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Assessment of the CONTAIN Direct Containment Heating (DCH) Model: Analyses of DCH Integral Experiments*

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Abstract

Models for direct containment heating (DCH) in the CONTAIN code for severe accident containment analysis have been reviewed and a standardized input prescription for their use has been defined. The code has been exercised against a large subset of the available DCH data base. Generally good agreement with the experimental results for containment pressurization (ΔP) and hydrogen generation has been obtained. Extensive sensitivity studies have been performed, which provide guidance for users and which permit assessment of many of the strengths and weaknesses of specific model features. These include models for debris transport and trapping, DCH heat transfer and chemistry, atmosphere-structure heat transfer, interactions between nonairborne debris and blowdown steam, potential effects of debris-water interactions, and hydrogen combustion under DCH conditions. Containment compartmentalization is an important DCH mitigator in the calculations, in agreement with experimental results, and a major contributor to this mitigation is atmosphere-structure heat transfer together with delayed or incomplete combustion of DCH-produced hydrogen in oxygen-starved subcompartment volumes. The CONTAIN model includes parametric treatments for some processes that are not well understood, including the interactions of nonairborne debris with steam and gas, debris-water interactions, and debris-gas slip in the transport model. The contribution of these uncertain processes to the results is expected to be important in some DCH scenarios and unimportant in others. The results of the assessment described here are employed to develop guidance for use of the CONTAIN DCH model in nuclear power plant analyses. The guidance includes possible sensitivity calculations for quantification of uncertainties.

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Executive SummaryExecutive Summary

Overview of the ReportOverview of the Report

This report presents an assessment of the models for direct containment heating (DCH) in the CONTAIN code and offers insights into DCH phenomenology developed in the course of the assessment. The CONTAIN code has been developed for the Nuclear Regulatory Commission (NRC) as a detailed analysis tool for evaluating containment response to severe reactor accidents. The principal methodology used is to compare calculated results with the results of experiments in which DCH processes are simulated using high-temperature, chemically reactive melts. These melts are ejected from a melt generator by high-pressure steam into scaled models of reactor cavities that are connected to a pressure vessel that simulates, in varying degrees, a nuclear power plant (NPP) containment building.

Two important purposes that the report is intended to serve are (1) providing a model assessment study based upon analyzing and interpreting the DCH integral data base to examine the extent to which the CONTAIN code can reproduce the experimental results, and (2) providing a tool to assist future users of CONTAIN in designing calculational matrices for particular studies, and in interpreting the significance of the results.

In support of these goals, direct comparison with the integral results of experiments has been supplemented with examination of specific model sensitivities that explore alternative explanations of the results obtained and investigate sensitivity to uncertain inputs and model assumptions. Considerable emphasis is placed upon understanding the reasons for the results obtained, in order to guide judgments as to whether the calculated behaviors are reasonable. In the process, significant insights into DCH phenomena are also obtained that contribute to the evaluation of model uncertainties. It is the complete body of understanding obtained, not just the goodness-of-fit to the experimental data, that must be applied when assessing the uncertainties in code calculations for DCH scenarios not studied experimentally, including analyses of hypothetical full-scale NPP events. The development of this understanding has required an extensive matrix of sensitivity calculations, and it must be emphasized that it is not expected that any code user will need to replicate more than a small fraction of these calculations.

Because the report is somewhat lengthy, it has been organized in a way that attempts to accommodate readers with different needs. After a brief introduction, the next three sections of the report give an overview of the DCH data base available for CONTAIN assessment, provide a high-level description of the CONTAIN DCH models together with a standardized input prescription for their use, and present the most important findings of this study. These sections are followed by a preliminary assessment of recently developed models for melt ejection from the reactor pressure vessel (RPV) and entrainment in the cavity, and a lengthy description of the details of the assessment of the various DCH-related models. The final section provides additional user guidance.

Data Base for DCH AssessmentData Base for DCH Assessment

It was not feasible to use the CONTAIN code to analyze every DCH experiment that has been performed, but a substantial subset of them has been analyzed. The selection of experiments for analysis has been guided by the desire to span as wide a range of relevant parameters as possible, by the prototypicality of the experiments, and by the availability of information on the details of the experiment required for analysis. The experiments selected for analysis include the six experiments of the limited flight path (LFP) series, the three experiments of the wet cavity (WC) series, eight of the integral effects test (IET) experiments performed at 1/10-scale in Zion geometry and the three counterpart Zion-geometry experiments performed at 1/40-scale, and three IET experiments performed at 1/5.75-scale in Surry geometry. The 1/40-scale Zion geometry experiments were performed at Argonne National Laboratory (ANL), the Surry-geometry IET experiments were performed in the Containment Technology Test Facility (CTTF) at Sandia National Laboratories (SNL), and all others were performed in the Surtsey DCH Facility at SNL.

Model Summary and Standardized InputModel Summary and Standardized Input

A high-level summary of the CONTAIN DCH model is provided, emphasizing features that need to be taken into account when assessing and/or using the models. An important part of the user-guidance function of the present work has been to develop a standardized input prescription for use in the experimental analysis which could also be applied to NPP analysis. This prescription is presented in conjunction with the model descriptions. A limitation of the standardized prescription is that it does not include the use of the newly developed CONTAIN models for debris ejection from the reactor pressure vessel (RPV) and cavity entrainment phenomena, because understanding of these phenomena is insufficient to justify defining a standard prescription at this time.

<u>Debris Sources and Blowdown</u>. The phenomena governing melt ejection from the RPV and dispersal from the cavity are believed to be especially uncertain, and it would be undesirable to allow uncertainties in these processes to distort the assessment of other DCH-related models. Hence, in the greater part of this work, experimental data were used to define

blowdown rates and debris sources so as to obtain the correct time dependence of the blowdown and debris sources, the correct degree of coherence between blowdown steam and debris entrainment, and the correct amount of debris dispersed from the cavity. Since this procedure depends upon the availability of experimental data, it cannot be directly used in a predictive mode. User guidance based upon experimental results is provided for how to define debris sources when analyzing other DCH scenarios (including NPP events). Sensitivity studies are given which indicate that uncertainties in these processes will not normally have a large impact upon the results of DCH calculations.

Debris Transport and Trapping. The physics governing debris transport and trapping is incompletely understood and, in addition, the lumped-parameter control-volume character of the CONTAIN code limits the detail that can be treated even when physical understanding would in principle permit a more refined treatment. Hence there are important uncertainties in the modeling of these processes. For practical purposes, the most important result of interest is f_{dome}, defined as the fraction of the debris dispersed from the cavity that is transported to the containment dome. (This statement presupposes a containment of the Surry or Zion type having a compartmentalized lower-containment geometry.) The standard prescription for use of the debris transport and trapping models has been defined in a way that is believed to tend toward conservatism in the sense that it is more likely to overestimate f_{dome} than to underestimate it; it is not guaranteed to be bounding, however.

DCH Heat Transfer and Chemistry. These parts of the CONTAIN DCH model have seen little recent change and the standard prescription relies heavily upon default settings of the input parameters. The most important exception is that the drop-side reaction rate limit is not used, i.e., an infinite drop diffusivity is assumed.

Nonairborne Debris. The inclusion of the interactions between blowdown steam and the CONTAIN nonairborne debris field (also called the trapped field) has been found to be important to obtaining good results in CONTAIN comparisons with experiments. The term "nonairborne" strictly applies only to the CONTAIN model; the debris configurations controlling the various processes involved are not known and may, for example, include debris dripping from structures following initial de-entrainment as well as debris films adhering to structures.

Because the processes involved are not completely understood, the nonairborne model is parametric in the sense that it includes a user-defined effective particle size, d_t. The present effort has devoted considerable attention to assessing the nonairborne model. The standard input prescription developed includes modeling the nonairborne interactions in the cavity and the subcompartments (but not the dome) using a value of d_t equal to 0.01 m in 1/10-scale experiments. A scaling rationale is provided which was used in analyzing the 1/40-scale ANL/IET experiments and the 1/5.75-scale Surry IET experiments. Appendix B of the report presents details of the scaling rationale and also provides an analytical derivation supporting the choice of $d_t \approx 0.01$ m at 1/10-scale in the standard prescription, which was originally developed on empirical grounds.

Interactions with Water. CONTAIN has no model for fuel-coolant interactions, but some of the potential effects of water co-dispersed with debris can be investigated by introducing a source of low-enthalpy steam (i.e., enthalpy equivalent to that of liquid water) in parallel with the debris. The treatment permits a simulation of the quenching effect of the water as well as the effect of the increase in the supply of coherent steam resulting from the vaporization of the water. However, the modeling for debris-water interactions is insufficiently complete to offer a mechanistic prediction of how much of the water will actually interact with the debris.

Water was not included when the standard prescription was defined, but subsequent results suggest that water in the cavity is a significant contributor in the Zion-geometry IET experiments. Hence, sensitivity studies including cavity water will be required for NPP analyses unless it is known that the reactor cavity will be dry. Guidance for performing the sensitivity studies is provided.

DCH-Related Use of Other Models. There are several CONTAIN models whose use in DCH calculations differs from use in other CONTAIN applications, and the standard prescription includes specifications for the use of these models in DCH calculations. The most important of these are the hydrogen combustion models. Others include the atmosphere-structure radiation model and input controlling convective flow velocities calculated by the code.

Principal Results of the StudyPrincipal Results of the Study

For each experiment analyzed, the following four cases were run:

Case 1. Standard input prescription.

Case 2. Case 1 except nonairborne debris interactions were modeled in the cavity only (not included in the subcompartments).

Case 3. As in Case 1 except no nonairborne debris interactions were modeled.

Case 4. As in Case 1 except that a slip factor, s_d, equal to 5 was specified for the subcompartments, instead of s_d equal to 1 as in the standard prescription.

It was found that the standard input prescription (Case 1) gave generally good results for containment pressurization due to DCH (ΔP), for hydrogen production, and for amounts of hydrogen burned. The Surry-geometry results fell in line well with the Zion-geometry results and comparison between the ANL and SNL Zion-geometry results revealed no obvious scale distortions, although there may be some tendency to overpredict hydrogen production at the smaller scale. The same standard prescription predicted both the compartmentalized-geometry experiments and the open-geometry experiments reasonably well. The poorest ΔP results obtained were for four LFP experiments in which ΔP was overpredicted by 35-75%.

Effect of Nonairborne Debris and Cavity Water. The Case 3 analyses correspond to the traditional interpretation of DCH, which considers only the interactions between airborne debris and the coherent portion of the blowdown steam (and interactions with the containment atmosphere, within the restrictions imposed by compartmentalization). A very important finding of this study was that Case 3, in which no nonairborne debris interactions were modeled, underpredicted hydrogen production in every case but one, and underpredicted ΔP for all experiments in which hydrogen could burn. By a substantial margin, the largest effects were observed in the Zion-geometry IET experiments, in which hydrogen production was underpredicted by a factor of about two, and ΔP was also underpredicted by a factor of two for those cases in which hydrogen could burn. The results of these analyses indicate that the Zion-geometry IET experiments cannot be understood in terms of the interactions between airborne debris and coherent steam alone.

Several convergent lines of evidence support the conclusion that additional processes (i.e., nonairborne debris interactions and/or debris-water interactions) make important contributions to both ΔP and hydrogen production in the Zion-geometry experiments. In the standard input prescription, these "additional processes" are assumed to be the nonairborne debris interactions. However, cavity water was present at condensate levels in all cases, and sensitivity studies show that debris-water interactions also have the potential to account for much of the difference between the Case 3 analyses and the experimental results. Neither the experimental data nor the modeling are sufficient to permit an unambiguous determination of the relative importance of the nonairborne debris interactions and the debris-water interactions. Comparisons of experimental versus calculated pressure-time histories suggest that both processes make significant contributions.

Effect of Slip in the Subcompartments. The overprediction of the LFP results noted above for the standard input prescription was due to a substantial overprediction of f_{dome} for these experiments, while the calculated f_{dome} was approximately correct (within the experimental scatter) for the Zion IET experiments and somewhat underpredicted for the Surry IET cases. In Case 4, specifying $s_d = 5$ reduced f_{dome} substantially in all cases, which improved agreement for both f_{dome} and ΔP in the LFP experiments. Case 4 substantially underpredicted f_{dome} for the Zion and Surry IET experiments, but ΔP and hydrogen production were insensitive to this change and agreement remained good. However, it is believed that the underprediction of f_{dome} is potentially nonconservative for other scenarios differing from those studied experimentally, and hence the standard prescription is defined with $s_d = 1$ in the subcompartments.

Mitigation Effects. The principal processes that act to mitigate DCH are debris trapping, which slows or terminates debris interactions with the atmosphere, and atmospheric heat transfer to containment structures. Containment compartmentalization can enhance the effect of trapping by preventing most of the debris from ever reaching the dome. It can also enhance the heat transfer effects, in part because hydrogen hold-up in oxygen-starved subcompartments can delay hydrogen combustion and thus give heat transfer more time to be effective. Sensitivity calculations indicate that the effect of atmosphere-structure heat transfer is as important as the effect of trapping.

