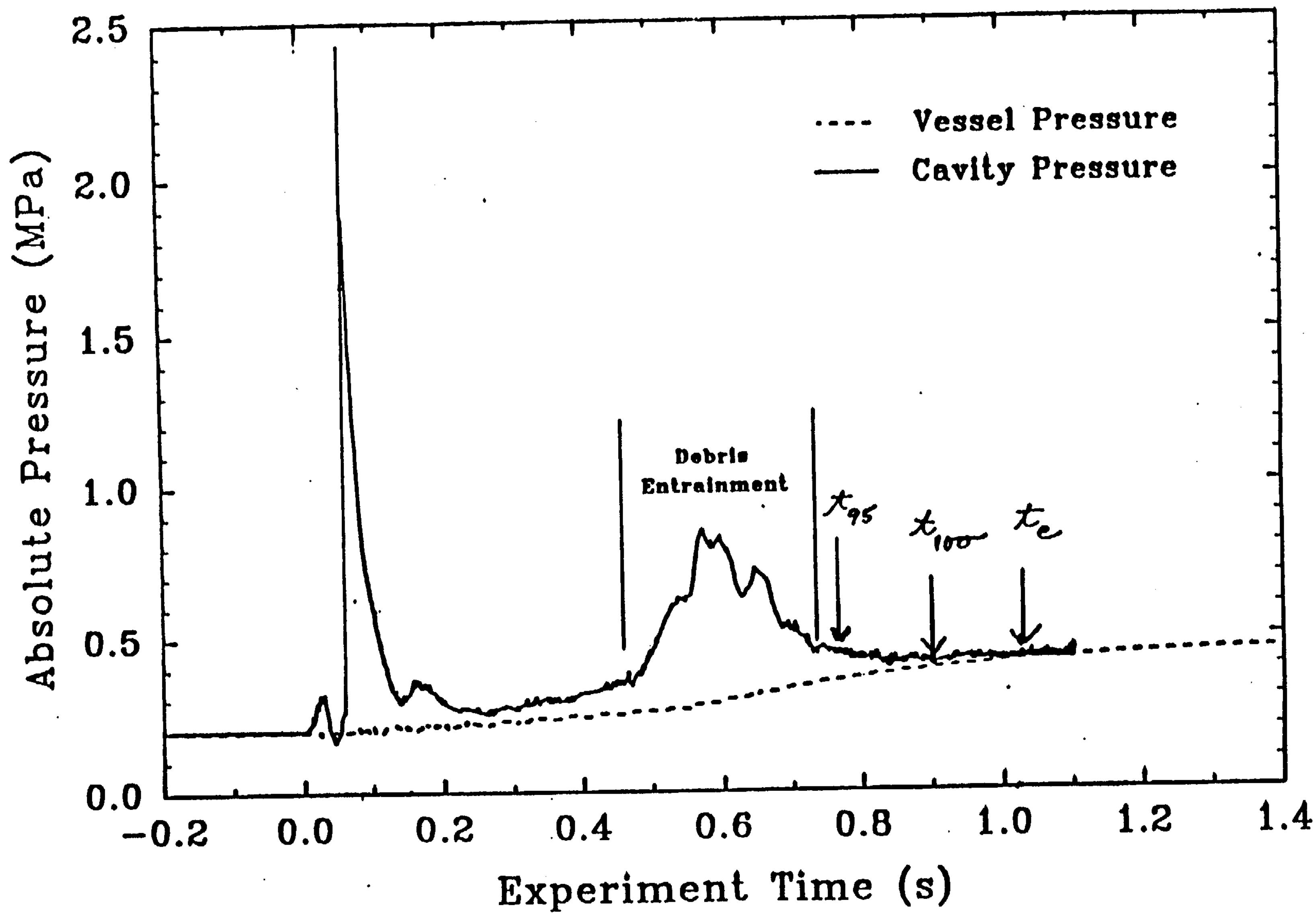

Figure B-4. Cavity pressurization history for the SNL/IET-6 experiment.

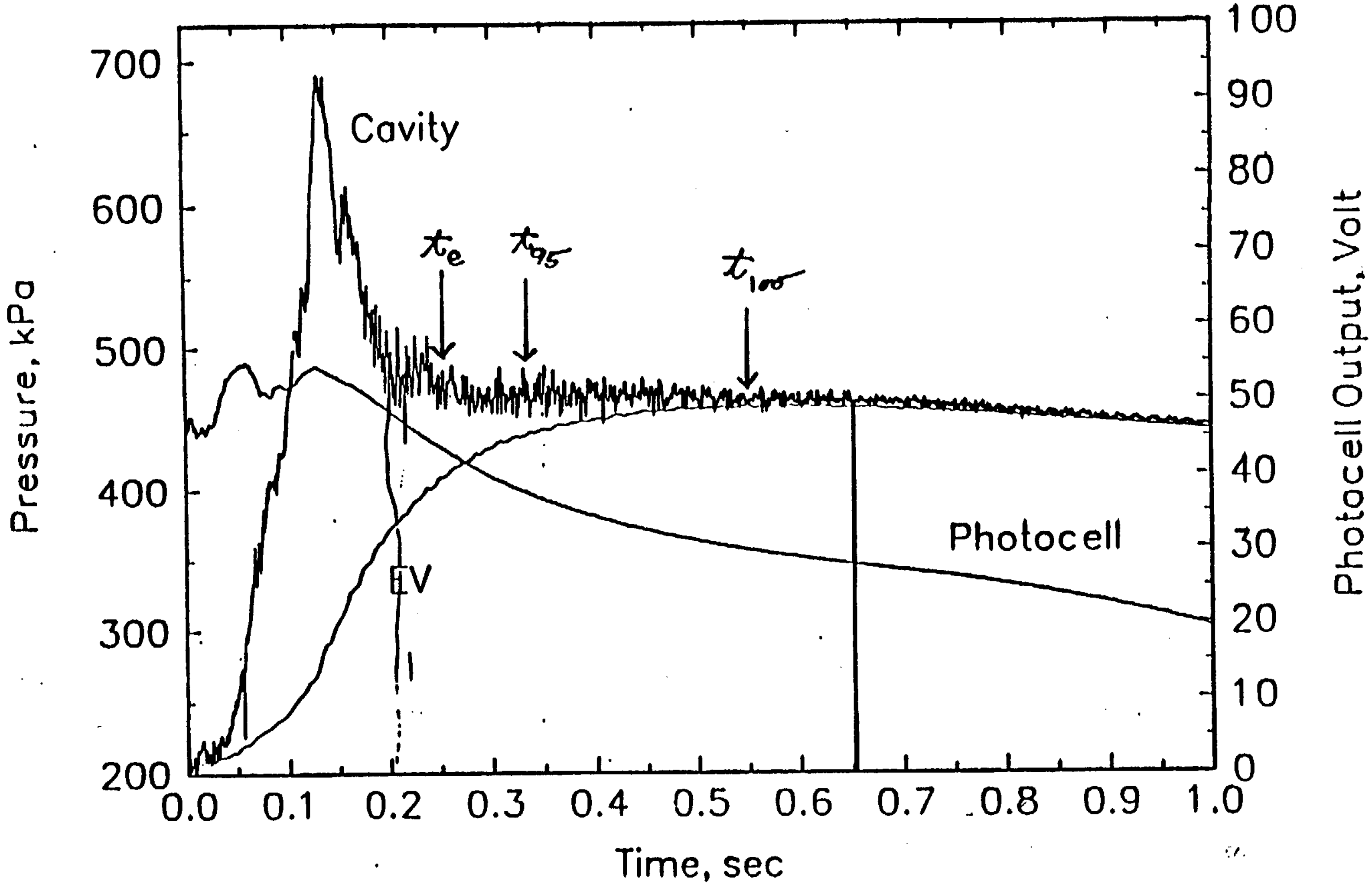

Figure B-5. Cavity pressurization history for the ANL/IET-6 experiment.

ratios, the approach is to use the cavity pressure curves to identify the time t_e at which dispersal ends, read off the pressure in the accumulator (P_e) at this time, and estimate the fraction of the blowdown steam that is coherent with debris dispersal from the ratio P_0/P_e, where P_0 is the initial pressure in the steam accumulator.

The coherence ratio is then calculated from this pressure ratio and the assumption that the accumulator depressurizes isentropically, yielding Eq. E.91 of NUREG/CR-6075:

$$R_\tau = \frac{\tau_e}{\tau_b} = \frac{2}{\gamma - 1}\left[\left(\frac{P_0}{P_e}\right)^{\frac{\gamma-1}{2\gamma}} - 1\right], \qquad \text{(B-1)}$$

where γ is the ratio of specific heats for steam, taken here to be 1.33. Another representation of coherence is f_{coh}, the fraction of the total steam that is coherent with debris dispersal; again assuming an isentropic depressurization of the accumulator, f_{coh} is given by

$$f_{coh} = 1 - \left(\frac{P_0}{P_e}\right)^{-\frac{1}{\gamma}}. \qquad \text{(B-2)}$$

Since f_{coh} is directly proportional to the amount of steam that gets to interact with debris in the TCE model, it is the most direct measure of the potential significance of uncertainties in the coherence.

This process would be straight-forward if the cavity pressurization histories exhibited an abrupt cut-off, but it is apparent from the figures that this is anything but the case: the curves tail off gradually, which raises the question as to how to choose t_e. The amount of debris represented by the tail may be small, but the uncertain time interval is a time at which the accumulator is depressurizing rapidly (see Figure B-2) and the total amount of steam credited as being "coherent" can be rather sensitive to the "cut-off" time, t_e. Note here that TCE is a "batch" model in which all steam considered to be "coherent" is allowed to interact with all the dispersed debris, even though steam entering the cavity during the tail end of the dispersal process might reasonably be supposed to interact with only a limited amount of debris; on the other hand, all "noncoherent" steam undergoes no interaction with debris at all in the model.

Pilch et al. (1994a) describe TCE as a "principle-based" model and the responses to reviewers' comments deny *any* tuning to fit the data [see, e.g., Response F35, Appendix A, Pilch et al. (1994b)]. This claim seems difficult to defend in view of the difficulty in defining *a priori* a criterion for deciding where to take the cut-off point for t_e. One legitimate option might be to admit a certain amount of empiricism in the model and define a procedure for choosing the cut-off point by fitting to give the best over-all fit to the ΔP data, being careful to use this same procedure for every experiment. The model would then be semi-empirical with a tuning parameter, not fully "principle-based" as currently claimed; however, much of engineering is based upon such semi-empirical correlations and there is nothing illegitimate about their use when they are developed and applied in a valid manner that is adequately explained and justified.

Comparison of the figures reproduced here reveals an important complication to pursuing the approach just suggested: with the partial exception of SNL/IET-1 and SNL/IET-6, which are somewhat similar, the cavity pressurization curves differ considerably from one another (this variability is the rule, not the exception). Hence it could be difficult to define and apply consistently "the same procedure" for every instance. This difficulty raises concerns as to the degree of consistency actually achieved. Inconsistent definition of the cut-off point can distort or obscure trends in the data and can invalidate the use of the approach even as an empirical correlation. Since the "experimental" values of coherence are input to the TCE model in the comparisons of the model predictions with experiment, inconsistent definition of the cut-off point would raise questions concerning the adequacy of the validation claimed for TCE.