Debris Source Characteristics. Sensitivity to debris particle size, cavity dispersal fraction, and debris dispersal coherence with blowdown steam was examined. These sensitivities were not large, which supports the belief that DCH calculations can be performed using experimental results to specify these parameters through the input without introducing large uncertainties into the calculation.

Assessment of RPV and Cavity ModelsAssessment of RPV and Cavity Models

The suite of RPV and cavity models has many options, including some in which the user specifies the fraction dispersed. These options also include several nonmechanistic features which require the user to estimate in advance the conditions that will exist in the cavity during debris dispersal. The present work was limited to studying the most fully mechanistic option, in which the code calculates single-phase and two-phase melt ejection from the RPV, the timing of gas blowthrough, conditions in the cavity, entrainment rates, and total quantity of debris dispersed. The modified Whalley-Hewitt correlation and the Levy correlation were both assessed in simulations of the SNL/IET-3 experiment. The findings include the following:

- Blowthrough occurs too early if a realistic diameter for the RPV is specified.

- For both the Whalley-Hewitt correlation and the Levy correlation, it was found that values of the cavity coefficient (K_c) obtained from experiments using low-temperature simulants were not applicable to the high-temperature tests (this result was expected). K_c must be tuned to the experimental data to obtain reasonable results.

- Neither the Whalley-Hewitt correlation nor the Levy correlation can match both the dispersed fraction (f_{disp}) and the coherent steam fraction (f_{coh}) simultaneously: if f_{disp} is matched, f_{coh} is too large; if f_{coh} is approximately matched, 100% dispersal results. The Levy correlation is somewhat better than the Whalley-Hewitt correlation in this regard.

- In the calculation, the rate of melt ejection from the RPV, rather than the entrainment rate, sets a lower limit to the value of f_{coh} that can be achieved, and this limit is actually somewhat greater than the experimental value; with a large hole size, blowdown might be complete before the calculated melt ejection is complete. It is possible that the model exaggerates the degree to which the melt ejection rate can limit f_{coh}.

- ΔP and H_2 results are fairly insensitive to dispersed fraction and coherence when the standard prescription (including nonairborne debris) is used, and agree reasonably well with experimental data. The results are more sensitive when nonairborne debris is not included and tend to underpredict experimental results.

- Use of the Weber number particle size model did not change the integral results substantially. The calculated value of f_{dome} was increased in some cases but this effect was not very large.

- The cavity models were not designed to be used in conjunction with a simulation of co-dispersed water, and evidence obtained in other parts of this assessment suggests co-dispersed water may be important. Hence this limitation may be a significant one.

Sensitivity Studies for Assessment of Specific Model FeaturesSensitivity Studies for Assessment of Specific Model Features

A large number of sensitivity studies were carried out in order to refine the assessment of specific model features. Not all the results can be mentioned in this summary. Some of the more significant results include the following:

- DCH sensitivities can depend strongly upon the scenario under consideration; the quantitative results of sensitivity studies described here cannot be assumed to apply without qualification to other scenarios that differ substantially from those that have been studied experimentally. In some instances, therefore, the user should perform the indicated sensitivity studies for the case at hand, and not assume that the sensitivities given here will apply.

- There appear to be some important dependencies upon cavity and containment geometry (open versus compartmentalized geometries and Zion versus Surry geometries).

- There was some sensitivity to nodalization in both the Zion and Surry geometries, but this sensitivity is less than some other uncertainties (nonairborne debris, debris-water interactions, hydrogen combustion). The nature of the sensitivities to nodalization differed for the Zion and the Surry geometries.

- When the containment geometry is open (as in the WC experiments), the effect of cavity water appears to be considerably less than may be the case in compartmentalized geometry, at least for Zion. Thus, one cannot use the WC-2 result, in which water did not cause large effects, to infer the absence of important effects in compartmentalized geometries. In compartmentalized geometries, small amounts of water tend to enhance loads while large amounts may mitigate loads.

- The standard prescription for the diffusion-flame burn (DFB) model yields good results for typical containment conditions, although it erroneously predicts efficient combustion in the IET-5 experiment, which was more heavily inerted than is expected to be the case for NPP scenarios. The temperature threshold needs to be lowered or eliminated when large amounts of co-dispersed water are involved (e.g., as in SNL/IET-8B). The data do not permit full assessment of the bulk spontaneous reaction (BSR) prescription; it could be either reasonably close to the best estimate or overly conservative.

- Comparison between the ANL/IET and SNL/IET counterpart experiments reveals no dramatic overall scale effects or substantial overall scale distortion in the CONTAIN model. Cancellation of opposing effects may be involved, as there do appear to be significant scale effects in some specific phenomena. These include the degree of debris-steam coherence and the efficiency and reproducibility of hydrogen combustion.

- Analysis of the Surry-geometry IET experiments suggests that differences in the initial conditions of the containment atmosphere were the dominant factor controlling the differences in ΔP measured between the IET-9, IET-10, and IET-11 experiments. In the CONTAIN analyses, this factor was more important than the other differences between the experiments, including differences in accumulator steam supply, melt generator hole size, debris-steam coherence, debris dispersal fraction, annular gap around the RPV, and ablated insulation.

User GuidanceUser Guidance

Some modifications to the standard prescription are needed in order to reflect lessons learned from the present work and/or reflect differences between NPP analysis and experimental analysis. The modified standard prescription is recommended as a starting point for NPP calculations, but it does have a number of limitations. The resulting uncertainties should be explored in sensitivity studies, depending upon the nature and purpose of the particular study the CONTAIN user is supporting. The need for sensitivity studies is minimized if acceptable loads are calculated even when conservative input assumptions are used. Some suggested guidelines include the following:

- Debris sources. Whether user-defined sources or the new RPV and cavity models are used, the reasonableness of the results should be judged by comparing f_{disp} and f_{coh} with experimental results. The present results suggest that sensitivity to f_{disp} and f_{coh} will be limited in at least some cases; however, studies to check this sensitivity are recommended, especially in view of the lack of substantial experience with NPP-scale analyses using the current DCH model and the standard input prescription.

- Debris trapping and transport. The standard prescription seems to give reasonable results for Surry and Zion geometries for the scenarios studied experimentally. In scenarios differing substantially from those studied experimentally, appropriate sensitivity studies are suggested, especially if transport beyond the subcompartments appears to play an important role.

- Hydrogen Combustion. The standard prescription for the DFB model appears to give good results for typical containment conditions, but the burn temperature threshold should be eliminated in scenarios involving large amounts of co-dispersed water. The standard prescription for the BSR model is recommended as a starting point but it may be overly conservative; sensitivity studies are warranted if resulting loads appear to be excessive. Care is needed to ensure that the deflagration model does not cause unwonted suppression of BSR. If containment atmospheric conditions can support a deflagration, the default flame speed correlation should be overridden with a higher user-specified value to take into account the presence of multiple ignition sources in DCH events.

- Nonairborne Debris Interactions and Debris-Water Interactions. Because these models are parametric, and proper scaling difficult to predict, uncertainties in their use can be relatively large in some instances. The uncertainties are expected to be smaller if the metal content of the melt is low. Recommendations include sensitivity studies involving conservative combinations of nonairborne interactions and/or debris-water interactions. If loads are nonthreatening even with conservative input, additional analysis may be unnecessary.

Perspective on UncertaintiesPerspective on Uncertainties

This report acknowledges that there are many phenomena associated with DCH that are quite uncertain as to their details. However, this fact does not mean that the DCH loads calculated by CONTAIN will normally be heavily affected by a large number of uncertainties, because the results in any given instance will commonly be insensitive to most of the uncertain phenomena. For example, there are important uncertainties in the phenomena controlling debris trapping and transport, yet the analyses of the Zion and Surry- geometry experiments were found to be quite insensitive to these uncertainties. Typically, the results of a given analysis will be sensitive to at most a small number of uncertain parameters or modeling assumptions; however, the identity of the more important uncertainties can be different for different DCH scenarios.

The impact of any given uncertainty on the results of DCH calculations can depend strongly upon the initial and boundary conditions of the scenario of interest. It is therefore impossible to give a quantitative estimate of the magnitudes of these uncertainties that would be applicable to all DCH analyses. Hence the approach adopted has been to define a set of suggested sensitivity calculations in the User Guidance section of the report. These recommendations are designed to provide the user with a reasonable understanding of the uncertainty for the particular case at hand.

To date, there has been only limited application of the approaches developed in this report to NPP analyses. Hence, some of the suggestions offered here must be considered tentative.

1 Introduction Introduction

In some reactor core melt accident sequences, the reactor pressure vessel (RPV) may not fully depressurize prior to failure of the vessel lower head, and probabilistic risk assessments [NRC90] indicate that these sequences can constitute a nonnegligible fraction of the total core melt frequency. 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 large amounts of 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 large amounts of 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). Early analyses [NRC85] employing simple bounding models showed that the energy source potentially available was sufficient to threaten containment integrity, but that determining whether a significant threat actually existed would require improved understanding of the many complex processes involved in DCH.

As part of an extensive effort to resolve this issue, 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). The analytical program has included the development of various models for DCH, of which the most detailed and mechanistic is the model incorporated into the CONTAIN code. The CONTAIN code has been developed for the NRC as a detailed analysis tool for evaluating containment response to severe reactor accidents [Mur89, Was91]. Modeling of direct containment heating (DCH) has been a major focus of the CONTAIN development program [Was95]. Results of a detailed independent peer review of the CONTAIN code, including a review of the CONTAIN DCH models, were published recently [Boy95]. Much of the work presented in this report was performed in support of the peer review effort.

The present report describes results obtained using the CONTAIN code to analyze a number of DCH experiments that have been carried out with melts generated by the iron oxide/aluminum thermite reaction to simulate DCH processes. The purposes of this work are twofold:

1. To provide an overview of the strengths and weaknesses of the CONTAIN code's ability to analyze DCH events and summarize insights concerning DCH phenomenology that resulted from the analysis of the experimental results and that are important to the assessment.

2. To provide a tool to assist future users of CONTAIN in designing calculational matrices for particular studies, and in interpreting the significance of the results.

One important goal of the user guidance effort has been to develop what is called here the "standard input prescription" for DCH calculations. This prescription is intended to provide what appear to be good choices of input parameter settings from among the wide range of options available. The model assessment also emphasizes the standard input prescription results.

In addition, a large number of sensitivity studies have been performed, largely in connection with the user guidance role of the report. Documenting these results is considered important to support the guidance offered to users. There is no expectation that any user will ever need to replicate more than a small fraction of these sensitivity calculations. These studies have been performed for many different reasons: to demonstrate that uncertainties in many of the input parameters actually matter little to the results, to explore the sensitivity of the results to those input parameters and modeling assumptions that do matter, to determine how important certain specific phenomena such as atmosphere-structure heat transfer are to the results, to examine model behavior and compare (as best possible) the model behavior with the behavior observed in the experiments, and to examine the degree to which alternative explanations exist for the experimental trends. Furthermore, the identity of the more important uncertainties in DCH analysis can depend heavily upon the initial and boundary conditions of the scenario (e.g., melt mass and composition, vessel failure mode, vessel pressure at breach, containment geometry) and it is not possible to know what scenario any particular user may wish to study. Hence consideration of a wide range of sensitivities was appropriate for this work. For any given scenario, however, it is expected that results will be sensitive to at most a small number of the uncertain phenomena that are considered in this report.

Section 2 summarizes the experiments that have been analyzed with CONTAIN, and also highlights some major lessons that can be learned from the systematics of the experimental results without resorting to detailed computer models. In Section 3, the main features of the CONTAIN DCH and DCH-related models are reviewed, and a standardized input prescription for the use of these models is presented.

Section 4 summarizes the major results of the present study. It includes results obtained using the standardized input prescriptions, results of the more important sensitivity studies that have been performed, and the principal insights into DCH phenomenology that have been obtained from these analyses. Uncertainties in the interpretation of the results are considered when these are potentially important for applications of the code to NPP analyses.

In Section 5, results are presented for a more limited assessment of recent modeling incorporated for ejection of debris from the RPV, entrainment in the cavity, and particle size. For reasons discussed in Section 3.2.2, these models were not used in the results presented in Sections 4 and 6.

In Section 6, sensitivity calculations are used to assess a number of specific model features and the key underlying DCH phenomena in more detail than is done in Section 4. Topics considered include debris trapping and transport, sensitivity to particle size, possible effects of nonairborne debris and co-dispersed water, hydrogen combustion, the importance and role of mitigation effects, and the effects of geometric scale.

In Section 7, guidance is suggested for use of the models in plant calculations. This includes recommendations for possible sensitivity calculations to explore uncertainties relevant for the particular case of interest to the user.

Appendix A presents additional details of the nodalizations used for analyzing the DCH experiments. Appendix B discusses the interactions of nonairborne debris with blowdown steam and includes a scaling rationale for the CONTAIN model for these interactions. Appendix C presents a simplified analytical estimate of the degree to which atmosphere-structure heat transfer and incomplete hydrogen combustion might be expected to mitigate DCH, as a check of CONTAIN's treatment of these effects. Appendix D presents, with little discussion, a compilation of sensitivity study results obtained after the standard prescription was defined.

Finally, we have attempted to take into account the fact that different readers will have different purposes and requirements in examining a lengthy document such as the present one. Some readers may be reasonably familiar with DCH and the CONTAIN code, and may be primarily interested in the principal results obtained. Readers in this category may wish to skim through Sections 2 and 3 only as needed to assure themselves that they are familiar with the material covered there, and then concentrate upon Section 4. On the other hand, readers needing the most complete evaluation of the CONTAIN DCH model's capabilities and limitations, and/or wishing to form an independent evaluation of the models, may find that the more detailed information given in Section 6 is needed, as well as the detailed model descriptions given in Reference Was95.

2 Overview of the DCH Data Base and DCH Systematics Overview of the DCH Data Base and DCH Systematics

Of the various experimental studies of DCH phenomena that have been performed, the most prototypic have been those in which high-temperature melts generated by thermite-type reactions have been expelled by high-pressure steam into scaled reactor cavities that were connected to pressure vessels simulating the reactor containment building to various degrees. Local and global pressure rise ($\triangle P$), temperature distributions, amounts of hydrogen produced and burned, and debris transport parameters were among the experimental results reported in these tests. Results are most directly applicable to pressurized water reactor (PWR) large dry containments, because the pressure suppression systems of BWR and PWR ice condenser containments have not been simulated in any of the experiments.

In this section, we briefly summarize the DCH data base obtained using high-temperature melts that is potentially applicable to assessing the CONTAIN DCH model, cite references providing more detailed information on the experiments, and discuss some systematic trends in the data that have proven helpful in guiding the assessment of the CONTAIN model. We do not consider the many less prototypic separate-effects experiments which have been performed because the scope of the present work does not include explicit comparisons between CONTAIN and the results of those experiments. One important part of this auxiliary data base includes the experiments that have been performed using low-temperature simulants to study dispersal of debris from the cavity. These results were used to select the cavity entrainment correlations that have been incorporated into CONTAIN [Wil96].

2.1 Summary of DCH Experiments.1 Summary of DCH Experiments

Experimental parameters and results for a total of 47 DCH experiments employing high-temperature melts have been summarized in a review by Pilch that was conducted as part of the NRC's DCH issue resolution effort [Pil94a]. It was not feasible to use the CONTAIN code to analyze all these experiments. The more recent experiments were emphasized because they included the more nearly prototypic cases; detailed information on these experiments was more readily available; and many of the important insights resulting from the earlier work had been incorporated into the design of the later experiments. A total of 23 experiments were analyzed with the CONTAIN code.

The summary of the DCH data base 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, 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) [Tar88], five performed at Argonne National Laboratory (ANL/CWTI series) [Spe88], and four experiments performed at Fauske and Associates, Inc. (FAI/DCH series) [Hen91]. 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 [Wil87]. 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 [Wil87, Wil88].

SNL Technology Development Series (TDS) [All94a]. 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. They were also sufficiently similar to certain experiments in the LFP and WC series (see below) that they have not been analyzed here, although it may prove useful to analyze some of them at a future time.

The experimental technique developed in the TDS series is basically the same as that used in the subsequent experiments which have been analyzed with CONTAIN, 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 that have been analyzed with the CONTAIN code. 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, some recent work [Pil94b] indicates that the metal content of actual core debris may be considerably lower than that used in the DCH experiments.

Limited Flight Path (LFP) Tests [All91a]. 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" [Zub91]. This terminology will be used in the present report, 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.

All of the LFP experiments were analyzed in the present work. Some test parameters for these experiments are summarized in Table 2.1-1.

Table 2.1-1

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

		LFP-1A	LFP-1B	LFP-2A	LFP-2B	LFP-2C	LFP-8A	WC
Flight path (m)		0.91	0.91	1.85	1.85	1.85	7.70	7.
Initial thermite mixture mass (kg)		80	50	50	50	50	50	5
Fraction dispersed from cavity		0.725	0.209	0.484	0.616	0.620	0.392	0.8
Steam driving P(MPa)		3.7	2.6	3.0	3.6	3.3	2.9	4
Moles of steam		262	180	229	249	246	188	37
Exit hole diameter (cm)		6.41	3.5	3.5	5.97	8.57	3.5	3
Initial pressure in Surtsey (MPa)		0.161	0.158	0.160	0.160	0.160	0.159	0.1
Initial gas	Ar	99.6	99.6	99.7	99.2	99.7	99.5	99
composition	N_2	0.31	0.33	0.2	0.63	0.29	0.38	0.
in Surtsey (mole%)	O_2	0.08	0.07	0.0	0.16	0.06	0.08	0.

[a] 11.76 kg water in cavity. Cavity was dry in all other experiments.
1

Wet Cavity (WC) Tests [All92a, All92b]. 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 more rapid melt ejection, vessel blowdown, and melt dispersal from the cavity.

Experimental parameters for the WC series are also given in Table 2.1-1. All three WC experiments were analyzed in the present work.

SNL Integral Effects Tests, Zion Geometry (SNL/IET Zion) [All94b]. 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 2.1-2. 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 [Zub91] 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. 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.

Table 2.1-2

Initial Conditions for the SNL/IET Zion Experiments

		IET-1	IET-1R	IET-3	IET-4	IET-5	IET-6	IET-7
Steam pressure (MPa)		7.1	6.3	6.1	6.7	6.0	6.3	5.9
Steam temperature (K)		600	585	585	555	586	571	599
Steam driving gas (g-moles)		468	507	485	582	453	505	416
Cavity water (kg)		3.48	3.48	3.48	3.48	3.48	3.48	3.48
Basement water (kg)		0	0	0	71.1	71.1	0	71.1
Surtsey pressure (MPa)		0.200	0.197	0.189	0.200	0.205	0.199	0.200
Surtsey temperature (K)		295	275	280	295	302	308	303
Surtsey gas moles (g-moles)		7323	7737	7291	7323	7318	6961	7129
Initial gas	N_2	99.90	99.78	90.60	90.00	16.90	87.10	85.95
composition	O_2	0.03	0.19	9.00	9.59	4.35	9.79	9.57
in Surtsey	H_2	0.00	0.02	0.00	0.00	2.76	2.59	3.97
(mol.%)	CO_2	0.01	0.00	0.02	0.02	75.80	0.00	0.03
	Other	0.06	0.01	0.38	0.39	0.19	0.52	0.48
Initial hole diameter (cm)		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
Debris fraction dispersed from cavity		0.768	0.654	0.601	0.720	0.585	0.790	0.619
Freeboard volume inside subcompartment structures						$4.65\ m^3$		
Freeboard volume in Surtsey dome						$85.15\ m^3$		
Total freeboard volume						$89.8\ m^3$		

2

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).

CONTAIN analyses of all the experiments except SNL/IET-8A are presented in this report. 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 present effort and is not included in the results summarized in Section 4. 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 [Dav93]. Some exploratory CONTAIN analyses of SNL/IET-8B were subsequently performed, however, and these results are included in Section 6.4.5.

ANL Integral Effects Tests (ANL/IET) [Bin94]. 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 2.1-3. 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.

Table 2.1-3

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

ANL/U Experiments [Bin94]. 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. 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 NPP analyses. The ANL/U experiments have not been analyzed with the CONTAIN code.

SNL Integral Effects Tests in Surry Geometry (SNL/IET/S) [Bla94]. 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 2.1-4 for all four experiments.

Table 2.1-4

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

The three CTTF experiments are probably 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. Furthermore, the melt generator was located inside the containment facility which permitted the study (in IET-11) of the effect of 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.

The three CTTF experiments have been analyzed using CONTAIN. IET-12 has not been analyzed.

2.2 Overview of DCH Systematics.2 Overview of DCH Systematics.2 Overview of DCH Systematics

The first conceptual descriptions of DCH emphasized dispersed particulate debris interacting thermally and chemically directly with the main volume of the containment atmosphere; hence the name "direct containment heating." Early CONTAIN analyses of DCH [Wil87, Wil88] suggested that this description of DCH needed some modification when applied to compartmentalized containment geometries. The calculations indicated that much of the debris dispersed from the reactor cavity would likely be de-entrained in the subcompartments without reaching the dome. Thus compartmentalization was a potentially important source of mitigation. However, the calculations also indicated that interactions between debris and steam in the cavity and/or the subcompartments could result in effective transfer of thermal and chemical energy (in the form of hydrogen generated by metal-steam reactions) to the dome. Given sufficiently large steam supplies, rapid flows, and conditions such that pre-existing and DCH-produced hydrogen could burn, containment-threatening loads could still be calculated for large melt masses with a high metal content.

The subsequent experimental results [All94b, Bin94, Bla94] have confirmed several features of this description. Compartmentalization prevented transport of all but a minor fraction of the debris to the dome for the conditions that have been studied; large amounts of hydrogen have been shown to be generated by metal-steam reactions; and combustion of this hydrogen has been shown to be an important contributor to DCH loads.

In the existing data base, the dominant trends can be explained in terms of just three factors: compartmentalization, hydrogen combustion, and the magnitude of the steam supply in the experiments performed in compartmentalized geometries. These three factors are sufficiently dominant that they can be displayed using a very simple correlation of the experimental data with the total steam supply in the accumulator, without resorting to detailed models or computer codes. The correlation starts with the assumption that the energy transfer to the containment, including both thermal and chemical energy, is proportional to the total steam supply, which implies a containment pressure rise, △P, given by

$$\Delta P = C_1 \frac{R\, N_{H_2O}}{V_{con}\, C_v} .$$

1 (2.2-1)

Here, N_{H2O} is the number of moles of steam in the accumulator in the experiment, V_{con} is the containment volume, C_v is the constant-volume molar heat capacity of the containment atmosphere, and R is the universal gas constant. The constant C_1 is to be 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 except that tests performed in open geometries are not included in the fitting. Note that C_1 is not dimensionless; it is not expected that Eq. (2.2-1) could be of use in estimating DCH loads generally. Here we are only examining its ability to correlate the existing data base.

In Figure 2.2-1, △P values given by Eq. (2.2-1) are plotted against the experimental values for all DCH experiments in which steam was the driving gas. Data required for evaluating Eq. (2.2-1) were taken from Reference Pil94a. Results obtained by evaluating Eq. (2.2-1) for the open-geometry experiments, all of which had inert atmospheres, are also included in the figure, even though they were not used in fitting Eq. (2.2-1) to the data.

Figure 2.2-1. Correlation of experimental DCH loads based upon the total steam in the accumulator, illustrating some of the differences between open-geometry and compartmentalized cases.

1

It is evident that the ΔP results fall into two groups: compartmentalized cases and open-geometry cases. For the compartmentalized cases, 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., $R^2 = 0.86$). This result is consistent with the hypothesis that, for these geometries, loads are largely governed by debris-steam interactions in the cavity and subcompartments followed by transport of the energy to the dome.

For the open-geometry experiments, loads implied by Eq. (2.2-1) are substantially less than the experimentally observed loads. In these open-geometry experiments the loads are heavily influenced by direct debris interactions with the main volume of the containment atmosphere, interactions Eq. (2.2-1) does not take into account.

At one time, it was considered important to determine the low-pressure cutoff for debris dispersal from the cavity. Figure 2.2-1 implies that, for compartmentalized containment geometries, determination of the low-pressure cutoff could be de-emphasized once it was established that any such cutoff is at relatively low primary system pressures. Low pressures generally imply low steam supplies and, hence, relatively low DCH threats in compartmentalized geometries even if the debris is dispersed from the cavity. An additional reason for de-emphasizing the cutoff concept is provided by experimental evidence suggesting that blowdown steam can interact reasonably efficiently with debris in the cavity even when the latter is not dispersed [All91a, Wil92]. However, the low-pressure cutoff is still expected to be important for plants in which the principal exit path from the cavity leads directly to the open volume of the containment dome.

It is not to be supposed that a simple correlation with total accumulator steam can provide a useful tool for predicting DCH loads. Indeed, the steam correlation only works, even as a zero-order approximation, because scaled melt masses were fairly large in most of the experiments, and the interactions tended to be more steam-limited than melt-limited.
Any useful DCH model must be able to capture the gross trends displayed in Figure 2.2-1, but it is also clear that there are many other parameters potentially important to DCH that a complete model must be able to represent. These include melt properties (mass, composition, temperature), vessel failure size, geometry of the cavity and/or subcompartments, cavity water, atmospheric versus subatmospheric containments, other atmospheric parameters, etc.

The DCH data base has proven enormously useful for DCH model assessment and has provided innumerable insights, confirming some long-standing suppositions and disproving others. However, the fact that the accumulator steam supply, together with hydrogen combustion, can explain most of the observed variation in DCH loads for the experiments in compartmentalized geometries necessarily implies that any variations in other DCH parameters did not have a large effect upon the experimental results. One reason is that these parameters have not been varied as extensively as the driving pressure (and hence the steam supply), or have not been varied under conditions for which substantial sensitivities would be expected.

The simplicity of DCH systematics means that the data base can be fit reasonably well by models based upon quite different physical assumptions, and which could have different implications when applied to DCH scenarios that differ substantially from those that have been studied experimentally. It necessarily follows that there are important limitations to the degree to which any DCH model can be fully validated by comparisons with the integral data base. For example, one cannot demonstrate that the model dependencies upon parameters such as melt characteristics, vessel failure mode, etc., match the experimental dependencies upon these parameters, because the data base exhibits little variability ascribable to these parameters.