There is evidence that this distortion has, in fact, occurred. Table E.8 of (Pilch et al., 1994a) tabulates data for the coherence ratio correlation and includes values of the ratio P_0/P_e. As part of the present review effort, the corresponding values of t_e were backed out from the tabulated P_0/P_e values together with the experimental accumulator depressurization curves (Allen et al., 1994); see Figure B-2 for the SNL/IET-1 example. These values are indicated in the cavity pressurization plots by the vertical arrows labeled "t_e". Table E.8 of (Pilch et al., 1994a) itself does tabulate values of t_e also; in most instances these agree reasonably well with the values backed out here but in a few cases they do not. In all cases, the values of R_τ tabulated correspond to the values of P_0/P_e tabulated and it therefore appears that the values of t_e derived here are close to the values that were actually used in the validation of TCE and its coherence ratio correlation as presented by Pilch et al. (1994a).

Even a casual inspection of these plots shows there is inconsistency in the treatment. For the SNL/IET-6 case (and also SNL/IET-3; see Figure B-6), the criterion for choosing the cut-off point appears to have been quite stringent; that is, all the tail is included in the coherence interval. (As an aside, one might question such a liberal allowance for the coherence interval because the steam entering the cavity during this time would see only the small amount of dispersed debris responsible for the tail. Note also that even the accumulator blowdown can produce some cavity pressurization. However, the main issue here is consistency.) On the other hand, for SNL/IET-1 and ANL/IET-6 the definition of the coherence interval is much less liberal, with a significant portion of the tail being excluded. The inconsistency is especially noteworthy for SNL/IET-1 and SNL/IET-6, since their cavity pressure histories are more nearly similar than is usually the case which should make it easier to define the cut-off consistently. It may be noted that, even with these values of t_e, TCE overpredicts SNL/IET-1 ΔP somewhat and underpredicts SNL/IET-6 slightly; a more nearly consistent treatment would worsen agreement for one or both of these experiments.

An even more important concern is illustrated by the ANL/IET-6 versus SNL/IET-6 comparison. A fundamental premise of the DCH issue resolution modeling is that scale-dependencies are negligible, with the possible exception of some weak scale-dependencies in hydrogen combustion. Both TCE and its coherence correlation are fundamentally scale-independent. Returning to SNL/IET-6 and ANL/IET-6, the values of R_τ tabulated in Table E.8 of (Pilch et al., 1994a) are 0.31 and 0.35, which appear to be reasonably consistent with scale effects being minor (and less than the random variability in the experiments). However, the inconsistency in the cut-off definition raises doubts as to this conclusion: if the tail in the ANL/IET-6 curve were included as rigorously as was the case for SNL/IET-6, the ANL/IET-6 coherence would clearly be larger. Furthermore, inspection of the IET Zion results generally revealed a similar pattern: except for SNL/IET-1, t_e was defined for the SNL cases so as to quite rigorously include the tail (especially in the cases for which DCH-produced hydrogen could burn), while significant amounts of the tail were omitted in the ANL cases.

In order to examine this inconsistency more quantitatively, the following procedure was adopted in the present review:

1. As best possible, define t_{100} to be the time at which cavity pressures returned to the containment value, to within the uncertainty in evaluating the curves.

2. Integrate the area between the cavity pressure history curve and the containment vessel curve out to t_{100} (the portion of the pressure histories attributed to FCIs was excluded in this integration).

3. Define t_N to be the time at which the running integral of the area between the two pressure curves achieves N% of its final value.

4. Base coherence estimates on the amount of depressurization that occurs up to time t_N.

Because the cavity pressurization does tail off gradually, the definition of t_{100} is subject to some of the same subjectivity as the definition of t_e that was discussed above. However, the actual area between the two curves over the questionable time period is very small and thus the definition of t_N is considerably less sensitive to this subjectivity unless N is chosen to be very close to 100%. For present purposes, N = 95% was chosen, although N = 85% was also used as a check. Leaving 15% of the debris outside the coherence interval is almost certainly too much if the purpose were to obtain values suitable for use in TCE; however, the only purpose here was to examine sensitivity of the consistency arguments to N. Indeed, there is no claim that N = 95% represents a "best" value for use in TCE.)

This technique was applied to the three SNL and three ANL IET experiments that were designed to be direct scaled counterparts of one another: ANL/IET-1RR, ANL/IET-3, and ANL/IET-6; and SNL/IET-1, SNL/IET-3, and SNL/IET-6,* respectively. Since

*Re-examination of SNL/IET-6 indicated that the value of t_{100} initially chosen (0.9 s) did leave out a small tail in the cavity pressurization curve (Figure 2.4); refiguring with t_{100} = 1.025 s shifted t_{95} from 0.77 s to 0.81 s and increased f_{coh} from 0.144 to 0.167, a change considerably too small to affect any conclusions of interest here. This result illustrates the limited sensitivity of the t_{95} method to ambiguity in t_{100}.

SNL/IET-1R was designed to be a replicate of SNL/IET-1, it was also included. Figures B-6 to B-8 present cavity pressurization curves for the three experiments not previously illustrated. For all the experiments, t_e values used by Pilch et al. (1994a), t_{100} values, and t_{95} values are shown (vertical arrows). It would appear from the figures that the t_{95} values do provide a significantly more consistent treatment of where to choose the coherence interval cut-off time than do the t_e values used by Pilch et al. (1994a). Furthermore, it is Pilch et al. (1994a) and the subsequent documents, not this critique, that claim to "resolve" DCH; hence, the burden of proof is on demonstrating that either the DCH issue resolution interpretation of these data is superior to the interpretation offered here, or else demonstrating that the difference is not significant.

Demonstrating that this difference is insignificant would appear to be difficult. Its potential importance is illustrated in Table B-1. The first column identifies the experiments, and the next two columns give the values of f_{coh} and R_τ used by Pilch et al. (1994a). The fourth and fifth columns give corresponding values obtained from the present analysis using t_{95} and the last two columns give results based upon t_{85}. Also shown in the table are the averages for the three ANL/IET experiments considered, the averages for the four SNL/IET counterpart experiments, and the ratio of the averages.

Table B-1
Scale-Dependence of the Coherence Ratio

Experiment	NUREG/CR-6075		t_{95} Values		t_{85} Values	
	f_{coh}	R_τ	f_{coh}	R_τ	f_{coh}	R_τ
ANL/IET-1RR	0.453	0.634	0.474	0.678	0.338	0.426
ANL/IET-3	0.244	0.286	0.419	0.568	0.259	0.307
ANL/IET-6	0.291	0.354	0.415	0.560	0.259	0.307
SNL/IET-1	0.291	0.354	0.291	0.354	0.248	0.291
SNL/IET-1R	0.281	0.339	0.248	0.291	0.160	0.176
SNL/IET-3	0.259	0.307	0.193	0.218	0.139	0.151
SNL/IET-6	0.263	0.313	0.167	0.185	0.117	0.126
ANL avg	0.329	0.425	0.436	0.602	0.285	0.347
SNL avg	0.273	0.328	0.225	0.262	0.166	0.186
ANL/SNL	1.204	1.294	1.94	2.23	1.721	1.864

Based upon the NUREG/CR-6075 values of the coherence, one would be justified in concluding scale effects are minor; the ANL f_{coh} average is only 20% higher than the SNL average and most of this difference is due to the ANL/IET-1RR result, with all the remaining

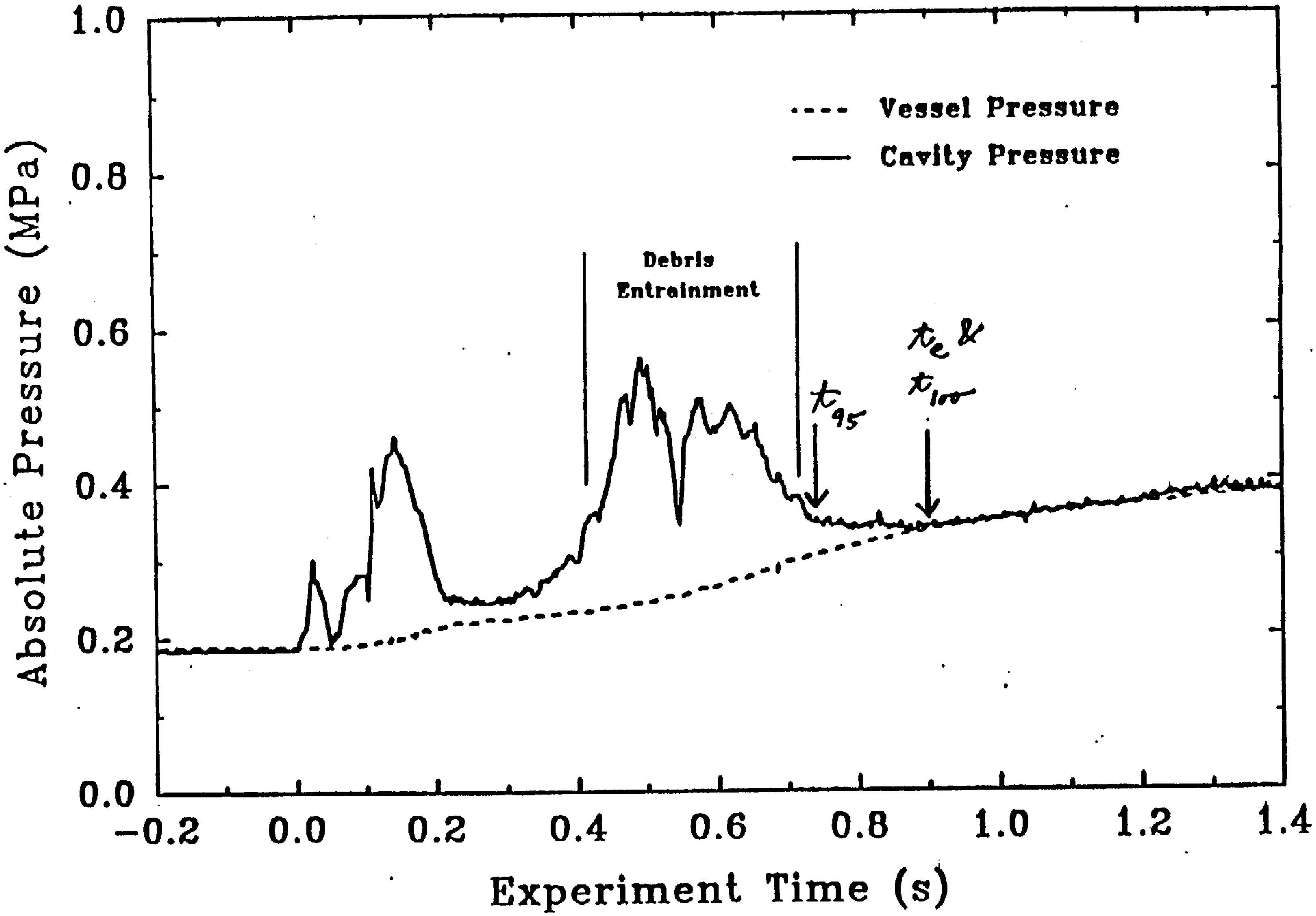

Figure B-6. Cavity pressurization history for the SNL/IET-3 experiment.