3 The CONTAIN DCH Model and Standardized DCH The CONTAIN DCH Model and Standardized DCH The CONTAIN DCH Model and Standardized DCH Input Prescription

In this section, major features of the CONTAIN DCH model are summarized and the standardized input prescription is given where a standard prescription has been defined. Certain other code models related to DCH (e.g., hydrogen combustion) are included when their use in DCH calculations may differ from standard use in other CONTAIN calculations. The model descriptions are given here only to provide a conceptual basis for reference in subsequent discussion. The descriptions omit many details and do not, for the most part, present the actual equations solved by the code (if given at all, equations are usually simplified). Detailed documentation of the DCH models is given in References Was95 and Gri94. Complete documentation of the CONTAIN code, including the DCH models, is currently in progress and will be forthcoming as the CONTAIN 1.2 Code Manual.

3.1 Conceptual Basis of the DCH Model.1 Conceptual Basis of the DCH Model.1 Conceptual Basis of the DCH Model

The CONTAIN DCH model was originally based upon the concept that DCH is governed by dispersed ("airborne"), finely divided core debris particles interacting with the atmosphere within the containment, including the reactor cavity. Despite the recent addition of a parametric treatment of the interactions of so-called "nonairborne" debris (Section 3.2.7), the greater part of the detailed CONTAIN DCH modeling remains based upon this concept.

The CONTAIN DCH model uses a multifield representation of airborne debris in which the debris is distributed among a number of different fields within each computational control volume (called a "cell"). The user specifies the number of fields to be used and, except as described in Section 5, specifies the initial distribution of debris among the fields. Each field can have its own characteristic particle size and composition at the time the debris is introduced into the calculation, and each field can be further subdivided into time-resolved "generations" such that each generation represents debris introduced into the problem at different times. The latter feature permits the code to keep fresh, unreacted debris separate from cooler, reacted debris, which might otherwise quench chemical reactions in the fresh debris. However, when the standard input prescription was used, it was found that there was no tendency for this quenching to occur in these analyses, and the multigeneration feature was not used. In NPP calculations, debris airborne residence times are longer, and difficulties resulting from combining fresh debris with aged debris can be greater than in the experimental analyses described here.

The airborne debris fields move with the gas as it flows from cell to cell, although not necessarily at the same rate (a simple parametric model for debris-gas slip is provided). Thermal and chemical interactions between the debris and the atmosphere are modeled in each cell. De-entrainment of airborne debris due to interactions with structures ("trapping") is modeled in each cell. Trapped debris is placed in an additional field, referred to as the "trapped field." A parametric model is provided to allow interactions between debris in the trapped field and the atmosphere to continue; this provides the basis of the "nonairborne debris" model.

DCH is phenomenologically an extremely complex subject, with tightly coupled interactions between such disparate phenomena as transient multiphase multicomponent transport through complex three-dimensional geometries, debris-structure interactions, debris-atmosphere-structure heat transfer, debris-atmosphere chemical interaction, gas combustion, etc. For some of the phenomena involved, understanding is sufficiently good that reasonably mechanistic models are provided. Examples include debris-gas heat transfer and chemical reaction, atmosphere-structure heat transfer, and intercell gas flow.

For other DCH-related phenomena, the controlling physics is not well understood at a detailed level, or else cannot be modeled accurately within a control-volume, lumped-parameter code such as CONTAIN. Even in these cases, the effect of such phenomena upon "downstream" calculations may be reasonably well understood. Typically, representations of these phenomena are parametric, and the user is allowed to specify model options and/or user-controlled parameters which control how the calculation is to be performed. In this report, a model is referred to as "parametric" if the following is true:

- Use of the model requires the user to specify an input quantity whose value is not dictated by the initial and boundary conditions and is not derivable from reasonably well-established physical principles.

- The output of the model is heavily influenced by the parameter value chosen when this value is varied over an uncertainty range that is consistent with the uncertainty in the current state of understanding of the controlling physics.

Parametric models, by this definition, may still have many mechanistic features that permit the model output to respond reasonably as a function of the other dynamic variables of the calculation.

An example is provided by the modeling for debris trapping and debris transport. Current physical understanding is not sufficient to permit development of detailed, validated models for all the physical processes that govern rates of debris trapping or rates and directions of debris transport. Even if the basic understanding were available, it would be difficult or impossible to adequately represent the detailed physics in CONTAIN, due to its limitations as a lumped-parameter code. However, for any given residence time of airborne debris prior to de-entrainment, and for any given degree of debris transport (e.g., beyond the subcompartments), the net effect upon DCH loads can be evaluated reasonably well. Hence, the CONTAIN model for debris transport includes a parametric representation of debris-gas slip, and a number of modeling options for trapping are provided.

This flexibility is important for a number of reasons. One essential use is to investigate the impact of uncertainties in the phenomena represented by parametric models upon the results of interest for the particular case at hand. It can be important to perform studies of this type in any careful CONTAIN analysis because the sensitivity to a particular uncertainty may depend strongly upon the specific scenario of interest. Hence, there may be little sensitivity to a particular parameter or phenomenon in one analysis while analysis of some other scenario may exhibit substantial sensitivity to the same parameters.

In addition to the models unique to DCH, there are some other models important to DCH analyses in ways not normally encountered in other CONTAIN calculations. These models and their use in DCH calculations are discussed in Section 3.3.

3.2 DCH Models and Standard Input Prescription.2 DCH Models and Standard Input Prescription.2 DCH Models and Standard Input Prescription

3.2.1 Role of the Standardized DCH Input Prescription.2.1 Role of the Standardized DCH Input Prescription.2.1 Role of the Standardized DCH Input Prescription

The flexibility in CONTAIN DCH modeling acknowledged above is currently viewed as being essential in order to permit the user to study uncertainties in the results of DCH calculations, as well as to permit the user to take advantage of any future refinements in DCH understanding. However, it obviously presents problems with respect to quality control and consistency for DCH analysis if some type of control on DCH input is not available. Hence an important goal of this effort has been to develop a standardized input prescription that will allow users working independently to obtain comparable results when consistency is desired.

One consequence of the variety of CONTAIN input options is that there is the potential for a degree of complexity that can be overwhelming. In defining the standardized input prescription, therefore, the tendency has been to favor the simplest of the available options except when there is some justification, experimental or theoretical, for doing something more complex.

Where possible, the standard inputs have been based upon separate-effects measurements obtained in the DCH experiments and/or stand-alone modeling. Separate effects measurements for phenomena such as hydrogen behavior obtained from DCH experiments were preferred to results of non-DCH experiments because the conditions of the latter often differ sufficiently from DCH conditions that applicability to DCH is doubtful in many instances. Parameters were not chosen by tuning directly to the integral results themselves (i.e., tuning to ΔP or hydrogen production results), with the partial exception of the nonairborne debris parameter d_t discussed in Section 3.2.7.

Another principle guiding the specification of the standard prescription is the desire to be mildly conservative when applying the prescription to scenarios differing from those that have been studied experimentally, especially in scenarios thought likely to be more severe than those studied experimentally. By "mildly conservative" is meant that, when available options appear to be equally defensible, the option expected to result in more conservative extrapolations is selected. The standard prescription should not be thought of as bounding, however.

One ground rule in the present work has been that the assessments against the data base described in Section 4 were all to be run using the standard prescription, other than for explicitly identified sensitivity studies. If this rule were to be violated, it would not be possible to present the results of Section 4 as an assessment of CONTAIN using the standard prescription. Redefining the standard prescription would therefore require rerunning the entire set. Hence the standard prescription could not reflect every insight obtained in the course of analyzing all the experiments unless the entire data set were re-analyzed, which would not have been feasible. The most important example of this limitation currently known is that the standard prescription does not take into account more recent insights concerning the effects of cavity water in the Zion IET experiments; see Sections 4.2, 6.4, and 6.5 for details.

It should be clear that the standardized prescription is not offered as a "cookbook" that must be followed, or that will guarantee good results if it is followed. It is offered as a suggested starting point or guideline. The standard prescription has potentially important limitations, and sensitivity studies to explore uncertainties are likely to be a part of any study that uses CONTAIN. One recommended use is to take the standard prescription as a starting point and to document deviations when reporting results.

In the remainder of Section 3.2, DCH models are summarized and the standard prescription for the associated input is given along with the model summaries, except when the appropriate values are clearly dictated by the problem initial and boundary conditions or when the default value of some parameter is used. The latter is often the case, and parameters not mentioned in the discussion should be assumed to be left at their normal CONTAIN code default values. A summary of the standard prescription input values is given in Table 3.2-1.

Table 3.2-1
Summary of the CONTAIN Standard Input Prescription for DCH Experimental Analyses

Parameter or Model Option	Values	Report Section Discussed
Debris Sources*		
Total mass, m_d	Experiment initial conditions	3.2.2
Composition	Al_2O_3/Fe/Cr/Al = 0.373/0.505/0.108/0.014 (weight)	2.1, 3.2.2
Temp., T_d^0	2500 K (from measurements)	---
Time Depend.	$S_d(t)$ from experimental cavity pressurization curves	3.2.2
Frac. Dispersed	f_{disp} from experimental results	3.2.2
Debris Particles		
Mass median d	1.0 mm	3.2.2
Size distribution	Log-normal, geom. std. dev. σ_g = 4, 5 size groups	3.2.2
Composition	Bulk composition all fields	3.2.2
Debris Transport		
Slip, s_d	5 in cavity and chute, 1 elsewhere	3.2.3
Trapping		
Model	None in cavity & chute, TOF/KU elsewhere	3.2.4
L_1	Experimental geometry ($6V_{cell}/S_{str}$ if ambiguous)	3.2.4
L_2	$6V_{cell}/S_{str}$	3.2.4
L_3, L_{gft}	$L_3 = L_{gft}$ = cell height	3.2.4

In Section 3.3, the discussion is extended to other code models important to DCH and whose use may differ from that of other problems; the "standard prescription" for these models given in this report applies only to DCH problems.

There are two important limitations to the status of the standard prescription as it currently stands. The first is that no general prescription can be given for the question of how to nodalize an arbitrary containment volume. Sensitivity to nodalization of the Zion and Surry-geometry experiments is considered in Section 6 and some suggested guidance is given in Section 7, but nodalization will always require judgment upon the part of the user (especially for containments not previously studied). Nodalizations used in this work are briefly summarized in Section 3.4, with additional details given in Appendix A.

The second important limitation to the standard prescription is that assessment of the new models for ejection of melt from the RPV, entrainment from the cavity, and debris particle size has been too limited to support a specific recommendation. The input parameters used in obtaining the results described in Section 5 are given there, however.

In the following discussions of the DCH-related models in CONTAIN, the standard prescription for their use is given as it was applied in the experimental analyses described in this report. Modifications appropriate for NPP analysis, and modifications reflecting lessons learned in the course of the current study, are deferred to Section 7 on user guidance, with at most brief cross-references in this section. The same organizing principle applies to the arguments given for the choice of the standard prescription.

3.2.2 Debris Sources, Particle Sizes, and Particle Compositions.2.2 Debris Sources, Particle Sizes, and Particle Compositions.2.2 Debris Sources, Particle Sizes, and Particle Compositions

In the past, debris sources always had to be introduced into a CONTAIN DCH problem via user-specified source tables. The associated input also specified how debris sourced into the problem was to be distributed among the debris fields, for which the particle sizes were also user-specified. Recently, models for debris ejection from the vessel, entrainment within the cavity, and particle size have been incorporated into CONTAIN. There is at present limited experience in using these models, and it is thought that the phenomena which they represent are especially complex and uncertain [Boy95]. These new models and some limited results obtained with them are summarized in Section 5.

For the purposes of this study, it was considered undesirable to permit assessment of the remainder of the DCH model to be heavily perturbed by the uncertainties in the new models, and they were not used in the majority of the work to be described here. User-defined sources, particle sizes, and compositions based upon experimental results were employed as described later in this subsection. This approach minimizes the effect of uncertainties in processes related to debris ejection from the vessel and entrainment in the cavity upon the assessment. Obviously, it also means that the new models for these processes are not being assessed in the calculations employing user-specified sources.

When user-specified sources are employed, time-dependent source tables are defined for each constituent in the debris. Each source table specifies the input rate and the temperature (or specific enthalpy) of the constituent as a function of time. The user also specifies the number of fields to be used to represent the airborne debris, the particle size for each field, and how the various constituents are to be apportioned among the fields as they are introduced from the source tables.

Standard Prescription for Blowdown, Sources, and Particle Size. In the CONTAIN analyses of the ANL and SNL IET experiments, care was taken to match the experimentally observed blowdown rates, debris dispersal rates, and the degree of temporal coherence between debris dispersal and blowdown. Coherence is potentially important because only blowdown steam entering the cavity during the debris dispersal interval (called "coherent steam") has an opportunity to interact efficiently with airborne debris, and therefore very rapid dispersal can mitigate DCH. Pilch and Theofanous [Pil94a] have examined the potential significance of this effect in detail. Early CONTAIN calculations [Wil88] also illustrated the effect, although the sensitivity to coherence found in those calculations was not large. Although most DCH models, including CONTAIN, predict that there should be some sensitivity of DCH loads to coherence, no experimental proof of this dependence is available.

A useful measure of coherence is the coherent steam fraction f_{coh}, defined as the fraction of the total blowdown steam that leaves the accumulator during the period that debris is being dispersed from the cavity. If we assume the steam remaining in the accumulator expands isentropically as the accumulator depressurizes, f_{coh} is given by

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

2 (3.2-1)

where P_0 is the initial pressure in the accumulator, P_e is the accumulator pressure at the end of the debris entrainment and dispersal interval, and γ is the ratio of specific heats for steam, taken here to be 1.33.

In the experimental analyses, the accumulator and the melt generator were modeled as two cells filled with steam such that the steam mass and pressure would correspond to the specified initial conditions. An orifice with a time-dependent area between the melt generator cell and the cavity cell was then defined and adjusted until the depressurization curve calculated for the accumulator provided a good match to the experimental curve; see Figure 3.2-1 for two typical examples (SNL/IET-3 and SNL/IET-6).

Figure 3.2-1. Comparison between the experimental blowdown curves and the calculated

Debris sources were then derived from the experimental cavity pressurization histories as follows. Debris source tables were defined to introduce the debris into the trapped field in the cavity, prior to the onset of the blowdown. A second set of source tables was then defined to transfer the debris from the trapped field to the airborne debris fields in the cavity. This transfer to the airborne debris fields represents entrainment of the debris by the blowdown steam.

The time dependence of the debris transfer to the airborne debris fields was derived from the experimental cavity pressurization histories. Experimental results show that there is always a period during which the cavity pressurizes with respect to the main containment volume, and pyrometers focussed on the cavity exit provide qualitative confirmation that it is principally during this time interval that debris is ejected from the cavity. The relevant pressure curves are presented for SNL/IET-3 and SNL/IET-6 [All94b] in Figure 3.2-2. The pressurization of interest is the broad peak on the interval 0.5-1.0 s; the earlier irregular peaks are believed to be due to fuel-coolant interactions (FCIs) and are not taken into account in defining the debris sources. Dispersal rates were assumed to be proportional to the net pressurization of the cavity, and the time-dependent sources were normalized to give the experimentally observed amount of debris dispersed from the cavity.

This method of defining sources probably gives a slightly greater degree of debris-steam coherence in the cavity than is strictly correct. The reason is that, in the calculation, the debris enters the cavity at a rate proportional to the experimental cavity pressurization curve, while in reality the pressurization curve probably reflects the amount airborne in the cavity and the exit chute more nearly than it reflects the instantaneous entrainment rate. Thus, the actual pressurization curve may lag the entrainment rate by an amount approximately equal to the airborne residence time of the debris in the cavity. In the CONTAIN simulations, this residence time is on the order of 0.1 s or less, which is short in comparison with the total entrainment time (~0.5 s) and any error in the debris-steam coherence introduced is therefore small.

In the calculation, all melt not dispersed was assumed to remain in the trapped field. In the experiments, some melt (5-10%) actually froze in the melt generator and remained behind in all the Zion-geometry IET experiments other than SNL/IET-8A, and this melt is also included in the trapped field of the cavity cell. Including this melt matters only when the interactions of the nonairborne debris are being modeled. The rationale for including it is the belief that thermal interaction with the steam is one reason why this melt solidified before it could be ejected from the melt generator. If this assumption is correct, significant chemical interaction is also likely to have occurred [Wil92]. These interactions are included in those represented by the nonairborne debris model when it is used.

It might be argued that melt froze and remained in the melt generator due to heat transfer to the melt generator structure, not the blowdown steam. However, in IET-8A, no steam was present at the time of melt discharge; only a small amount of nitrogen was in the melt generator (see Table 2.1-2). In this experiment only, over 99% of the melt was ejected despite the fact that the absence of high driving pressure would lead one to expect slower melt ejection and, hence, more opportunity for heat transfer to the melt generator. It is therefore believed that steam interactions were largely responsible for melt freezing in the other IET experiments.

Sources for LFP and WC Experimental Analyses. Analysis of these experiments was initiated at an earlier phase of this work, and the detailed procedure defined above was not used in defining the blowdown and the debris sources. First, no attempt was made to tailor the melt generator orifice area to match the experimental blowdown curve; instead, this orifice area was simply set equal to its final size at the start of the calculation. Next, the fraction of the steam which was coherent with the debris dispersal was estimated from the experimental blowdown and cavity pressurization curves analogous to Figures 3.2-1 and 3.2-2. Sources with a simple trapezoidal time dependence were then defined such that, when combined with the calculated blowdown curve, the degree of coherence in the calculation was reasonably close to that inferred for the experiment.

One difficulty with this approach is that it requires identification of a time, t_e, at which debris entrainment from the cavity could be said to end. As is apparent from Figure 3.2-2, the interval of cavity pressurization tails off without an abrupt end, introducing a considerable degree of subjectivity in the definition of t_e. Since the accumulator is depressurizing rapidly at this time (see Figure 3.2-1), the coherent steam estimate is sensitive to t_e. Experience showed that this subjectivity could result in different investigators getting different coherence estimates when the same data were analyzed using this method. Furthermore, comparison with the results obtained using the more detailed method suggests that there may be some tendency for this subjectivity to distort trends when different experiments are analyzed using this method, even by the same investigator.

Identification of these difficulties prompted the development of the more detailed method that was used on all the IET experiments. The more detailed method includes the assumption that debris dispersal rates are proportional to the net cavity pressurization. However, results given in Section 6.3.3 indicate that sensitivity to this assumption is low, and furthermore, the shapes of the cavity pressurization histories obtained in calculations using the sources generated in this way closely match the shapes of the experimental pressurization histories (see Section 6.5.2), indicating that the procedure is at least consistent with the CONTAIN model. The procedure is also reasonably objective and should be capable of yielding similar results when repeated by different investigators. In addition, it should not distort trends when comparing results of different experiments. The LFP and WC analyses have not been repeated using the more detailed approach, however, as it is somewhat tedious to apply.

Particle Size Distributions. In some of the Surtsey experiments with open geometries (e.g., the WC series), most of the debris could be recovered as solidified particles after the experiment and the size distribution determined by sieving. In WC-1, the sieve mass median diameter (mmd) was 1.45 mm and the distribution was approximately lognormal, with a geometric standard deviation, σ_g, of about 4. Size distributions in several other experiments were found to be rather similar despite variations that one might suppose would affect the size distribution. Thus, the sieve mmd was 1.25 mm in WC-2 (wet cavity), 1.45 mm in WC-3 (large melt generator hole size), and 1.1 mm in LFP-8A (Surry cavity geometry instead of Zion). The widths of the size distributions were also similar.

When the pretest analyses for the first SNL/IET experiment were performed, it was thought that the experimental results for the WC-1 experiment were the most nearly relevant. Since the recovered debris particles were more or less irregular in shape and somewhat porous, it was thought that use of the sieve mmd would underestimate actual surface/mass ratios when used in the CONTAIN model, which assumes fully dense spherical particles. Hence, the analyses were performed assuming a particle size of 1 mm.* (Only a single-field model was available at that time and a size distribution could not be specified.)

For experiments performed in compartmentalized geometries, including all the IET experiments, meaningful particle size distributions can only be obtained for the relatively small fraction (typically ~10%) of the debris which is transported beyond the subcompartments. Debris de-entrained within the subcompartments evidently coalesces while liquid, because it is recovered as a solidified slag which yields no meaningful particle size distribution. Size distributions of the debris recovered outside the subcompartments show mmd values averaging somewhat smaller (~0.5 mm is typical) than noted above, with wide size distributions and with considerable variability among the experiments. However, there is little reason to suppose these distributions are representative of those existing in the cavity or the subcompartments, where most of the interactions with steam occur; one would expect the debris carried beyond the subcompartments to be weighted in favor of the smaller particle sizes.

Experimental results, then, have provided little basis for varying the particle size as a function of the parameters of the experiment. Hence the standard prescription remains specification of a lognormal size distribution with mmd = 1 mm, $\sigma_g = 4$. Sensitivity studies performed for the SNL/IET-1 posttest analysis* indicated that five logarithmically spaced particle sizes, with equal amounts of debris assigned to each field, were adequate to represent the distribution. However, in analyzing the smaller-scale ANL/IET experiments, ten particle sizes were used, based on arguments that the smaller-scale experiments might be more sensitive to the degree of resolution in the size distribution representation. (Using an unnecessarily large number of debris fields does no harm except to increase computer execution times.)

Particle Compositions. Since core debris oxide constituents and metallic constituents are not fully miscible, and the same is true of thermite melts, it might be supposed that metals and oxides would be segregated on the scale of individual drops, which would then tend to be either metal-rich or oxide-rich but would not tend to have the mean bulk composition of the entire melt. This assumption was invoked in early DCH analyses [Wil87, Wil88]. In the current multifield debris model, segregation can be represented by explicitly assigning the metallic constituents and the oxidic constituents in the debris sources to separate fields. The issue is potentially important because, in the chemistry model (Section 3.2.6), only the surface

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* *D. C. Williams, "Pretest Calculations for the First Integral Effects Experiment (IET-1) at the Surtsey and CWTI DCH Experimental Facilities," Sandia National Laboratories, Letter Report to the U.S. NRC, August 23, 1991.

* *D. C. Williams, "Posttest Calculations for the First Integral Effects Experiment (IET-1) at the Surtsey DCH Facility," Sandia National Laboratories, Letter Report to the U.S.NRC, January 22, 1992.

area of drops containing metals is included in calculating the mass transfer rates assumed to control reaction rates. Hence, if metals and oxides are segregated into separate drops, reaction rates will be less than if each drop is treated as having the mean bulk composition of the melt.

In Reference Wil92, analyses are described that use general heat/mass transfer analogy arguments to correlate experimental ΔP results with hydrogen production for the LFP and WC experiments. A high degree of correlation ($R^2 > 0.98$) was obtained without using CONTAIN or other detailed modeling assumptions, but the analysis did require the assumption that the surface area for heat transfer was equal to that available for chemical reaction. Hence, this result is believed to support the well-mixed assumption. The rationale for this assumption is that the turbulence of the DCH event keeps the debris well mixed. In addition, once the multifield model became available (during the SNL/IET-1 posttest analyses), sensitivity studies were performed which suggested that the segregated-drop assumption tended to underestimate hydrogen production somewhat in calculations that were otherwise satisfactory, and better results were obtained if it was assumed that each drop had the average bulk composition (well-mixed assumption).

Hence the current standard prescription specifies that each field is assigned the same composition, equal to the bulk composition of the entire debris mass. The source composition is independent of time. Note that this uniformity applies only to the assignment of fresh debris as it enters the problem. Since the small size fields interact chemically and thermally much more rapidly than do the larger fields, the compositions (and temperatures) of the fields often diverge rapidly as the calculation proceeds.

RPV Insulation. In many NPP, there is an annular gap between the RPV and the biological shield wall that provides a path for debris dispersed from the cavity to enter the dome volume, without first being transported through the subcompartments. The vessel exterior is typically fitted with a high-temperature insulation that consists of thin sheets and foils of stainless steel. The RPV gap and insulation were modeled in only one experiment, SNL/IET-11. Prior to the experiment, it had been thought possible that displaced insulation might block the gap, thereby preventing debris from being transported directly from the cavity to the dome via this gap. However, the insulation was almost totally removed, opening the gap, with no tendency to block it; therefore, blockage of the gap by the insulation is not considered to be a likely outcome. In addition, the ablated insulation may have contributed to hydrogen production in this experiment [Bla94].

Debris recovered from the dome regions indicated that the insulation had been largely stripped by ablation, with melting, rather than simply removed by mechanical fragmentation. In the CONTAIN calculations, therefore, the iron and chromium content of the insulation was added to the debris sources; the nickel content was not modeled. Half of the insulation was added to the airborne debris in the cavity and half was added in the dome. The rationale is that insulation ablated from the vessel bottom should mix with the other debris in the cavity, while insulation ablated from the sides of the vessel within the gap would mix with debris that is already committed to entering the dome via the gap, and it would not have a chance to return to the cavity. The insulation was assumed to be homogenized with the debris and to have the same size distribution. Sources representing the insulation had the same time dependence as sources representing the debris. The sources representing the ablated insulation were introduced at the initial containment temperature (399 K), and the insulation therefore contributed no thermal energy. It could, however, contribute chemical energy and hydrogen production.

Application to NPP Calculations and Other Analyses. The procedure used here to define time-dependent debris sources is not applicable to NPP analyses, or analysis of any other scenarios for which experimental results are not available. Whether the new RPV and cavity entrainment models or user-specified inputs are employed, the goal should be to ensure that the fractions dispersed from the cavity and the debris-steam coherence are reasonable, based upon the experimental results available. Section 7.3 provides guidance for using the experimental results and a semi-empirical coherence correlation [Pil94a] for achieving these goals. Fortunately, sensitivity of the calculated DCH loads to uncertainties in these parameters is not large in the cases that have been examined (see Sections 6.3.2 and 6.3.3).