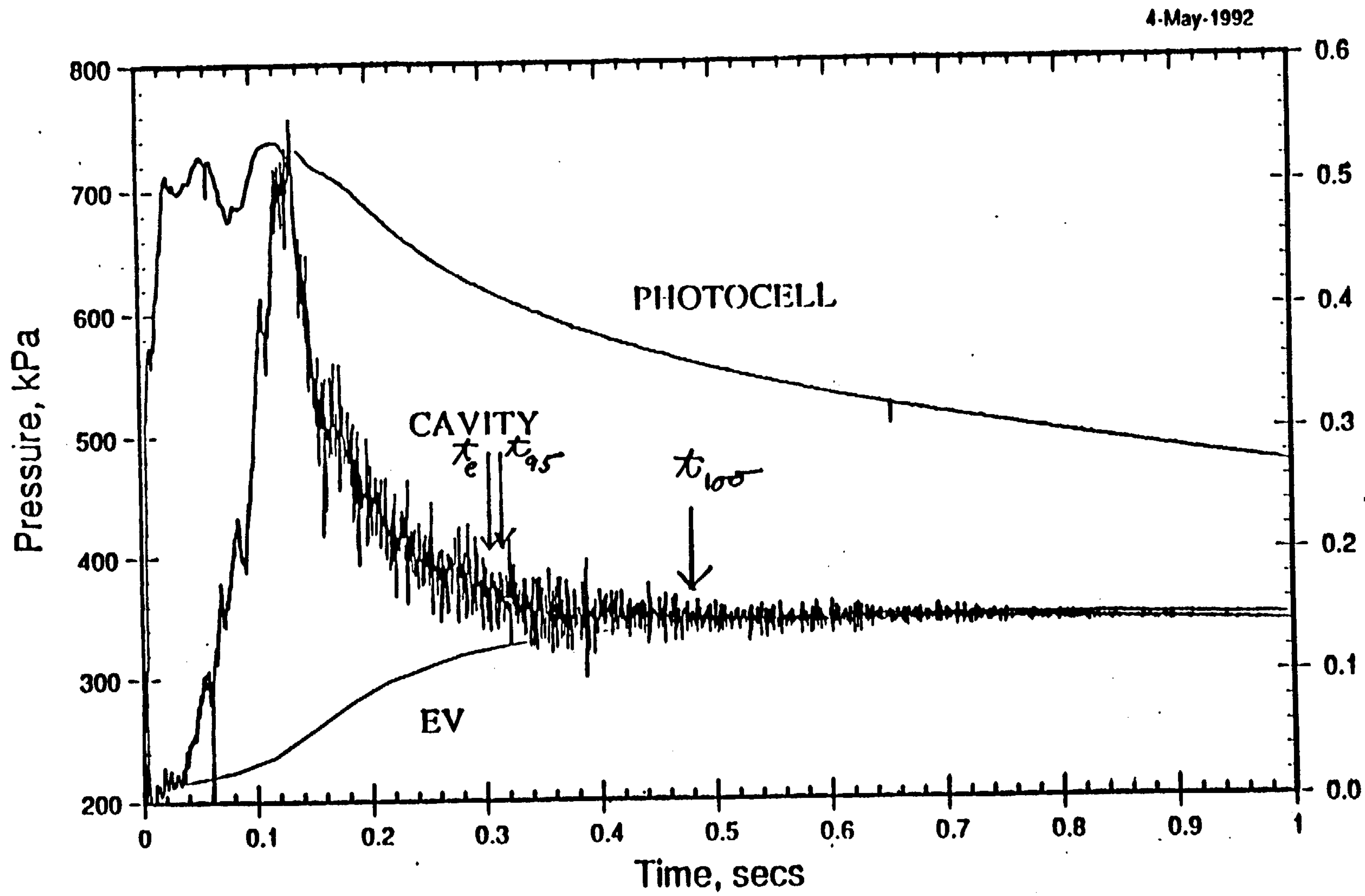

Figure B-7. Cavity pressurization history for the ANL/IET-1RR experiment.

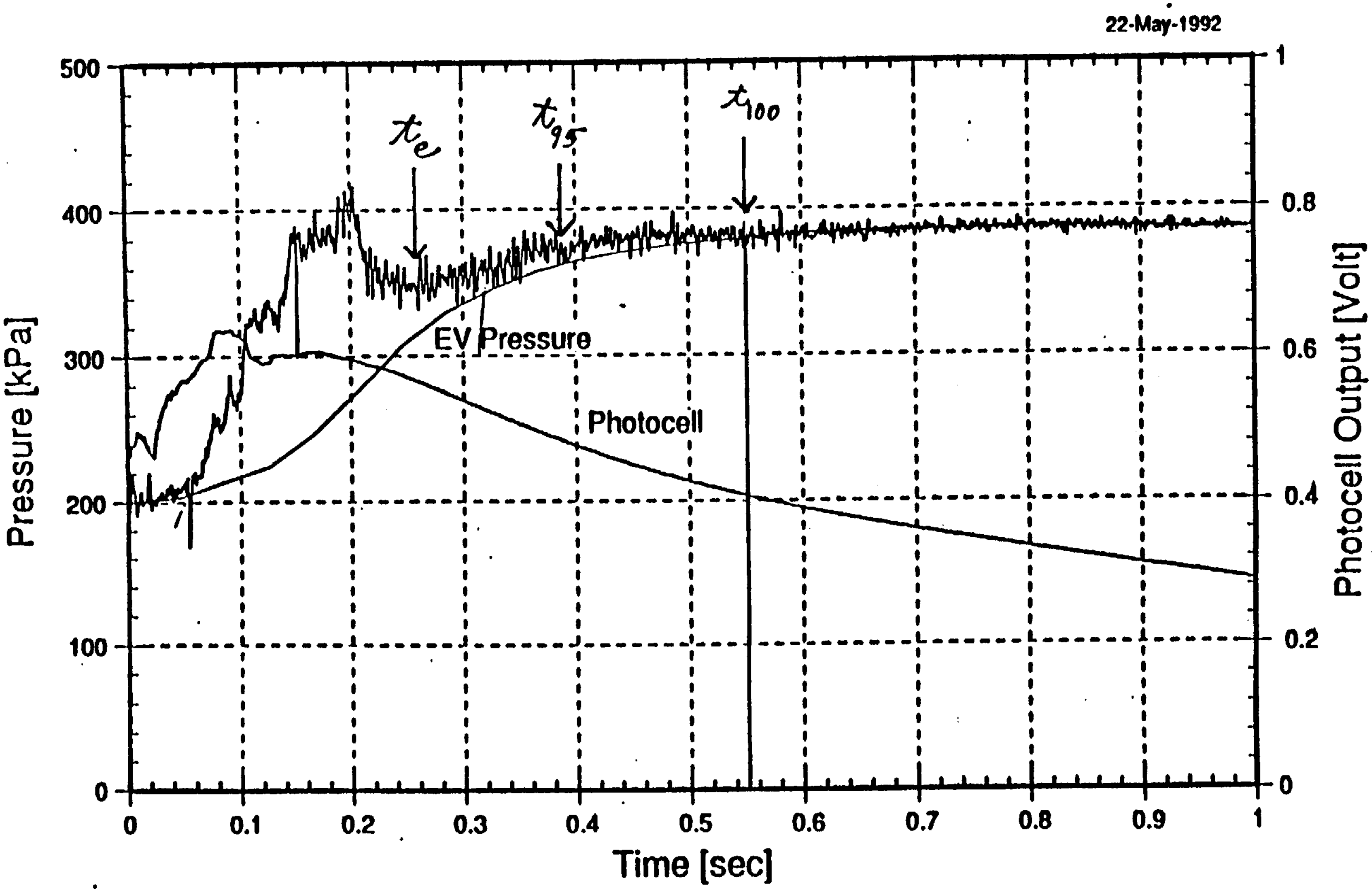

Figure B-8. Cavity pressurization history for the ANL/IET-3 experiment.

values being in good agreement with one another. (It should be recalled here that, other than scale, the parameters varied in these experiments did not include parameters that might reasonably be expected to have large effects upon the coherence.)

A quite different picture emerges when coherence estimates are based upon t_{95} as defined above. Here the ANL values of f_{coh} average almost twice as large as the SNL values and the spread within either the ANL group or the SNL group is considerably smaller than the difference between the group means; i.e., all of the three ANL values are significantly larger than any of the four SNL values. This method of analysis would justify a conclusion that scale effects are substantial. Even use of the t_{85} values would not change the qualitative picture, although the magnitude of the effect would be reduced somewhat.

It is also apparent that all the t_{95} coherence values for the ANL experiments other than ANL/IET-1RR are greater than values given by Pilch et al. (1994a), while all the SNL/IET t_{95} coherence estimates are less than the estimates of Pilch et al. (1994a) with the exception of SNL/IET-1, for which the two estimates are the same. Results in Table E.6 of (Pilch et al., 1994a) indicate that, for those IET experiments in which DCH-produced hydrogen burned (the most nearly prototypic experiments), TCE overpredicts ΔP slightly for the ANL experiments while it underpredicts ΔP for the SNL Zion experiments. Clearly, use of the t_{95} coherence estimates would increase this tendency, worsening agreement with experiment. Furthermore, use of the t_{95} coherence estimates would mean that TCE would predict a negative dependence of ΔP upon scale, while the experimental results suggest a moderate positive dependence upon scale for those experiments in which hydrogen could burn.

The results summarized here support a belief that *any* consistent method of obtaining coherence ratios from the cavity pressurization data would lead to considerably larger coherence ratios for the ANL experiments than for the SNL experiments; that use of these more consistent coherence estimates in TCE would worsen the agreement with experiment; and that TCE would then predict a scale dependence that is the reverse of that actually implied by the experimental data. Unless these conclusions can be disproven, they raise important doubts as to the adequacy of the treatment of scaling in the DCH issue resolution work.

Correction for Melt Volume. Both the analysis given here and that employed by Pilch et al. (1994a) assume that all the accumulator depressurization prior to t_e results from the discharge of coherent steam, which is not entirely correct. In reality, some of this depressurization represents the increase in free volume due to melt ejection. Correcting for this effect would reduce P_0/P_e by a factor of about 0.96. The relative impact on f_{coh} is not large, but it is not completely trivial when f_{coh} itself is small. For example, if the uncorrected value of P_0/P_e is 1.3, making the correction reduces the value of f_{coh} from 0.18 to 0.153. Thus, making the correction would reduce the amount of coherent steam by about 15%. It would also increase the ANL/SNL f_{coh} ratio to about 2.15, based upon the average t_{95} results. If the correction were to be applied in NUREG/CR-6075, the tendency of TCE to underpredict the SNL/IET Zion data would be increased slightly, for the cases in which hydrogen could burn.

Appendix C
Independent Analyses Supporting the Importance of Phenomena Neglected in the DCH Issue Resolution Models

In Section 3.2 of the main report, evidence was summarized from CONTAIN analyses of the DCH experiments (Williams et al., 1997) that indicated certain mitigation processes neglected in the DCH issue resolution models are actually very important. These processes include atmosphere-structure heat transfer and the effects of incomplete or delayed combustion of DCH-produced hydrogen, both of which are ignored in the two-cell equilibrium (TCE) and the convection-limited containment heating (CLCH) models. However, not all investigators find it convincing to use systems code calculations to draw conclusions concerning the underlying phenomenology, and this skepticism may well be increased by the fact that the document providing the principal validation basis for the CONTAIN DCH model (Williams et al., 1997) is not generally available, as permission to publish has been withheld precisely because the results do conflict with the basic assumptions of TCE and CLCH. Hence Section C.1 of this Appendix provides a simple analytic treatment of these mitigation effects that supports the CONTAIN results. This treatment is taken from Appendix C of (Williams et al., 1997).