For particle size distributions, the potentially relevant properties (densities and surface tensions) of core debris and thermite do not differ greatly, and the understanding of the processes governing particle size is not sufficiently great to justify attempting to take into account the differences that do exist. Hence the standard prescription defined here for particle sizes and compositions is defined to apply generally. To recapitulate, the standard prescription consists of specifying five particle sizes, lognormally distributed, with mmd = 1 mm, $\sigma_g = 4$, and with the core debris constituents being distributed uniformly among the fields. In analyzing experiments smaller than 1/10-scale, the standard prescription specifies ten particle sizes.

3.2.3 Intercell Transport of Debris.2.3 Intercell Transport of Debris.2.3 Intercell Transport of Debris

In the CONTAIN DCH model, the movement of the airborne debris fields is governed by the flow of gases between the cells. In the past, debris-gas slip was not included, which meant that the fraction of airborne debris transported from an upstream cell to a downstream cell in a timestep was the same as the gas fraction transported. Airborne debris mass was included in the gas density in solving the flow equations, and the model was sometimes referred to as the "heavy gas" model.

Recently, a simple representation of debris-gas slip, analogous to models for two-phase water systems [ElW62], has been incorporated into the model. The user must specify the slip factor, s_d, for each cell (unless it is to be unity, which is the default). There is no internal model for calculating s_d. The slip factor definition is the conventional one, $s_d = v_g/v_d$, where v_g and v_d are, respectively, the gas velocity and the debris velocity in the flow path. A limitation of the current model is that the same slip factors apply to all paths leading out of a given cell. The slip factor can, however, be specified separately for each debris field. The flow equations are solved using a self-consistent formalism that conserves mass and momentum flux properly, but the treatment does not model all the potential implications of debris-gas slip.

The transport of debris through complicated containment geometries is an extremely complex problem, and the CONTAIN model is obviously highly simplified. The user would do well to keep this simplification in mind. One symptom of the oversimplification is that analyses to date have not been able to reproduce both the extent of cavity pressurization and the experimentally measured debris velocities exiting the cavity. If low values (s_d close to unity) are used, cavity pressurization is approximately correct but debris dispersal velocities are considerably higher than the experimental values. Increasing s_d decreases the debris velocities but also decreases the extent of cavity pressurization.

A fundamental limitation of the model is that debris transport is always assumed to be governed by the gas flow and, hence, is always in the same direction as the gas flow, even if s_d values different from unity are specified. In reality, debris particle trajectories may decouple from the gas flow; that is, debris motion may be governed by the momentum inherited from driving forces acting upon the debris upstream of the current cell, more than it is governed by the gas flow patterns within the current cell. In such instances, neither the direction nor the velocity of debris transport will be controlled by the gas flow. One example of this problem is that momentum-governed debris transport through the seal table room to the dome is known to occur in both the Zion and Surry experimental geometries, and CONTAIN does not model this process. It may also arise more generally in calculating transport through the subcompartments when flow velocities within the subcompartments are not very large. In these instances, it is possible that momentum inherited from the ejection of the debris from the cavity will dominate forces exerted by the gas flow through the subcompartments.

Cross-sectional areas available for flow through the subcompartments are sufficiently large that, in all the experiments performed to date, this "low velocity" situation probably applies to transport within the subcompartments to at least some degree, even aside from the seal table room path. Given higher driving pressures and larger vessel failure sizes than those studied experimentally, flow rates through the subcompartments might become sufficiently high to re-establish better coupling between debris transport and gas flow. There is no experimental confirmation of this supposition, however.

Standard Prescription. For the cavity and the chute connecting the cavity to the subcompartments (if the chute is modeled as a separate cell), $s_d = 5$ is specified. The justification for this value is based largely upon estimates of slip factors from experimental measurements of debris velocities plus the belief that $s_d = 1$ results in cavity airborne residence times that are too short. The latter would risk underpredicting debris-steam interactions in the cavity, which would tend to be nonconservative. The value of $s_d = 5$ is also in order-of-magnitude agreement with slip measurements in two-phase flow experiments involving water [ElW62]. Sensitivity studies performed for the IET experiments (Section 6.1.3) indicated that containment pressurization, hydrogen production, and debris transport to the dome were all insensitive to the value of s_d specified for the cavity and chute. Cavity pressurization, however, was more sensitive to the value of s_d and values greater than unity underpredicted the extent of cavity pressurization.

In the subcompartments (and also the dome) $s_d = 1$ is specified. Because of the way slip interacts with the trapping model, larger values will tend to reduce transport beyond the subcompartments in the standard prescription; also, larger values can result in debris velocities within the subcompartments that are believed to be excessively small when gas velocities within the subcompartments are only moderate. Sensitivity studies performed for all experiments analyzed in this work include one case run with $s_d = 5$ in the cell(s) representing the subcompartments. Results presented in Section 4 tend to support the choice of $s_d = 1$ in the subcompartments as the standard prescription.

3.2.4 Trapping.2.4 Trapping.2.4 Trapping

Trapping can be an important mitigating effect in CONTAIN calculations of DCH events. If debris de-entrainment rates within a cell exceed rates for debris-gas thermal and chemical interactions, the extent of the latter may be substantially reduced. If trapping rates exceed rates of debris transport through the cell, transport of debris to cells further downstream will be limited. The latter effect is one of the ways that compartmentalization can mitigate DCH.

It should be noted, however, that sensitivity studies in which trapping was artificially switched off have shown that trapping is far from the only factor governing the degree of mitigation resulting from compartmentalization. Atmosphere-structure heat transfer is also very important; see Section 6.7 and References Wil87 and Wil88.

In CONTAIN, debris is removed from the airborne debris fields according to a simple first-order rate equation:

$$\dot{m}_d = - \lambda \; m_d \; , \qquad (3.2\text{-}2)$$

where m_d is the mass of airborne debris in any field and any cell, λ is the fractional trapping rate (s^{-1}), and $_d$ is the time rate of change of m_d due to trapping. Eq. (3.2-2) is applied separately to each debris field and in each cell. Debris removed from any airborne field within a cell is deposited in the trapped field for that cell.

In early versions of the DCH model, the user was required to specify λ, and this option is still available. However, the code now includes internal models for calculating λ. Two of these models have been used in the present work: the gravitation fall time (GFT) and the time-of-flight/Kutateladze number (TOF/KU) model. In the GFT model, λ is equal to v_{gft}/L_{gft} where v_{gft} is the gravitational terminal fall velocity of a particle in the field and is calculated by the code, and L_{gft} is a characteristic length for the cell geometry.

The TOF/KU model is considerably more complex and the code documentation should be consulted for details [Was95]. Briefly, the model attempts to determine, for each field, whether a particle will be de-entrained on either the first or the second impact with structures in the cell, and what the time of flight is between the time the particle enters a cell and the time it is de-entrained on a structure. This time of flight is taken to be the airborne residence time for calculating debris-gas chemical and thermal interactions, and the trapping rate, λ, is set equal to the reciprocal of the residence time. The criterion for de-entrainment is based upon a Kutateladze number (Ku) criterion. De-entrainment upon the jth impact (j = 1 or 2) is assumed to occur if the following relationship is satisfied:

$$Ku_j = \frac{\rho_{g,j} \, v_{g,j}^2 \; + \; \delta_{mix} \, \rho_{vol,d,j} \, v_{d,j}^2}{\sqrt{g \, \rho_{mat,d} \, \sigma}} \; le \; Ku_{T,j} \; . \qquad (3.2\text{-}3)$$

In Eq. (3.2-3), δ_{mix} is either 0 or 1, depending upon which of two modeling options discussed below has been selected. The volumetric density ($\rho_{vol,d}$) is defined as the mass of debris per unit volume of debris-gas mixture while $\rho_{mat,d}$ is the density of the actual debris material itself; g is the acceleration of gravity and σ is the surface tension. Ku_T is the critical or threshold value such that de-entrainment will not occur if Ku is greater than Ku_T. [Some investigators have defined Ku to be the square root of the quantity defined by Eq. (3.2-3).] The default values of Ku_T are equal to ten, although the user may specify either or both of these quantities.

The rationale for the use of Ku to determine whether de-entrainment occurs is that it represents a measure of the competition between the momentum forces (momentum flux) at the surface, which tend to prevent debris from sticking to the surface, versus forces of gravity and/or surface tension, which tend to make debris adhere to the surface. In CONTAIN, if the option "rhodg = gas" is specified in the input, $\delta_{mix} = 0$ is used and only the momentum flux of the gas is used in evaluating Ku. If the input option "rhodg = mix" is specified, $\delta_{mix} = 1$ is assumed and the momentum flux corresponding to the entrained debris is also credited in evaluating Ku. The latter choice is the more conservative option, since it tends to reduce trapping.

Velocities at the first structure impacted are based upon the entering flow velocities while velocities at the second structure impacted are based upon gas convection velocities calculated for the second structure as defined in the structure definition input block; see Section 3.3.3 for additional information on use of this input in a DCH calculation. Slip factors specified for the upstream cell can affect the velocity of the debris at the first structure impact, while slip factors specified for the current cell can affect the velocity of the debris at the second impact. In addition to the velocities at impact used to evaluate Ku, mean debris velocities are also evaluated in order to estimate airborne residence times. The latter velocities are assumed to be at least as large as v_{gft}, in order to avoid unrealistically long residence times when flow velocities are small. There are a number of other complications involved in estimating the various velocities; details may be found in the model documentation [Was95].

In addition to the velocities, calculation of the airborne residence time also requires specification of travel distances from the point of entry in the cell to the location of the first impact point (L_1), and the distance from the location of the first impact to that of the second impact (L_2). These values depend upon the cell geometry and the user therefore must provide them through the code input; the standard prescription for these values is discussed below.

Another input model option involves a velocity which the code uses to calculate residence time in the event that de-entrainment does not occur on either the first or the second structure. If the user specifies "vnost = cnvel," the estimated residence time following the second impact will be a length L_3 divided by the debris transport velocity through the cell (or v_{gft} if it is greater); here, L_3 is a characteristic length determined by cell geometry (typically the cell height in the standard prescription). If "vnost = vgft" is specified, the velocity used is v_{gft}, independently of flow conditions. It can be shown that, as flow velocities through the cell increase without limit, the fraction of debris trapped in the cell will converge to some nonzero value if the first option is used, while the second option will allow the trapped fraction to approach zero in this limit. The latter option is more conservative and may be qualitatively more realistic, since one would expect de-entrainment within a cell to become very small in the limit of very large flow velocities.

Since there are many approximations and uncertainties in the trapping model, sensitivity studies are always recommended. It will often happen that results of interest will seem rather insensitive to many of the trapping assumptions and parameters, yet substantial sensitivity may arise in some other problem. There are enough nonlinearities in the trapping model that it is difficult to offer general rules as to when results are likely to be sensitive to trapping uncertainties.

Standard Input Prescription for Trapping. In the standard input prescription, zero trapping rates are specified for the cavity cell (and chute cell when one is modeled). The reason is that dispersal fractions are set to match experimentally determined values and these fractions already take into account any trapping in the cavity and/or chute (that is, debris trapped in the cavity is counted as "not dispersed"). The same is true of the experimental data base used to develop the entrainment rate and dispersal fraction correlations employed by the CONTAIN cavity entrainment models. Hence, this prescription applies even in the results of Section 5, for which the cavity models were used.

In the subcompartment and dome cells, the standard prescription employs the TOF/KU model in all instances. However, in the dome, sensitivity studies using the GFT model are recommended. TOF/KU may overestimate trapping on the first impact with a structure when flight paths are long, which could be nonconservative in some instances.

For the TOF/KU model, the standard input prescription is as follows:

" The more conservative "rhodg = mix" and "vnost = gft" options are used.

" If the dominant path for entry of debris into a cell can be identified, and the actual distance along the debris trajectory to the first structure can be estimated from the cell geometry, this distance should be equated to L_1 in the TOF/KU input. Otherwise, $L_1 = 6V/S_{str}$ is used, where V is the cell volume and S_{str} is the total surface area of all structures defined within the cell.

" For the distance to the second structure, $L_2 = 6V/S_{str}$ is specified in the standard prescription.

" $L_3 = L_{gft}$ in the standard prescription (this is the default; L_3 need not be specified)

" L_{gft} is the actual cell height determined by the cell geometry. If this cannot be determined for some reason, $6V/S_{str}$ may be used.

The quantity $6V/S_{str}$ is used as a generic mean free path for debris when a distance based upon actual cell geometries and debris trajectories cannot be defined. This quantity is equal to the dimension for a cubic cell with no internal structure and no openings in the walls, and provides a first-order representation of reductions due to internal structure and of increases when openings into or out of the cell represent a significant fraction of the cell boundary. Definition of more specific values of the trapping lengths generally requires identification of a preferred direction for debris trajectories and a length in that direction. For L_1, the entrance path may define the preferred direction, and gravity is assumed to define the preferred direction for L_{gft}. Following the first impact, "splattering" is assumed to result in considerable randomization of debris trajectories, and the generic length $6V/S_{str}$ is therefore prescribed for L_2 unless there is a definite reason based upon the specific geometry for doing otherwise.

All other trapping input is left at default values in the standard prescription, including the critical values of Ku that govern de-entrainment, $Ku_{T,1}$ and $Ku_{T,2}$.

3.2.5 DCH Heat Transfer.2.5 DCH Heat Transfer.2.5 DCH Heat Transfer

Heat transfer from debris to gas associated with conduction/convection is calculated using a Nusselt number based upon the Reynolds analogy [Bir60]:

$$h = \frac{k_g}{d}\left(2.0 \ + \ 0.6 \ \sqrt{Re_g} \ \ Pr_g^{1/3}\right),$$

5 (3.2-4)

where h is the heat transfer coefficient, k_g is the thermal conductivity of the gas, d is the diameter of the debris particle, Re_g is the Reynolds number based upon the particle diameter and the debris-gas relative velocity, and Pr_g is the gas Prandtl number. Gas properties are evaluated at the film temperature equal to the mean of the gas and the debris temperatures [Bir60] and the debris-gas relative velocity is evaluated from information developed in the flow and the trapping models; see the code documentation for the details of the latter.

Debris-gas heat transfer due to thermal radiation is modeled using a gray-body model:

$$\dot{Q}_{rad} = \varepsilon_{d-g} \, \sigma \, A_d \, (T_d^4 \ - \ T_g^4),$$

6 (3.2-5)

where $_{rad}$ is the rate of heat transfer by radiation, ε_{d-g} is the effective emissivity for debris-atmosphere radiation, σ is the Stefan-Boltzmann constant, A_d is the debris surface area, and T_d and T_g are, respectively, the debris and gas temperatures. There is also a model for direct radiation from debris to structures analogous to Eq. (3.2-5) except that A_d includes a correction for self-shielding and ε_{d-g} is replaced by ε_{d-s}, a black-body multiplier for debris-structure radiation.

Standard Prescription for DCH Heat Transfer. The standard prescription specifies $\varepsilon_{d-g} = 0.8$ and $\varepsilon_{d-s} = 0$. The rationale for these values is that, experimentally, dense aerosol clouds accompanying debris dispersal from the cavity appear to result in very short optical paths within the atmosphere during DCH [All94b], rendering debris-atmosphere radiant transfer quite effective while debris-structure radiation is rendered ineffective. All other DCH heat transfer input is left at default values in the standard prescription (see, however, Section 3.3 for the treatment of atmosphere-structure radiation in DCH calculations).

3.2.6 DCH Chemistry.2.6 DCH Chemistry.2.6 DCH Chemistry

The DCH chemistry model includes metal-oxygen reactions, metal-steam reactions, and the hydrogen recombination model. Four reactive metals are recognized: Zr, Al, Cr, and Fe. A reaction hierarchy is imposed with the order being that given. All reactions are assumed to proceed to completion except that the iron-steam chemical equilibrium is modeled. For all practical purposes, steam and oxygen react in parallel at rates controlled by mass transport through the gas phase to the surface of the reacting debris particle (gas-side limit). There is also a diffusion-based model for reaction rate limits associated with mass transport within the debris particle (drop-side limit).

For both oxygen and steam, the gas-side mass transfer rate is based upon a Sherwood number, Sh, given by applying the heat/mass transfer analogy to the Nusselt correlation assumed in Eq. (3.2-4):

$$Sh = 2.0 + 0.6 \sqrt{Re_g}\ Sc_x^{1/3} ,$$

7 (3.2-6)

where Sc_x is the Schmidt number for oxidant x (x = oxygen or steam). Additional details are given in the code documentation.

If metal-steam reactions occur in a cell which still contains oxygen in the atmosphere, the hydrogen produced is normally assumed to immediately recombine with oxygen. Hence, the net effect is energetically equivalent to all the metal reaction occurring directly with the oxygen except that the hydrogen recombination energy is deposited in the gas, not the debris. If desired, the user can turn off this hydrogen recombination model in the code input.

<u>Standard Prescription</u>. The most important nondefault specification in the present analyses is that the drop-side reaction rate limit is not imposed (infinite drop diffusivity assumed). The default treatment assumes a drop-side limit based upon a diffusivity within the drop of 10^{-8} m^2/s. However, it now appears that this assumption can result in serious underprediction of reaction rates and this default treatment is not recommended. The rationale for specifying no drop-side limit in the standard prescription is essentially the same as that for specifying well-mixed debris in the definition of debris sources in Section 3.2.2. In particular, the analyses based upon the heat/mass-transfer analogy described in Reference Wil92 involve the assumption that drop-side reaction rates are not limiting, and the success of this analysis supports the belief that significant drop-side limits should not be modeled. In addition, Appendix D includes calculations for the SNL/IET-1R and SNL/IET-3 experiments in which the drop-side limit was imposed. For both experiments, hydrogen production was underpredicted by more than a factor of two. For SNL/IET-3, in which hydrogen combustion is a major contributor to containment pressurization, ΔP was underpredicted by 35% when the default drop-side limit was imposed. Note that the assumption of no drop-side limit is also the conservative choice, and sensitivity studies are not needed unless it is desired to try to defend a less conservative modeling option.

The threshold for chemical reaction was specified to be 1200 K, which had little effect because temperatures were well above this value at any time and location for which reaction might be important. Caution is needed in using this value for scenarios involving substantial water, in which lower temperatures might cause premature quenching. The default value, 273.15 K, is obviously safe and is now recommended; see Section 3.2.8.

In analyses of experiments with inert atmospheres (O_2 mole fractions always $\leq 0.2\%$), the hydrogen recombination option was switched off. Otherwise, hydrogen produced by metal-steam reaction would scavenge the trace of oxygen very efficiently, a result considered unrealistic when the oxygen is extremely dilute. In analyses with anything approaching realistic oxygen concentrations, the hydrogen recombination model should be left on, which is the default.

3.2.7 Nonairborne Debris.2.7 Nonairborne Debris.2.7 Nonairborne Debris

In the past, most DCH analyses have emphasized the interactions of airborne debris with coherent blowdown steam; i.e., that portion of the blowdown which is discharged during the time interval that debris is being dispersed from the cavity. However, Reference All91a presented evidence that considerable hydrogen could be generated even by debris that was not dispersed from the cavity. In addition, Reference Wil92 presented evidence that the total hydrogen production in the SNL/LFP and SNL/WC experiments was larger than could be accounted for by the coherent steam alone, and it was argued that debris not dispersed from the cavity also contributed by interacting with the later, noncoherent part of the blowdown. (Many of the results to be presented in Sections 4, 5, and 6 of this report reinforce the belief that DCH events are not always controlled by the airborne debris/coherent steam interactions alone, especially in the Zion geometry.)

These observations motivated the installation of the so-called "nonairborne debris" (NAD) model in CONTAIN. The term "nonairborne debris" may be fully accurate only in the context of the CONTAIN model, in that it is based upon allowing debris in the trapped field to interact with the cell atmosphere using almost the same modeling as is used for the airborne debris fields. Appendix B presents analyses indicating that interactions of steam with debris films on structural surfaces are significant, and the nonairborne model is intended to represent the effects of these interactions. However, other processes may be involved also and the "nonairborne debris" model serves as a surrogate for any debris interactions contributing to DCH other than those represented by the interactions of the airborne debris fields. Among other things, the nonairborne model provides the only means by which substantial interactions between debris and the noncoherent blowdown steam can occur in CONTAIN, because trapping in the subcompartments is usually calculated to remove airborne debris too rapidly to permit significant interaction with blowdown steam to continue once debris dispersal from the cavity is complete.

As an example, splashing, re-entrainment, and dripping of molten debris from the surfaces upon which it is initially deposited may prolong interactions in the subcompartments, and the nonairborne debris model is the only means by which such prolongation could be represented. Visual evidence of molten debris dripping from the Surtsey dome was obtained in early DCH experiments and this dripping may have contributed to containment pressurization [Tar88], although this interpretation has been questioned [All91b]. If any such effects do prolong the de-entrainment process, the "nonairborne" model is the only means that CONTAIN has of representing this contribution. For this type of process, the term "nonairborne" could be a misnomer. A considerable range of processes may be involved.

CONTAIN Modeling of Nonairborne Debris. By default, CONTAIN models no interactions of debris in the trapped field. However, if the user specifies a nonzero value for the parameter "diatrap" in any cell, an effective particle diameter, d_t, equal to the specified value is assigned to the trapped debris in that cell. Time-dependent values of d_t may be specified. Debris-gas thermal and chemical interactions are then modeled for the trapped debris using Eqs. (3.2-4)-(3.2-6), essentially as for the airborne debris fields. The gas velocity used in evaluating the Reynolds number is the flow velocity through the cell as calculated for the second structure in the cell (see Section 3.3). Since the trapped field is still being modeled as spherical particles, the surface area is inversely proportional to d_t; hence, total interaction rates vary approximately as $d_t^{-3/2}$. By default,* radiant energy transfer from the nonairborne debris to the gas is modeled with the same value of ε_{d-g} as is used for the airborne debris. Nonairborne debris cannot be transported from one cell to another.

An important limitation of the nonairborne model is that there is no modeling of heat transfer from the nonairborne debris to structures. Insofar as one is actually dealing with debris residing as films on structures, rapid heat transfer to the structure may occur. Neglect of this cooling may permit an excessive amount of interaction to occur late in the problem relative to what occurs earlier; see Appendix B for additional discussion.

Scaling. Since the CONTAIN model for nonairborne debris is computed using an effective particle size, it does not scale properly if the actual interaction is with films on surfaces unless one varies d_t as a function of scale in order to compensate. In Appendix B, a scaling rationale based upon debris films on surfaces is outlined. It is based upon the assumption that, for such surfaces, Nu and Sh vary as Re_g^m, and that the characteristic length L of the structures is proportional to scale. The result is

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* *Reference Was95 erroneously states that the default is to neglect the debris-atmosphere radiation.

$$d_t(S) = d_t(S_e)\left(\frac{S}{S_e}\right)^{\frac{2(2-m)}{3}} = d_t(S_e)\left(\frac{S}{S_e}\right)^{0.8} \text{ for m = 0.8,}$$

8 (3.2-7)

where $d_t(S)$ is the appropriate value for a problem of scale S, $d_t(S_e)$ is a value found to be appropriate for a scaled experiment with scale factor S_e, and the value of m = 0.8 corresponds to the Nusselt and Sherwood number correlations used by CONTAIN to calculate heat and mass transfer resulting from forced flow across structure surfaces [Mur89, Was91]. With m = 0.8, Eq. (3.2-7) yields a nonairborne interaction that declines slightly in efficiency with increasing scale, while m = 1 would yield a scale-independent interaction efficiency.

With so much uncertainty concerning the actual configuration of the interactions being represented by the nonairborne model, Eq. (3.2-7) must be used with considerable caution. The arguments given in Appendix B neglect many potentially important effects and it is possible that Eq. (3.2-7) (with m = 0.8) can yield nonconservative results when extrapolated to NPP scale. Note, for example, that the analysis based upon films may be quite inappropriate if the actual process is governed by dripping from surfaces upon which de-entrainment initially occurs.

Standard Prescription for Nonairborne Debris. In the standard prescription, the nonairborne model was active in all cells other than those representing the dome; thus, nonairborne debris interactions in the subcompartments were also included. For all experiments analyzed, sensitivity studies were performed without nonairborne debris and with nonairborne debris included in the cavity only.

In both the cavity and the subcompartments, d_t was specified to be 0.01 m for the first 3 s; it then increased linearly to 0.025 m at 4 s and to 1 m at 5 s. The blowdown and DCH processes are almost complete at or before 3 s, and the subsequent increase in d_t was introduced to terminate interactions at times too late to contribute to the processes of interest. If this were not done, chemical reaction would continue to occur as long as steam (or oxygen) were available, which would complicate the interpretation of the CONTAIN calculation of quantities of hydrogen produced and hydrogen burned. Continued interaction at late times would be unrealistic because, in reality, debris-structure heat transfer would be expected to terminate the interactions.

The value of 0.01 m was selected initially because it gave reasonable results in the analysis of the SNL/IET-1 and SNL/IET-3 experiments for both ΔP and hydrogen production. It was then "frozen" for all other 1/10-scale analyses, with no attempt made to tune the value to optimize fit to a wider data base. Subsequently, an independent stand-alone analytical model for d_t that involves no tuning to experimental results was developed, and this model also supports the choice of $d_t \approx 0.01$ m for 1/10-scale experiments. The model is described in Appendix B.

For experiments at other scales, Eq. (3.2-7) with m = 0.8 was used, which gives $d_t = 0.00335$ m for the ANL/IET analyses and 0.0156 m for the CTTF analyses. This specification was also based upon the model described in Appendix B. It was made *a priori*, before any of the ANL/IET or CTTF experiments were analyzed. Inspection of the results yields some limited evidence that it may overpredict interactions in the small-scale ANL/IET experiments (see Sections 4 and 6.8), in which case it might be nonconservative to employ Eq. (3.2-7) with m = 0.8 to extrapolate to NPP scale. A choice of m = 1 is now preferred. Recommendations for use of the NAD model, including recommended sensitivity calculations, are provided in Section 7.8.