The TCE models claim approximate agreement with the DCH ΔP data. Since mitigation processes neglected by TCE and CLCH are believed to be important, it necessarily follows that these models also neglect equally important processes that contribute to the DCH energy release. Williams et al. (1997) cite reasons for believing that these processes include interactions of the noncoherent portion of the blowdown steam with nonairborne debris (NAD), and the interactions of debris with co-dispersed cavity water (or co-ejected RPV water). Section C.2 summarizes a stand-alone analysis supporting the plausibility of the nonairborne debris hypothesis; Appendix B of Williams et al. (1997) presents additional details. Section C.3 summarizes some of the arguments for believing that, under certain conditions, debris-water interactions can augment DCH significantly.

The CONTAIN models for NAD interactions and debris-water interactions are partially parametric, and the calculated effects of NAD and water on both ΔP and hydrogen production were found to be rather similar. Neither the experimental data nor the available models are adequate to permit a clean separation of these effects. The status of the validation of the CONTAIN treatment based upon the experimental analyses is summarized by Williams et al. (1997). It is acknowledged that the evidence for the importance of NAD interactions and debris-water interactions is considerably less conclusive than the evidence for the importance of the mitigation effects neglected by TCE and CLCH. It is the mitigation effects that provide the conclusive evidence that the TCE and CLCH descriptions of DCH are not adequate; disproof of the nonairborne debris and debris-water interaction hypotheses would simply mean that the processes compensating for the mitigation effects have not even been identified and that DCH is even more mysterious than is argued here.

C.1 Independent Evaluation of Mitigation Effects

In Section 3.2 of the main text, it was noted that CONTAIN analyses of the Zion-geometry IET experiments greatly underpredicted ΔP if neither NAD interactions nor debris-water interactions were modeled, but that this conclusion depended upon the model for the mitigation effects neglected by TCE; if the mitigation effects neglected by TCE were also omitted from the CONTAIN calculations, the latter showed approximate agreement with TCE for the cases that were considered there. Hence it is important to provide an independent check upon the mitigation calculated by CONTAIN for the effects of atmosphere-structure heat transfer and incomplete (or delayed) combustion of DCH-produced hydrogen. Since an approximate check can be obtained using simple analytical methods, it is included here. Specifically, we develop an estimate of the mitigation effect for the SNL/IET experiments in which DCH-produced hydrogen could burn and compare results with the mitigation calculated by CONTAIN for the SNL/IET-3 and SNL/IET-4 experimental analyses that included neither NAD nor debris-water interactions.

We start by noting that, to a good approximation, the pressurization, ΔP, of the Surtsey vessel due to transfer of energy ΔU to the atmosphere is given by

$$\frac{\Delta P}{\Delta U} = \frac{R}{VC_v} = 0.00381\ MPa/MJ, \qquad \text{(C-1)}$$

where R is the universal gas constant, V is the Surtsey free volume (89.8 m^3 in the Zion IET experiments), and C_v is the molar heat capacity at constant volume (~24.3 J/g-mole K). We estimate the reduction in ΔP by estimating the reduction in energy input into the containment, relative to what it would be if there were no atmosphere-structure heat transfer and if all DCH-produced hydrogen could burn. We consider only the experiments in which the Surtsey atmosphere contained sufficient oxygen to support combustion of the DCH-produced hydrogen.

We estimate the atmosphere-structure heat transfer rates, $\dot{Q}$, using correlations that are similar to those employed by the CONTAIN code (Washington et al., 1991):

$$\begin{aligned} h_{nc} &= 0.141\frac{k}{L}Gr^{1/3}Pr^{1/3}, \\ h_{ff} &= 0.037\frac{k}{L}Re_L^{0.8}Pr^{1/3}, \\ h_{rad} &= \sigma\epsilon_{g-s}(T_g^2 + T_s^2)(T_g + T_s), \\ \dot{Q} &= (h_{rad} + \max(h_{nc},h_{ff}))A_s(T_g - T_s). \end{aligned} \qquad \text{(C-2)}$$

Here h_{nc}, h_{ff}, and h_{rad} are, respectively, the heat transfer coefficients for natural convection, forced flow, and thermal radiation. Gr is the Grashof number, Pr the Prandtl number, Re_L the Reynolds number based upon gas flow velocities across structures with a characteristic length L, k is the gas thermal conductivity, and ϵ_{g-s} is the effective emissivity for gas-structure thermal radiation. A_s is the area of structure surfaces and T_g and T_s are, respectively, the temperatures of the gas and the structure surfaces.

Conditions in the dome and the subcompartments are very different and Eq. (C-2) must be evaluated separately for the two regions. During the period of debris dispersal, gas entering the subcompartments would consist of almost pure hydrogen at temperatures close to the debris temperature (2500 K) if debris-steam equilibrium were to be achieved; since the chromium reaction energy is sufficient to compensate for the energy needed to heat the hydrogen, the debris would not cool. However, in CONTAIN calculations with the standard particle size distribution, equilibrium is approached but not achieved, and it would be more representative to take the gas temperature to be 2000 K and the composition to be 75% hydrogen, 25% steam. In the subcompartments, gas flow velocities may be calculated assuming a cross section for flow of about 1 m^2 and a flow rate of about 300 g-moles/s (the approximate blowdown rate during debris dispersal), and characteristic lengths of the structures are taken to be 1 m.

Atmosphere emissivities are expected to be high due to the presence of dense aerosol clouds; an emissivity value of 0.8 is assumed here as in the CONTAIN standard DCH input prescription. Structure surface emissivities are also about 0.8. Taken together, these values imply $\epsilon_{g\text{-}s} \approx 0.67$. Structure temperatures, T_s, were assumed to be 500 K in the subcompartments. Structure areas in the subcompartments total about 40.6 m^2. Hot debris films may render some small fraction of the subcompartment surfaces ineffective as heat sinks, but no correction is applied for this effect, since we are comparing with the CONTAIN case without NAD interactions modeled. In any event, the correction would be small.

In the dome, maximum experimental temperatures observed are in the range 600-700 K; 600 K is assumed here. Structure surfaces in the dome do not heat significantly during the event, and T_s was therefore taken to be 300 K. Surface areas are about 156 m^2.

Using these values, approximate heat transfer coefficients and heat transfer rates implied by Eq. (C-2) were evaluated on a small spreadsheet program. Results are summarized in Table C-1.

Table C-1
Mitigation by Heat Transfer

Region	A_s (m^2)	h_{nc} W/m^2-K	h_{fc} W/m^2-K	h_{rad} W/m^2-K	T_g-T_s (K)	$\dot{Q}$ MJ/s
Subcomp.	40.6	42	96	404	1500	30.5
Dome	156	24.2	---	15.4	300	1.85

The extreme temperatures assumed here for the subcompartments prevail only for a time period comparable to the time during which debris is being dispersed from the cavity, typically about 0.4 s in the Zion-geometry SNL/IET experiments. Hence, about 12 MJ would be lost from the subcompartments during this period. Eq. (C-1) indicates this energy loss would reduce ΔP by about 0.046 MPa, relative to the adiabatic case.

At the end of the debris dispersal time, much of the hydrogen produced will still remain in the 4.6 m^3 volume of the subcompartments, which contain no oxygen at this time. Assuming the pressure is about 0.3 MPa at this time (which is well before the time of maximum pressure), the subcompartments at 2000 K would contain about 111 g-moles of gas. If we assume the same composition as was assumed above (75% hydrogen), the number of hydrogen moles remaining in the subcompartments at the end of entrainment, $n_{H2,e}$, is about 83 g-moles. Since hydrogen combustion releases 0.2406 MJ/g-mole, failure to burn any of this hydrogen would reduce ΔP by another 0.076 MPa, relative to the adiabatic complete combustion case.

This estimate neglects the fact that, in the SNL/IET Zion experiments, the coherent steam fraction, f_{coh}, was only 0.20-0.40; that is, only 20-40% of the total accumulator steam was discharged at the time debris dispersal was effectively complete. As the blowdown continues, some of the hydrogen present at the end of entrainment will be carried to the dome, where it can burn. If we assume that the subcompartment atmosphere is well mixed during the blowdown, it can be easily shown that the hydrogen remaining in the subcompartments at the end of the blowdown, n_{H2}, is approximately given by

$$n_{H_2} = n_{H_2,e} e^{-V_{blo,e}/V_{sub}},$$

$$V_{blo,e} = \frac{n^0_{H_2O}(1-f_{coh})RT_{blo}}{P_{sub}}, \qquad \text{(C-3)}$$

where V_{sub} is the subcompartment volume, $V_{blo,e}$ is the volume of blowdown steam entering the subcompartments after the end of entrainment, P_{sub} is the pressure in the subcompartments (essentially equal to the Surtsey pressure, ~0.4 MPa at this time), T_{blo} is the temperature at which the blowdown steam enters the subcompartments (~450 K, due to cooling as a result of expansion). The initial steam inventory in the accumulator, n^0_{H2O}, is about 500 g-moles in the SNL/IET Zion experiments. The SNL/IET-3 and SNL/IET-4 experiments, used in the examples below, had $f_{coh} \approx 0.25$. Using this value, Eq. (C-3) gives n_{H2} = ~39 g-moles for the amount of hydrogen remaining in the subcompartments at the end of the blowdown.

This hydrogen is unlikely to contribute to DCH pressurization because it can burn only insofar as natural convection between the subcompartments and the dome mixes it with oxygen, a relatively slow process. Furthermore, high steam/hydrogen ratios and reduced temperatures in the subcompartments at these later times may limit hydrogen combustion even as oxygen does become available. In any event, the experimental results show that peak pressures were achieved at or before the time the blowdown ends in the SNL/IET Zion experiments.

It appears, then, that the ~39 g-moles remaining in the subcompartments at the end of blowdown will not contribute, reducing ΔP by about 0.036 MPa. Since the time required for blowdown, ~3 seconds, is long compared with the entrainment time assumed previously, additional heat losses occur which were not previously accounted for. We neglect any additional losses in the subcompartments, because the entering steam is relatively cool; however, the estimated energy losses in the dome are about 5.5 MJ during this period (see Table C-1), reducing ΔP by an additional 0.021 MPa.

Relative to the adiabatic complete combustion case, then, the estimated mitigation is about 0.046 + 0.036 + 0.021 = 0.103 MPa, a very significant amount, since the total containment pressurization in these experiments was about 0.25 MPa. This result clearly lends good qualitative support to the general CONTAIN prediction that mitigation was important in these experiments.

In order to obtain a more quantitative comparison, the SNL/IET-3 and SNL/IET-4 CONTAIN analyses with no nonairborne debris and no debris-water interactions were recalculated with all structure areas set equal to 10^{-20} m^2 in order to eliminate heat transfer, and with the combustion model parameters reset to assure complete hydrogen reaction. For SNL/IET-3, the calculated ΔP in the original calculation was 0.110 MPa while the calculation without mitigation gave 0.183, a difference of 0.073 MPa. For SNL/IET-4, ΔP in the original calculation was 0.141 MPa, while the calculation without mitigation yielded ΔP = 0.235 MPa, for a difference of 0.094 MPa.

These results agree reasonably well with the simplified calculation, in view of the many approximations made in the latter. For example, in estimating the heat losses from the subcompartments during the debris dispersal period, the simplified calculation neglects the fact that some of the lost energy can be made up by continued heat transfer from the airborne debris that is still present in parts of the subcompartment volume at this time. The intent of the simplified analysis is only to provide a sanity check on the CONTAIN calculation; it is not to be expected that the simplified approach would be useful for quantitative DCH calculations.

The simplified analysis supports the belief that the mitigation effects are being evaluated reasonable well by the CONTAIN code. It is concluded, therefore, that there is little reason to doubt the implications of the CONTAIN calculations that the mitigation effects are important and must be properly taken into account in DCH analysis.

C.2 Interactions of Nonairborne Debris

The traditional approach to DCH analysis assumes that interactions of debris with gas and blowdown steam may be ignored except for debris that is present as airborne particulate, in part because the surface/volume ratio is so much higher for airborne debris than for debris that is deposited on structures. The TCE and CLCH models both adopt this approach, and it was the basis of CONTAIN code analyses of DCH until recently. However, the surface/volume ratio argument neglects the fact that the airborne residence time is very short, while nonairborne debris may have considerably longer times in which it can interact. Although airborne debris interactions are expected to dominate whenever airborne debris is present in good supply, these interactions are largely limited to the supply of coherent steam in compartmentalized geometries, while nonairborne interactions may continue after the coherence interval. Hence they constitute a potential source of hydrogen and energy transfer in addition to the airborne interactions, and ignoring them is nonconservative unless they can be shown to be negligible.

Interest in the nonairborne interactions was first highlighted by the observation (Allen et al., 1991) that a plot of hydrogen production versus mass of debris dispersed from the cavity in the SNL/LFP experiments did not come close to the origin when extrapolated back to zero debris dispersal. Allen et al. (1991) therefore suggested that substantial hydrogen production could occur even if no debris is dispersed from the cavity. Williams (1992) extended the analysis and concluded that coherent steam alone could not adequately explain the observed hydrogen production in the SNL/LFP, SNL/WC, SNL/IET-1 and SNL/IET-1R experiments. These conclusions were based upon simple bounding arguments and did not make use of detailed code calculations.

A more quantitative treatment of nonairborne interactions was given in Appendix B of Williams et al. (1997), and what follows is based upon the treatment given there. We address the problem using heat and mass transfer correlations similar to those used for interactions between containment structures and the atmosphere in the standard CONTAIN models for these processes (including non-DCH analyses). In a sense, the case for significant contributions from nonairborne debris is only the flip side of the case for significant mitigation due to heat transfer to those structures which are not coated with hot debris (Section C.1).

Depending upon the geometry and flow patterns, a number of correlations are available for the Nusselt number, Nu, for heat transfer (Bird et al., 1960). We consider here a subset of these correlations that can be at least approximately represented by the form

$$Nu = \beta Re_L^m Pr^{1/3}, \qquad \text{(C-4)}$$

where β and m are constants, Re_L is the Reynolds number for gas flow across a structure surface of characteristic length L, and Pr is the Prandtl Number. The correlation used in the CONTAIN code for atmosphere-structure heat transfer under forced flow conditions is of this form, with β = 0.037 and m = 0.8 (Washington et al., 1991).

Using the heat/mass transfer analogy, a corresponding relation for the Sherwood number, Sh, is obtained from which the gas-phase mass transfer coefficient, h, may be written

$$h = Sh\left(\frac{D_g}{L}\right) = \beta Re_L^m Sc^{1/3}\left(\frac{D_g}{L}\right), \tag{C-5}$$

where D_g is the binary diffusivity for hydrogen and steam, and Sc is the Schmidt number. In the present instance, we are interested in steam reacting with hot metallic debris and we have therefore assumed that the dominant constituents of the atmosphere are steam and hydrogen. During a DCH event, this assumption is usually valid for the cavity and the subcompartments, and the NAD model is not applied in the dome (Williams et al., 1997).

The extent of reaction of steam flowing through the cell will be governed by the ratio of the time constant for gas flow to sweep gas out of the cell, τ_{fl}, to the time constant for reaction, τ_h. An approximate measure of the efficiency, ϵ_h, of the steam-hydrogen conversion process is given by

$$\epsilon_h = \frac{\tau_{fl}}{\tau_{fl} + \tau_h}, \tag{C-6}$$

assuming well-mixed gases in the cell. (A correction for the iron-steam equilibrium is needed when iron is the only remaining metal.) In what follows, we take the ratio τ_{fl}/τ_h to be the figure of merit for evaluating the efficiency of the NAD interactions.

The ratio τ_{fl}/τ_h is estimated as follows. First, we assume that mass transport rate limitations within the film are negligible and that only gas phase mass transport limits the reaction rate, and assume that the film does not run out of metal. The time constant for reaction of steam with the debris-coated surfaces, τ_h, is equal to V/hA_d, where V is the volume of the cell of interest and A_d is the area of the surfaces coated with debris films. Given the blowdown rate in moles per second, $\dot{n}$, the gas velocities and other information needed to evaluate Eq. (C-5) may be estimated by applying the ideal gas law to obtain the volumetric flow rate (m^3/s) and dividing by the cell cross section for flow, A_h. The time constant for gas flow through the cell is equal to the cell volume divided by the gas volumetric flow rate. After a little algebra, one may obtain

$$\frac{\tau_{fl}}{\tau_h} = \beta A_d (R\dot{n}L)^{m-1} A_h^{-m}\left(\frac{PD_g}{T}\right)^{1-m} Sc^{1/3-m}. \tag{C-7}$$

Here, P and T are, respectively, the pressure and temperature of the gas, and R is the universal gas constant.

In CONTAIN, Eq. (C-5) with $\beta = 0.037$ and $m = 0.8$ forms the starting point of the model used for calculating condensation upon (or evaporation from) structures in the presence of forced flow, although the actual evaporation/condensation model includes many refinements not needed here. With these values of β and m, Eq. (C-7) becomes

$$\frac{\tau_{fl}}{\tau_h} = 0.037 A_d (R\dot{n}L)^{-0.2} A_h^{-0.8} \left(\frac{PD_g}{T}\right)^{0.2} Sc^{-0.467}. \qquad \text{(C-8)}$$

Quantitative results to be presented below will be based upon Eq. (C-8). Note also that, although we shall refer to Eq. (C-8) and similar relationships as representing "film models," they are in reality thin film models, in that various complications (e.g., wave action) that can arise when films are thick will be neglected in our discussion.

Examination of the various parameter dependencies in Eq. (C-8) shows that the net variations with pressure, temperature, gas composition and flow rate are weak and large changes in τ_{fl}/τ_h do not occur as the event proceeds. We evaluate Eq. (C-8) for conditions typical of the post-dispersal blowdown phase of the SNL/IET Zion experiments, which we take to be $\dot{n}$ = 250 g-moles/s, T = 1000 K, P = 4.5×10^5 Pa, and an H_2:H_2O ratio of 1:3.

We consider the cavity and chute in the SNL/IET Zion experiments and take A_h = 0.067 m^2 and L = 0.5 m. We assume that both the cavity and the chute surfaces are coated with debris films, since the experiments typically leave most chute surfaces as well as cavity surfaces coated with debris;* A_d is then equal to 3.7 m^2. Eqs. (C-8) and (C-6) then give $\epsilon_h \approx 0.30$. For the amounts of blowdown steam that exit the accumulator after debris dispersal terminates (typically ~300 g-moles), this efficiency is sufficient to generate another 60-100 g-moles of hydrogen, in addition to what is generated by the interactions with airborne debris. Applying a similar approach to estimate the heat transferred from the nonairborne debris results in an estimate of about 4 to 7 MJ. The latter is sufficient to account for 15-25% of the ΔP observed in the SNL/IET (Zion) experiments in which hydrogen could not burn, while this heat transfer plus the combustion energy of the additional hydrogen produced could account for 30-45% of the total ΔP observed in experiments in which the hydrogen did burn. (Both estimates neglect atmosphere-structure heat transfer.)

Application of a scaling analysis based upon Eq. (C-7) or Eq. (C-8) to the subcompartment volumes indicates that there is no basic reason why comparable nonairborne interactions cannot continue there. However, uncertainties related to debris location and flow distribution in the subcompartments are larger than in the cavity and chute, which have a relatively simple geometry (Appendix B, Williams et al., 1997).

The results summarized here provide good support for the NAD concept. Using relatively standard correlations for heat and mass transfer, the analysis shows that significant nonairborne interactions should be expected.

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*T. K. Blanchat, private communication to the author.

It is acknowledged that there are substantial uncertainties in the nonairborne debris analysis, and these uncertainties could either increase or decrease the extent of interaction. For example, the Nusselt correlation used in deriving Eq. (C-8) is based upon flow parallel to a dry surface and may be too low for DCH conditions involving flows impinging on surfaces at various angles, and surfaces covered with wavy liquid films. On the other hand, debris-structure heat transfer could act to cool the films sufficiently rapidly to reduce the contribution of nonairborne debris. An approximate treatment of film cooling was given by Williams et al. (1997), and it was concluded that this heat transfer could reduce the importance of nonairborne interactions, but it was unlikely to eliminate these interactions. A simple scaling analysis given in the reference suggests that cooling of debris films may be less likely to inhibit the NAD interactions at plant scale than at experimental scale. Other uncertainties, related to the thickness of the debris films and the duration of the event, may be more important at plant scale than at experimental scale.

The CONTAIN code models nonairborne debris by permitting the user to specify an effective particle size, d_t, for the nonairborne debris. Heat transfer and chemical reaction are then calculated using the same models as those applied to the airborne debris. An important limitation of the model is that heat transfer to the structures is not modeled. Empirically, d_t values of 0.01-0.02 m were found to give reasonable results for experiments conducted at 1/10-scale, and it was shown in Appendix B of Williams et al. (1997) that this result is in reasonably good agreement with Eq. (C-8). A scaling rationale was provided for applying the model to DCH events at other scales, including application to NPP events; in the recommended prescription, the calculated efficiency of the NAD interactions shows little dependence upon scale. This follows from the fact that the surface-volume ratio varies inversely with scale while the interaction time available increases with scale; hence the net effect on the ratio τ_{fl}/τ_h is small.

To a certain extent, the "nonairborne" model in CONTAIN is viewed as a semi-empirical means of representing any process that permits debris to interact with the noncoherent portion of the blowdown steam; the actual geometry of the debris-gas interface is considered to be uncertain. Since uncertainties in the treatment are acknowledged to be important, sensitivity studies exploring the potential impact of these uncertainties upon the results of interest are recommended (Williams et al., 1997).

The DCH issue resolution models do not include nonairborne interactions as contributions to containment loads. Including these interactions within the philosophy of the models would be difficult because a close approach to thermal and chemical equilibrium is not expected for the nonairborne interactions, and invoking an equilibrium assumption could be excessively conservative in many instances. On the other hand, the complete neglect of these interactions is nonconservative and unjustified, based upon what has been presented here.

C.3 Water and DCH

Water can play a role in DCH in various contexts: water on the basement floor can interact with debris dispersed from the cavity; water initially in the cavity can be codispersed with the debris; and RPV water overlying the debris prior to vessel breach can be coejected with the debris. Water is expected to be present on the basement floor in almost any accident scenario, and Pilch et al. (1994b) have concluded at least some water will be coejected with the debris in any DCH event. The presence of water in the reactor cavity is plant specific and often depends upon small details. A review of the industry's Individual Plant Evaluations (IPEs) for Westinghouse plants by Pilch et al. (1996) concluded that many U.S. reactor cavities will be deeply or partially flooded if the refueling water storage tank (RWST) has discharged; otherwise, most cavities will be almost dry or only partially flooded.

The DCH issue resolution models neglect water altogether and it is assumed by Pilch et al. (1996) that water will either have little effect or else mitigate DCH. Here we summarize some reasons for believing that water can augment DCH loads under some conditions and that its neglect results in underestimating the uncertainties in DCH loads prediction and may be nonconservative. In particular, water has the potential to augment DCH loads in compartmentalized containment geometries when the amount of water interacting with debris is less than the amount the debris can vaporize without substantial cooling of the debris; on the other hand, water quantities sufficient to completely quench the debris may mitigate containment loads.

Both systems code calculations and simple arguments based upon thermodynamic limits to the extent of debris/gas/water interactions indicate that water has the potential to either mitigate or augment DCH loads, depending upon the scenario. Independent reviews of DCH phenomenology (Zuber et al., 1991; Boyack et al., 1995) have concurred that the effect can be in either direction and that its potential importance to DCH loads is high. Controlling factors in model predictions include the debris/water mass ratio, the containment geometry, and whether debris-gas interactions would be steam-limited in the absence of additional steam generated by vaporizing water. Major uncertainties include the amount of water that actually interacts and the fate of that water which does not interact initially.

It is easy to understand why systems code calculations indicate that water can mitigate loads under some conditions and enhance loads under other conditions. One does not need to resort to complex code calculations in order to understand the basic issues involved. Possible mitigation effects include quenching of debris, suppression of hydrogen combustion by steam inerting, and quenching of hydrogen combustion energy by aerosolized water. Possible augmentation effects include increasing the supply of coherent steam available for thermal and chemical interactions with the debris, accelerating the transport of energy and hydrogen to the dome, and reducing subcompartment temperatures for the same amount of sensible heat transfer to the gas. The accelerated transport and reduced temperatures can reduce the mitigating effect of atmosphere-structure heat transfer (Williams et al., 1987).

Several of the potential effects of water noted above involve thermodynamic arguments that can be illustrated with simple hand calculations, without resort to elaborate computer codes. In compartmentalized containment geometries, reasoning similar in concept to the modeling used in TCE and CLCH imply that small or moderate amounts of water can augment DCH in scenarios for which debris-gas interactions would otherwise be steam starved, while large amounts of water can have a mitigating effect.

We can illustrate these potentials using the 1/10-scale SNL/IET Zion-geometry experiments as examples. All the experiments other than SNL/IET-8B had 3.48 kg (193 g-moles) of water in the cavity. Vaporization of the water to produce saturated steam would extract about 9 MJ of energy from the debris. Adding this 193 g-moles of saturated steam ($T \approx 400$ K) to the containment atmosphere (volume = 89.8 m^3) would contribute only $\sim$0.0071 MPa to ΔP. Adding 9 MJ of thermal energy to the containment atmosphere would contribute $\sim$0.034 MPa. Hence energy used to vaporize water is only 20-25% as efficient in pressurizing the containment as is atmospheric heating.

The Zion geometry, however, is highly compartmentalized, with most of the debris failing to reach the dome. In the cavity and subcompartments, the debris/steam heat capacity ratio, ψ, was generally in the range 5 to 10 in these experiments. If, as in the TCE model [see Eqs. (7-1) and (7-2) of Section 7.1 of this report], we assume that only a fraction $1/(1+\psi)$ of the debris energy is available for transfer to the blowdown steam, the 9 MJ lost to vaporizing the water actually reduces the energy available for containment heating by only 1-2 MJ. In addition, the 193 g-mole of steam produced is not enough to prevent the 250-300 g-moles of hydrogen that were generated in these experiments from burning. Thus the potential for mitigation is probably minor in this case.

On the other hand, if the 193 g-moles of steam equilibrate thermally with the debris, about 17 MJ of additional energy is transferred, sufficient to pressurize the containment by about 0.06 MPa. Furthermore, the hydrogen production in these experiments was heavily steam-limited if only the coherent blowdown steam is available to react with the metal; if the steam generated by vaporizing the water equilibrates chemically as well as thermally with the debris according to Eq. (7-4) of Section 7.4 of this report, and if the resulting hydrogen is burned, the additional thermal and chemical energy transferred is sufficient to pressurize the containment vessel by about 0.19 MPa. Evidently, the potential for augmentation is considerably greater than the potential for mitigation in this instance.

The situation is quite different when the amounts of water available are large. For example, in the SNL/IET-8B experiment, there were 62 kg of water in the cavity. The thermal energy of the debris would be sufficient to vaporize $\sim$89% of the 62 kg of water present in the SNL/IET-8B experiment, with no thermal energy left to heat the steam or the containment atmosphere. Furthermore, the 3060 g-moles of steam that would be produced could be sufficient to inert the $\sim$300 g-moles of hydrogen that were produced in the experiment against combustion. Unvaporized water might remain airborne long enough to provide an atmospheric heat sink, reducing pressurization further. For large amounts of water, therefore, the potential for strong mitigation clearly exists. Note that a key word here is "potential"; for example, the SNL/IET-8B experimental results indicated that the DCH-produced hydrogen did burn even though most of the cavity water was vaporized (Allen et al., 1994); evidently the steam generated did not prevent the hydrogen from burning in the actual experiment.

In open containment geometries it is less clear that there is a potential for substantial augmentation, whatever the amounts of water. With the full dome atmosphere available for debris-gas interactions, debris-gas heat transfer will not be heavily limited by the heat capacity of the atmosphere [$\psi < 1$ in Eq. (7-1) of Section 7.1], and steam and oxygen available for chemical reaction will be sufficient to oxidize all the metal in the dispersed debris. On the other hand, the potential quenching effects of the water on the debris and on hydrogen combustion can still arise. It is likely, therefore, that the balance between augmentation versus mitigation is shifted in favor of mitigation, relative to compartmentalized-geometry containments. Note, however, that these arguments are based upon thermodynamic limits; the possibility exists that the water could affect particle size and other parameters affecting rates of thermal and chemical interactions.

Experimentally, water on the basement floor appears to have at most a limited impact (Allen et al., 1994). Experimental evidence concerning the effect of co-dispersed cavity water has been reviewed by Pilch et al. (1997) with inconclusive findings. The experimental results indicate that cavity water does increase the amount of thermal energy extracted from the debris, but part of the energy typically goes into generating steam rather than heating the atmosphere. Measured impacts upon containment temperatures have ranged from eliminating any temperature rise to enhanced temperature rises and rates of rise. There are no examples in which water clearly had a large effect (in either direction) upon containment pressurization, and there are no clear tests of the prediction that water can result in either substantial augmentation or mitigation of DCH loads under the appropriate conditions. Where dry-cavity comparison cases are available, cavity water has increased hydrogen production to at least some extent. Pilch et al. (1997) give additional details.

Analysis of the Zion-geometry experiments with the CONTAIN code indicated that the co-dispersed cavity water could have contributed significantly to containment pressurization and hydrogen production in these experiments. However, the effects of the co-dispersed water could not be cleanly separated from the effects of nonairborne debris in these analyses, and there was no clean experimental test because no counterpart experiments with a completely dry cavity are available for comparison purposes. Calculated pressure-time histories in the containment tended to agree better with the experimental results when it was assumed that both the nonairborne debris and the cavity water did contribute significantly, however. There are important limitations to the ability of CONTAIN to model the effects of water in DCH scenarios (Boyack et al., 1995); Williams et al. (1995) summarize the approach used and the results obtained and Williams et al. (1997) provide considerably more detail.

Co-ejected RPV Water. Water coejected from the RPV with the melt is important in the DCH issue resolution context because all the scenarios defined for that work involve at least some co-ejected water. Furthermore, the amount assumed in Scenario VI [10000 kg; see Pilch et al. (1994b) and Pilch et al. (1996)] is in the regime for which the arguments given above indicate that augmentation of DCH loads is likely.

Co-ejected RPV water raises some of the same issues as codispersed cavity water, but there are also important differences. Co-ejected water accompanies and/or follows the melt, and therefore cannot be dispersed from the cavity as a slug in advance of the melt. Instead, much of the water may follow the dispersal event. RPV water will partially flash to steam upon depressurization, and the remaining water is likely to be highly fragmented. Flashing tends to add to the containment pressurization while aerosolized water can act as a heat sink.

CONTAIN calculations have been performed for the Sequoyah plant without ice in the ice condenser. The containment would be classified as having a compartmentalized geometry, although it differs in significant ways from dry containment geometries. The calculations indicated that substantial (factor-of-two) enhancement could result from small amounts (~10000 kg) of co-ejected water in a scenario in which thermal interactions of steam and debris would have been heavily steam-limited ($\psi \approx 4$) in the absence of water. In a different scenario with more blowdown steam available, sensitivity to either 10000 kg or 75000 kg of co-ejected water was less. In this particular case, compartmentalization prevented enough aerosolized water from reaching the dome to result in substantial mitigation; aerosolized water has been calculated to be a significant mitigating effect in other CONTAIN analyses, however.

Experiments involving true simulations of co-ejected water have proven difficult to perform. Pilch et al. (1996) assert that issues involving co-ejected water would be addressed in tests that were subsequently performed in Calvert Cliffs containment geometry (Blanchat et al., 1996). However, experimental difficulties prevented any actual co-ejected water experiments from being performed; instead, the thermite melt was generated in the *cavity* and then simply dispersed from the cavity by high-pressure water or steam. Resulting ΔP values showed only minor dependence upon steam-driven versus water-driven experiments. However, the contact mode between the melt and the water or steam in these experiments is sufficiently nonprototypic that there is some doubt as to what conclusions should be drawn concerning the actual effects of co-ejected water in NPP scenarios, even for the conditions nominally simulated. What is even more important in the present context is that these experiments were performed for conditions that are the reverse of those for which loads augmentation might be expected. That is, the amounts of water were large (100 kg, with only 30 kg of thermite melt), and the Calvert Cliffs geometry is better classified as an open geometry than a compartmentalized geometry because the dominant path for dispersal of debris and water from the cavity leads directly to the dome rather than the subcompartments.

The closest approach to a prototypic test of co-ejected water is probably an experiment designated SNL/CED-2 (Blanchat et al., 1994b), which was performed in Surry geometry. Strong cavity pressurization resulted in damage to the experimental system. This damage included tearing loose and launching the melt generator that simulated the RPV, and also damage to containment structures simulating the seal table room. A posttest CONTAIN analysis of this experiment (Blanchat et al., 1994b) gave ΔP and hydrogen production values agreeing with experiment to within 7.5%. It also yielded the correct order of magnitude of cavity pressurization and momentum transfer to the melt generator, and it provided a plausible explanation for the damage to subcompartment structures that was observed in the experiment. These results do provide some support for using the CONTAIN code to assess possible effects of co-ejected water. However, experimental results were used in the CED-2 analysis to estimate the time interval debris was dispersed from the cavity. There presently exist neither experimental correlations nor mechanistic modeling capabilities for predicting the dispersal rates when co-ejected water is involved. Hence large uncertainties in debris dispersal rates must be allowed for in plant calculations involving co-ejected water.

C.4 Implications for the DCH Issue Resolution Modeling Approach

The DCH issue resolution models employ bounding analyses based upon thermodynamic limits for those processes that are treated, while other processes are generally neglected. (The principal exception is that the treatment of pre-existing hydrogen attempts to include the effect of atmosphere-structure heat transfer.) In this Appendix, arguments have been presented for believing that three of the neglected processes are quite important. Here we summarize some of the difficulties these processes imply for any approach based upon simple bounding analyses such as those presented in the DCH issue resolution work.

Concerning the heat transfer processes considered in Section C.1, the key point is that analyzing these effects requires assessing the net effect of the competition between rates of energy addition to the containment atmosphere versus the rates of energy loss from the atmosphere. Analysis of process rates is inherently outside the domain of equilibrium thermodynamics, which deals with end states. Analyzing process rates requires more complex modeling for the rates of the various energy and mass transfers involved, and also requires assessment of the uncertainties in these models. While such models might be added to TCE or CLCH, doing so would mean abandoning the thermodynamic limit approach currently adopted. It is not entirely clear why such an effort should be attempted in any case, since the required capabilities already exist in systems codes such as CONTAIN and MELCOR.

Thermodynamic limit models could be defined for the nonairborne debris interactions and debris-water interactions considered in Sections C.2 and C.3, respectively. However, this treatment would probably be excessively conservative. For nonairborne debris, an equilibrium treatment would allow the noncoherent blowdown steam to equilibrate with all the debris not transported to the dome. In the notation of Section C.2, the limiting treatment is equivalent to assuming that $\tau_{fl}/\tau_h \gg 1$ so that $\epsilon_h = 1$, while the analysis given there indicated that $\epsilon_h \approx 0.3$ would be a more reasonable estimate for the case considered. Hence a limiting thermodynamic treatment is likely to be excessively conservative.

Similar considerations apply to debris-water interactions. The analyses summarized in Section C.3 were based upon thermodynamic limits, and the results indicated that, for the Zion-geometry IET experiments, the small amount of cavity water present could have contributed 0.19 and 0.06 MPa to the total ΔP in experiments with and without hydrogen combustion, respectively. Since the total ΔP for these experiments were about 0.25 MPa and 0.1 MPa, respectively, the thermodynamic limiting analysis indicates that water could have been the *dominant* contributor to the observed loads, which does not seem likely. For example, the CONTAIN analyses of these experiments indicated that the *combined* effects of debris-water interactions and nonairborne debris contributed about 50% of the total DCH energy release in the experiments in which hydrogen could burn, and about 30-40% in the inerted experiments.

To sum up, the mitigation effects considered here are inherently beyond the scope of a simple thermodynamic limiting treatment, and a treatment based upon thermodynamic limits for the augmenting effects will be too conservative to be very useful, especially if one must ignore the mitigating effects. On the other hand, the augmenting effects probably contribute at least 50% of the total DCH energy release in the Zion IET experiments with noninert atmospheres, and these effects obviously cannot be ignored in a valid treatment. Hence attempting to extend the DCH issue resolution modeling approach by simply including limiting models for some of the effects that are currently neglected is not likely to be a fruitful approach. More sophisticated modeling approaches are needed.

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Appendix D
Summary of DCH Experiments Involving High-Temperature Melts

For the benefit of those readers not intimately familiar with the DCH experimental program, this section provides a summary of the major DCH-related experiments that have been performed. Only those experiments involving high temperature melts are included here. In addition, there have also been a large number of separate-effects experiments involving dispersal of low-temperature, chemically unreactive melt simulants from scaled models of reactor cavities. These experiments are not very relevant to the issues raised in this report and they are therefore not considered.

The description that follows is taken with little change from Section 2.1 of SAND94-1174 (Williams et al., 1997). It therefore includes an emphasis on the experiments analyzed with the CONTAIN code as described by Williams et al. (1997). The more recent experiments were emphasized in that work because they included the more nearly prototypic cases, and many of the important insights resulting from the earlier work had been incorporated into the design of the later experiments. However, the experiments performed in Calvert Cliffs geometry are not discussed here, as they were performed after the CONTAIN analyses were concluded; they were briefly discussed in Appendix C.3 of this report and the details have been given by Blanchat et al. (1996).

The summary of the DCH experiments that follows omits many significant details, which may be found in the experimental reports cited. For those experiments that have been analyzed using the CONTAIN code, figures illustrating the experimental configurations are provided in Appendix A of Williams et al. (1997), which also includes summaries of the nodalization used to represent the experiments in CONTAIN.

Early Exploratory Experiments. Early experimental investigations of DCH included four experiments performed at Sandia National Laboratories (SNL/DCH series) (Tarbell et al., 1988; Allen et al., 1991b), five performed at Argonne National Laboratory (ANL/CWTI series; Spencer et al., 1988), and four experiments performed at Fauske and Associates, Inc. (FAI/DCH series; Henry et al., 1991). With the exception of one FAI/DCH test, none of these tests employed steam as a driving gas; instead, a chemically inert driving gas (N_2 or Ar) was used. These experiments provided much useful information which helped to guide subsequent experimental and analytical studies. However, predictions of large-scale hydrogen production due to metal-steam reactions during DCH events has always been a dominant feature of CONTAIN DCH analyses ever since the earliest version of the model (Williams et al., 1987), and later experiments have confirmed this prediction. Since this feature cannot be tested against these early experimental results, the latter will not be considered further here. However, analyses of the SNL/DCH-1 and SNL/DCH-3 experiments using an early version of CONTAIN have been reported previously (Williams et al., 1987; Williams and Louie, 1988).

SNL Technology Development Series (TDS) (Allen et al., 1994a). The basic purpose of these experiments was to develop the technology for performing experiments using steam-driven thermite melts. In addition, techniques were developed for enhancing melt chemical reactivity by adding chromium metal to the melt, in order to better simulate the higher chemical reactivity of molten core debris. The emphasis in these experiments was on technology development and they were all quite similar in terms of parameters thought to be important to DCH. Initial containment pressure was varied in these experiments and it was found that ΔP exhibited a weak positive dependence upon the initial containment pressure. The experimental technique developed in the TDS series is basically the same as that used in the subsequent experiments, and this technique merits a brief summary.

The TDS series was conducted at SNL using a 1/10-scale model of the Surry NPP cavity connected to the Surtsey DCH facility. Surtsey is a steel pressure vessel with a volume of approximately 103 m^3, when not reduced by the addition of internal compartmentalization. In the TDS experiments, the Surtsey volume was essentially open, without internal compartmentalization. The Surtsey atmosphere was chemically inert (argon gas).

The high-temperature melts were generated by the iron oxide/aluminum thermite reaction. This reaction was carried out in a crucible placed within a melt generator vessel that was connected to a pressure vessel, called the accumulator, filled with high-pressure steam. The volume of the accumulator was scaled approximately (not exactly) to the volume of the primary system of typical PWRs. Prior to thermite ignition, the melt generator and the steam accumulator were isolated from one another, and the accumulator was opened to the melt generator after ignition. Upon completion of the thermite reaction (within a few seconds), the melt contacted a fusible brass plug in the bottom of the melt generator, causing it to fail and initiating HPME.

The thermite mixture (including chromium) used in these experiments was the same as that used in the large majority of all the subsequent thermite-driven experiments, including all the experiments for which CONTAIN analyses were reported by Williams et al. (1997). The mixture prior to ignition was analyzed chemically and corresponds to an initial melt composition of Al_2O_3/Fe/Cr/Al equal to 0.373/0.505/0.108/0.014 by weight, assuming complete reaction of the thermite. Note that the Fe/Cr ratio is about equal to that of reactor internals stainless steel. Hence, the chemical reactivity of the metal fraction of the melt is comparable to that of molten core debris unless the latter contains significant unoxidized zirconium (or uranium) metal, in which case the core debris metal would possess greater reactivity. On the other hand, melt compositions assumed by Pilch et al. (1994b) and subsequent DCH issue resolution work have metal contents considerably lower than that used in the DCH experiments.

Limited Flight Path (LFP) Tests (Allen et al., 1991a). These six experiments were also performed in the Surtsey facility with an inert (argon) atmosphere. As in TDS, a 1/10-scale model of the Surry cavity and chromium-enhanced thermite melts were used.

The design of the LFP experiments was motivated by the observation that, in many (but not all) U.S. PWR containments, the dominant exit path from the cavity does not communicate directly with the main volume of the upper containment. Instead, the dominant path is often a keyway or instrument tube tunnel which communicates with a compartmentalized lower containment, the structures of which present additional barriers to debris transport to the main volumes of the containment. This compartmentalized lower-containment region is commonly referred to as "the subcompartments" (Zuber et al., 1991). This terminology will be used in the present discussion, which will also refer to the main open volumes of the upper containment as the "dome." Containments with this type of geometry will be referred to as "compartmentalized," while the term "open geometry" will be applied to containments or experiments in which the dominant exit path from the cavity communicates directly with the dome.

The purpose of the LFP tests was to examine sensitivity to the length of unobstructed flight path. In the LFP series, a concrete slab was positioned above the cavity exit chute to limit the unobstructed upward flight of debris dispersed from the cavity. The slab had a vertical steel plate extending downward from the edge to intercept debris splashed horizontally following its initial impact with the slab. The slab effectively blocked direct vertical transport of debris and inhibited horizontal transport, but there was ample space around the edges to permit an unrestricted flow of gases to the volume above the slab. The slab effectively divided the Surtsey volume into a lower compartment and an upper compartment, but in no way were the details of any actual containment geometry simulated.

Two of the LFP tests were performed with the slab 0.91 m above the cavity exit; three tests were done with the slab at 1.85 m; and one test (LFP-8A) was performed with the slab at 7.7 m. Since the height of the Surtsey vessel is about 10 m, most of the volume is below the slab in the latter test and this experiment is classified as an "open-geometry" experiment rather than a "compartmentalized-geometry" experiment. In addition to flight path, vessel hole size was varied. Steam driving pressures at the time of melt ejection were in the range 2.6-3.7 MPa.

CONTAIN code analyses of all the LFP experiments have been reported by Williams et al. (1997). Some test parameters for these experiments are summarized in Table D-1. Experimental results indicated that ΔP did increase with increasing flight path, but the results also indicated that substantial debris-gas energy transfer took place in the cavity. Hydrogen generation did not correlate with flight path length indicating that most hydrogen was generated in the cavity, which is not surprising in view of the inert containment atmosphere. Debris transport beyond the slab limiting the unobstructed flight path was small ($<$ 10% in all cases).

<u>Wet Cavity (WC) Tests (Allen et al., 1992a; Allen et al., 1992b)</u>. These three experiments were similar to LFP except that the 1/10-scale Surry cavity was replaced with a 1/10-scale Zion cavity and the concrete slab was at the 7.7 m level; hence, these are "open-geometry" experiments. WC-1 and WC-2 were very similar except that WC-2 had water in the cavity. WC-3 was similar to WC-1 except that it had a considerably larger melt generator hole size, resulting in correspondingly more rapid melt ejection, vessel blowdown, and melt dispersal from the cavity.

Experimental parameters for the WC series are also given in Table D-1. All three WC experiments have been analyzed using the CONTAIN code (Williams et al., 1997). Results indicated that the water in WC-2 did increase hydrogen production somewhat ($\sim$23%).

Table D-1

Initial Conditions for the SNL/LFP and SNL/WC Experiments

		LFP-1A	LFP-1B	LFP-2A	LFP-2B	LFP-2C	LFP-8A	WC-1	WC-2[a]	WC-3
Flight path (m)		0.91	0.91	1.85	1.85	1.85	7.70	7.70	7.70	7.70
Initial thermite mixture mass (kg)		80	50	50	50	50	50	50	50	50
Fraction dispersed from cavity		0.725	0.209	0.484	0.616	0.620	0.392	0.840	0.837	0.80
Steam driving P(MPa)		3.7	2.6	3.0	3.6	3.3	2.9	4.6	4.6	3.8
Moles of steam		262	180	229	249	246	188	374	337	265
Exit hole diameter (cm)		6.41	3.5	3.5	5.97	8.57	3.5	3.5	3.5	10.1
Initial pressure in Surtsey (MPa)		0.161	0.158	0.160	0.160	0.160	0.159	0.158	0.157	0.162
Initial gas	Ar	99.6	99.6	99.7	99.2	99.7	99.5	99.9	99.5	99.9
composition	N_2	0.31	0.33	0.2	0.63	0.29	0.38	0.06	0.48	0.10
in Surtsey (mole%)	O_2	0.08	0.07	0.0	0.16	0.06	0.08	0.01	0.05	0.02

[a] 11.76 kg water in cavity. Cavity was dry in all other experiments.

Neither the water nor the vessel failure size had a large effect upon ΔP, in agreement with CONTAIN analyses for these experiments.

SNL Integral Effects Tests, Zion Geometry (SNL/IET Zion) (Allen et al., 1994b). In these experiments, the thermite melts were ejected into a 1/10-scale model of the Zion cavity which was connected via a chute to the Surtsey vessel. Scale models (1/10-scale) of the Zion lower containment subcompartments and structures were included. The modeling of the Zion lower containment structures was quite detailed, in contrast with previous experiments in which the containment geometries were quite nonprototypic. Owing to geometric constraints, the length of the chute connecting the cavity to Surtsey was overscaled by a factor of about 2.7.

Some initial conditions for the SNL/IET Zion experiments are summarized in Table D-2. The thermite mass (43 kg) was scaled to the "most probable" estimate of melt masses and compositions developed in support of the Severe Accident Scaling Methodology (SASM) effort (Zuber et al., 1991) and thus does not represent an attempt to simulate highly conservative or bounding DCH scenarios. The Surtsey atmosphere was inert (nitrogen) in the first two experiments and included a nitrogen-air mixture giving an oxygen content of about 9-10% by volume in all the others except IET-5, which had about 76% CO_2 in the atmosphere and only 4.4% oxygen. The experiments with the nitrogen-air mixture were the first experiments in which DCH-produced hydrogen could burn, as all previous experiments either employed an inert atmosphere or else did not include steam.

In all these experiments, there was some water in the cavity: 3.48 kg (corresponding to estimated condensate levels) in all cases except SNL/IET-8A and SNL/IET-8B, in which the amounts were much larger (62 kg). Other experimental parameters studied were the presence or absence of water on the basement floor, the presence or absence of pre-existing hydrogen in the Surtsey atmosphere, and classical inerting of the containment atmosphere (in SNL/IET-5).

Williams et al. (1997) present CONTAIN analyses of all the experiments except SNL/IET-8A. SNL/IET-8A was excluded because melt generator pressurization failed in this experiment and no HPME occurred. SNL/IET-8B was not originally analyzed as part of the CONTAIN DCH assessment effort and is not included in the results summarized in Section 3 of this report. One reason for its exclusion was that the important role played by fuel-coolant interactions (FCIs) complicates the analysis, since CONTAIN does not have a true FCI model, and the methodology developed for analysis of the other experiments requires modification for application to SNL/IET-8B. This experiment, together with SNL/IET-8A, have been simulated using the FCI code IFCI (Davis, 1993). Some exploratory CONTAIN analyses of SNL/IET-8B were subsequently performed, however, and these results are also summarized by Williams et al. (1997).

The SNL/IET demonstrated the important role played by combustion of DCH-produced hydrogen, as the experiments with nitrogen-air atmospheres yielded ΔP values about 2.5 times as large as those with inerted atmospheres. Other parameter variations studied did not have a large effect for the conditions of these experiments.

Table D-2

Initial Conditions for the SNL/IET Zion Experiments

		IET-1	IET-1R	IET-3	IET-4	IET-5	IET-6	IET-7	IET-8A	IET-8B
Steam pressure (MPa)		7.1	6.3	6.1	6.7	6.0	6.3	5.9	1.06	6.2
Steam temperature (K)		600	585	585	555	586	571	599	421	554
Steam driving gas (g-moles)		468	507	485	582	453	505	416	4.1 (N_2)	545
Cavity water (kg)		3.48	3.48	3.48	3.48	3.48	3.48	3.48	62.0	62.0
Basement water (kg)		0	0	0	71.1	71.1	0	71.1	71.1	71.1
Surtsey pressure (MPa)		0.200	0.197	0.189	0.200	0.205	0.199	0.200	0.200	0.203
Surtsey temperature (K)		295	275	280	295	302	308	303	304	298
Surtsey gas moles (g-moles)		7323	7737	7291	7323	7318	6961	7129	2105	7360
Initial gas composition in Surtsey (mol.%)	N_2	99.90	99.78	90.60	90.00	16.90	87.10	85.95	85.32	85.80
	O_2	0.03	0.19	9.00	9.59	4.35	9.79	9.57	9.85	9.79
	H_2	0.00	0.02	0.00	0.00	2.76	2.59	3.97	4.33	3.91
	CO_2	0.01	0.00	0.02	0.02	75.80	0.00	0.03	0.03	0.03
	Other	0.06	0.01	0.38	0.39	0.19	0.52	0.48	0.47	0.47
Initial hole diameter (cm)		3.5	3.5	3.5	3.5	3.5	3.5	3.5	3.5	3.5
Final hole diameter (cm)		4.04	4.02	4.53	4.22	4.31	3.91	4.08	3.50	4.10
Debris fraction dispersed from cavity		0.768	0.654	0.601	0.720	0.585	0.790	0.619	0.167	0.832
Freeboard volume inside subcompartment structures						4.65 m^3				
Freeboard volume in Surtsey dome						85.15 m^3				
Total freeboard volume						89.8 m^3				

ANL Integral Effects Tests (ANL/IET) (Binder et al., 1994). These experiments were designed to be scaled counterparts of the SNL/IET Zion-geometry experiments. The linear scale factor was 0.0255 (approximately 1/40), relative to NPP scale. The initial conditions are summarized in Table D-3. A major purpose of these experiments was to study scale effects by comparing the results with the results of the SNL/IET experiments. Three of the experiments (ANL/IET-1RR, ANL/IET-3, and ANL/IET-6) were designed to be close counterparts of the corresponding SNL/IET tests. These experiments were analyzed with CONTAIN to assess the scalability of the model. The other ANL/IET experiments have not been analyzed with CONTAIN. Comparison with the SNL/IET experimental series did not demonstrate any dramatic scale dependencies, but the contribution of DCH-produced hydrogen to containment pressurization was somewhat larger and considerably more consistent in the larger-scale SNL experiments.

ANL/U Experiments (Binder et al., 1994). This series consisted of three experiments performed in the Zion geometry at 1/40-scale as in the ANL/IET series. Unlike the latter experiments, melts with prototypic core debris compositions (including UO_2 and metallic Zr) were used. Some difference with respect to the iron oxide/aluminum thermite experiments were observed. For example, hydrogen production appeared to be somewhat greater while ΔP values were somewhat lower in the ANL/U series; however, it should be noted that the initial conditions were not exact counterparts of the thermite experiments. Nonetheless, no dramatic differences with respect to the iron oxide/aluminum thermite experiments were observed. This result is important because it supports the belief that the nonprototypic melts used in most of the other DCH experiments do not introduce important uncertainties in the interpretation of the other experiments in the context of DCH model validation. The ANL/U experiments have not been analyzed with the CONTAIN code.

SNL Integral Effects Tests in Surry Geometry (SNL/IET Surry) (Blanchat et al., 1994). In these experiments, scaled models of the Surry NPP cavity and containment structures were used. Three experiments (SNL/IET-9, -10, and -11) were conducted in the Containment Technology Test Facility (CTTF) with a linear scale factor of 1/5.75, relative to NPPs. The fourth experiment, IET-12, was performed at 1/10-scale in the Surtsey facility; although the structures in the latter experiment were faithful replicas of the larger-scale CTTF experiments, the initial conditions were not designed to provide a scaled counterpart of any of the CTTF tests. Initial conditions are summarized in Table D-4 for all four experiments.

The three CTTF experiments are among the most nearly prototypical of all the DCH experiments that have been performed. In addition to the large scale of these experiments, the atmosphere contained steam rather than the nitrogen diluents (CO_2 in SNL/IET-5) used in the SNL/IET Zion experiments, and concentrations of pre-existing hydrogen ranging from 2.0 to 2.4% were also present; note, however, that these values are much less than prototypic (see Section 6.2.2 of the main report). Furthermore, the melt generator was located inside the containment facility which permitted the study (in IET-11) of the effect of RPV insulation and the annular gap between the reactor pressure vessel (RPV) and the biological shield wall. In the IET-12 experiment, there was no annular gap, pre-existing hydrogen concentrations were higher (5.7%), and the melt included no chromium.

Table D-3

Initial Conditions for the ANL/IET Zion Experiments

	IET-1RR	IET-3	IET-6	IET-7	IET-8
Exit hole diameter (cm)	1.3	1.1	1.1	1.1	1.1
Steam driving P (MPa)	6.7	5.7	6.6	6.1	6.5
Moles of steam	9.84	8.43	9.65	8.88	9.36
Thermite mass (kg)	0.82	0.82	0.71	0.71	0.71
Fraction dispersed from cavity	0.668	0.674	0.668	0.788	0.754
Initial containment P (MPa)	0.2	0.2	0.2	0.1	0.2
Initial containment T (K)	318	318	315	318	477
Initial containment atm (mole %)					
N_2	99.9	88.8	87.5	89.9	37.4
O_2	0.12	10.8	9.9	10.1	7.7
H_2O	~0	~0	~0	~0	50.0
H_2	~0	~0	2.0	~0	3.9

The three CTTF experiments have been analyzed using CONTAIN. IET-12 yielded anomalous results and is not well understood; it was not analyzed with the CONTAIN code.

Table D-4

Initial Conditions for the SNL/IET Surry Experiments

		IET-9	IET-10	IET-11	IET-12
Mass of the initial thermite charge (kg)		158.0	158.0	158.0	30.00[a]
Fraction dispersed from cavity		0.873	0.732	0.81	0.459
Mass of the RPV SS insulation (kg)		0	0	29	0
Gas pressure at plug failure (MPa)		12.9	12.1	13.2	11.2
Gas temperature at plug failure (K)		787	713	693	696
Moles of driving gas (g-moles)		3005	3275	3705	604
Initial hole diameter (cm)		7.0	7.0	7.0	5.6
Final hole diameter (cm)		7.4	9.8	7.6	5.6
Initial annular gap area (m^2)		0	0	0.0174	0
Final annular gap area (m^2)		0.012	0	0.0360	0
Water on basement floor (kg)		372	0	703	0
Initial vessel absolute pressure (MPa)		0.1351	0.1791	0.2209	0.1635
Initial vessel temperature (K)		392	410	399	408
Initial vessel gas moles (g-moles)		11870	15027	18802	2461
Initial gas composition in the containment vessel (mol.%)	Steam	67.24	48.20	32.25	57.98
	N_2	24.01	38.47	50.98	28.45
	O_2	6.14	10.17	13.66	7.28
	H_2	2.20	1.98	2.39	5.66
	CO	0.00	0.51	0.00	0.03
	CO_2	0.13	0.21	0.02	0.26
	Other	0.28	0.46	0.70	0.34
Freeboard volume inside subcompartment structures (m^3)		83.1		79.1	12.8
Freeboard volume in upper dome (m^3)		202.9		202.9	38.2
Total freeboard volume (m^3)		286.0		282.0	51.0

[a]Thermite mixture included no chromium metal.

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