3.2.8 Interactions with Co-Dispersed Water.2.8 Interactions with Co-Dispersed Water.2.8 Interactions with Co-Dispersed Water

CONTAIN does not have an FCI model, nor does it have a model for entrainment of water in the cavity and dispersal from the cavity. However, containment pressurization is primarily sensitive to certain integral quantities, not the details of the debris-water interactions. These integral quantities include energy absorbed in vaporizing water, the quantities of steam generated, energy transferred to the steam, and hydrogen generated and burned. In addition, the enhanced steam flow rates resulting from vaporization of water can affect (reduce) the degree of DCH mitigation provided by atmosphere-structure heat transfer and hydrogen hold-up in oxygen-starved subcompartments. The CONTAIN model can be used to simulate these effects of debris-water interactions, albeit with some important limitations acknowledged in the discussion that follows.

In calculations involving co-dispersed cavity water and/or co-ejected RPV water, the normal procedure is to specify an atmospheric source of low-enthalpy steam (i.e., steam with an enthalpy equivalent to that of the liquid water) in the cavity cell such that the timing of this source overlaps the time during which the debris is specified to enter the cavity. The water enters as an atmospheric component, and chemical and thermal interactions with the debris are modeled using the standard CONTAIN DCH heat and mass transfer models. No direct melt contact with liquid water is modeled, and no thermal resistance between liquid water and the heated atmosphere is modeled. Thus, the airborne water is assumed to be in thermodynamic equilibrium with the local atmosphere. On the other hand, since the standard DCH models for debris-atmosphere interaction rates are controlling, the debris is usually not in equilibrium with the atmosphere.

The treatment corresponds to the situation illustrated in Figure 3.2-3, in which debris and liquid water are both present as dispersed drops, with little direct liquid-liquid contact, and the water drops are small compared with the debris particles. In this case, the atmosphere does mediate the heat transfer to the water, and the controlling thermal resistance is the debris-to-gas thermal resistance, which is modeled. The controlling resistances to heat transfer (R_{hx}) and mass transfer (R_{mx}) are diagrammed schematically in Figure 3.2-4. The subscripts 1, 2, and 3 refer to debris-gas, gas-water, and direct debris-water interactions, respectively. Figure 3.2-4a corresponds to the configuration of Figure 3.2-3; here, $R_{hx,1} \gg R_{hx,2}$ and, because there is little direct debris contact with liquid water, $R_{hx,3} \approx \infty$ and $R_{mx,3} \approx \infty$ (represented as "open circuits" in the diagram). Hence the controlling processes are those that are included in the models of the code.

Figure 3.2-3. Dispersed debris and liquid water fields corresponding to the CONTAIN treatment.

(a) schematic corresponding to Figure 3.2-3

(b) schematic for FCI with direct debris-water contact

In an actual FCI involving direct debris-water contact, the schematic in Figure 3.2-4b may apply; in this case, the code may not capture all the important processes controlling the interactions. This situation may well apply when the amount of cavity water is large. It is less likely to apply when amounts of water are small because only small amounts of energy transfer, whatever the process, are required to vaporize all the water; subsequent processes are only those modeled for dry DCH scenarios.

Whether Figure 3.2-4a or 3.2-4b applies, given the amount of debris-water chemical and thermal interaction that occurs, the code does model the subsequent implications of the interaction using the same models as those used for DCH events not involving water. Effects modeled include the enthalpy required to vaporize the water (i.e., debris quenching), the effects of increased steam supply on debris-gas thermal and chemical interactions, effects upon debris transport, and effects upon DCH mitigation processes involving atmosphere-structure heat transfer and hydrogen holdup in the subcompartments.

If energy transferred to the gas is insufficient to vaporize all the water, CONTAIN assumes that the remainder of the water will condense in the atmosphere as water aerosol. Except for a small amount that may deposit on structures, this water aerosol will transport with the gas flow. This water remains available as a potential atmospheric heat sink since the water aerosol can subsequently re-evaporate as DCH energy is added to the containment atmosphere in the calculation. Since aerosols are not included in the mass treated by the flow solver, the effects of "tamping" by the water on cavity pressures are not modeled. This limitation can be important in predicting cavity pressurization, but is not expected to affect containment pressurization substantially.

Co-Dispersed Cavity Water. Not all the water initially in the cavity necessarily interacts with the debris; some may be blown out of the cavity by the initial interaction. The water blown out of the cavity may not interact efficiently with the debris (although debris-water interactions can occur in the subcompartments as well as in the cavity). CONTAIN has no models for calculating the amount of water that is dispersed without interacting. Comparisons between experimental and calculated results suggest that most of the water may have interacted with the debris in the compartmentalized Zion IET geometry, while only a small fraction appeared to interact in the WC-2 experiment, in which the containment geometry was open. Because the CONTAIN code cannot predict how much interaction with water will actually occur, it is perhaps more appropriate to refer to the calculations as evaluating the potential effects of water than to refer to them as actual predictions of these effects.

Given the amount of water in the cavity, the recommended approach is to run one calculation with the total amount sourced into the cavity in parallel with the debris source, and to perform sensitivity studies for smaller amounts of water in order to simulate the possible effects of some water not participating. In this way, an uncertainty range is developed for the effects of the water. The sensitivity studies may not be needed when the amount of water is small, since the usual effect of water on DCH calculations in compartmentalized geometries is to increase loads when amounts are small and decrease loads when amounts are large. (In open containment geometries, increased loads may not be predicted for any amount of water.) For small amounts, assuming all the water participates is usually the limiting case, but this assumption can be nonconservative for large amounts. Here, a "small amount" of water may be defined as an amount less than the amount the debris energy is capable of vaporizing without substantially cooling the debris, and conversely for a large amount.

Co-Ejected Primary System Water. A key difference between primary system water co-ejected with the debris and co-dispersed cavity water is that the temperature of the co-ejected water is likely to be substantially higher than the saturation temperature that corresponds to pressures in the cavity. Hence a significant fraction of the water flashes upon discharge. It seems likely that flashing and other atomization processes will result in the co-ejected water being present as fine drops, with a vapor fraction by volume that is 1-2 orders of magnitude greater than the liquid fraction. Even if ejection itself does not convert the water to a well-dispersed fine spray, dispersal criteria (e.g., Kutateladze numbers) indicate that the water will be dispersed under any conditions for which debris is dispersed, and Weber number arguments indicate that water drop sizes will be considerably less than debris particle sizes. Hence, the situation represented by Figure 3.2-3 and Figure 3.2-4a, rather than Figure 3.2-4b, is thought likely to apply; the co-ejected water scenario may be less likely to be controlled by processes not modeled by the code than are co-dispersed water scenarios involving substantial amounts of water.

Standard Prescription. In the standard prescription results presented in Section 4, no water was included in the IET analyses. In sensitivity studies, water is introduced into the problem in parallel with the debris sources and this may be taken to be the standard prescription for investigating the potential effects of water. This amounts to assuming that the debris and water have complete coherence, which is unrealistic; however, the effects of reduced coherence will be similar to the effects of reducing the amount of participating water in sensitivity studies. Additional user guidance on DCH analyses involving water is offered in Section 7.8.

3.3 DCH-Specific Use of Other CONTAIN Models.3 DCH-Specific Use of Other CONTAIN Models.3 DCH-Specific Use of Other CONTAIN Models

In addition to the DCH models themselves, certain other CONTAIN models are important to DCH calculations and these may be used in ways that differ from their normal use in non-DCH calculations. In this section, the standard (for DCH) prescription for these models will be summarized. The descriptions that follow are brief and leave out many features that are important for the models' use generally; what is given is only intended to be sufficient to define specialized use in the DCH analyses.

3.3.1 Gas Combustion.3.1 Gas Combustion.3.1 Gas Combustion

CONTAIN has three models for gas combustion: the deflagration model, the diffusion-flame burn (DFB) model, and the bulk spontaneous recombination (BSR) model.

Deflagration Model. All parameters in this model were left at default values. The deflagration model played at most a minor role in any of the experimental analyses, although some small deflagrations did occur in some of the calculations. In NPP analysis, default settings are not normally optimum; see Section 7.9 for user guidance on this subject.

DFB Model. In this model, combustible gas in a flow entering a cell is assumed to burn as it enters, provided certain conditions are satisfied. The model calculates the amount of receiving cell atmosphere required to burn the combustible gas entering in a timestep and assumes that this gas instantaneously mixes and reacts with the incoming stream; thus, combustion rates are limited only by the inflow rate. Combustible gas in the receiving cell atmosphere entrained into the flame is also assumed to burn, and the oxygen demand of this combustible gas is taken into account in calculating the amount of receiving cell gas entrained. Any oxygen in the incoming flow is neglected when evaluating the amount of receiving cell gas that must be entrained in order to burn the incoming combustible gas.

In the analysis of those experiments in which the DCH-produced hydrogen could burn, most of this combustion took place in the DFB model as hydrogen-rich gases from an oxygen-starved upstream cell entered receiving cells which still contained oxygen. In the DFB model, combustion occurs only if certain conditions are met. These include an incoming gas temperature greater than 'dftemp,' oxygen and steam concentrations in the receiving cell greater than 'mfocb' and less than 'mfscb,' respectively, and a (diluent gas)/(combustible gas) molar ratio less than 'shratio.' These parameters are specified through the code input.

The particular parameters used in the experimental analyses are summarized in Table 3.2-1. These values were deliberately defined to make combustion almost unconditional. In the subcompartments, it was assumed that high temperatures would favor combustion even for gas compositions that would normally be nonflammable. Hence, the composition parameters were set to quite permissive levels, but 'dftemp' was set to a high value (1000 K) to ensure that combustion of trace gases would not occur when the high-temperature assumption was not in fact valid. In the dome, where oxygen supplies are more plentiful, high incoming gas temperatures were assumed to be unnecessary to obtain combustion, and 'dftemp' was therefore set to 400 K, while the concentration limits were set to slightly less permissive values. In both locations, however, the intent was to ensure that DCH-produced hydrogen could burn during the main event (except when isolated from oxygen by compartmentalization), but allow combustion to eventually be snuffed out without consuming every trace of hydrogen at late times.

As had been expected, the DFB parameters in Table 3.2-1 erroneously predicted combustion would occur for the heavily inerted (75% CO_2) SNL/IET-5 experiment. Most analyses of this experiment were therefore run with default values of the DFB parameters (which suppressed combustion) in order to permit assessment of other features of the DCH model.

The rationale summarized above for the use of the DFB model in the experimental analyses is based, in part, upon a considerable amount of foreknowledge of the conditions that exist within containment during these experiments. In NPP analysis, a wide range of conditions may require consideration, and it may be less clear what conditions will exist during the event. Some modifications to this prescription are therefore suggested for NPP analysis in Section 7.9 under User Guidance. These modifications would have negligible impact if applied to the conditions of the experiments analyzed here, but are potentially important for some NPP scenarios.

<u>BSR Model</u>. In this model, it is assumed that hydrogen and oxygen will recombine at a user-specified fractional rate ('srrate', units s^{-1}) when <u>either</u> the gas temperature exceeds a temperature threshold ('srtemp') <u>or</u> the debris concentration exceeds a threshold ('debconc') <u>and</u> the debris temperature exceeds a threshold value ('debtemp'). The model is intended to reflect the fact that, if a mixture containing combustible gas and oxygen is heated to a sufficiently high temperature, rapid reaction is expected to occur even if the concentrations of the reactants are too low to result in a propagating deflagration. In the DCH experimental analyses, BSR was the principal mechanism by which pre-existing hydrogen in the dome was calculated to burn, for those analyses in which it did burn.

The values of 'srtemp' used (Table 3.2-1) were based upon chemical kinetics calculations performed with the SENKIN code [Lut91] combined with a scaling analysis estimating the temperature at which energy releases due to reaction would exceed energy losses from the gas volume.[*] The values used in the Zion-geometry IET experiments were based upon applying the scaling analysis to the 1/10-scale experiments, and the same values were used for the ANL/IET analyses, without rescaling.

When 'srtemp' is exceeded, the combustion characteristic time scale or e-folding time, τ_{rx}, is equal to the reciprocal of 'srrate.' This means that combustion is about 63% complete, not 100% complete, within a time of τ_{rx}. In the standard prescription, 'srrate' was set equal to $(v_{mix})/V_{cell}^{1/3}$, where v_{mix} is a mixing velocity (taken to be 5 m/s) and V_{cell} is the volume of the cell. The volume dependence is based upon the recognition that the CONTAIN assumption of a homogeneous well-mixed atmosphere cannot be correct for the situation at hand; in reality it is likely that pre-existing hydrogen and oxygen in the receiving cell burn only as the gas is mixed in with the hot DCH-produced plume.

The specific value of v_{mix} used here is believed to be reasonably consistent with the results of the IET experiments in both Zion and Surry geometries [All94b, Bla94], in which thermocouples spaced through the containment vessel volumes provided temperature-time histories at various locations. Typically the thermocouple traces implied that the heated zones expanded through 50% or more of the total volume within a time of 1-2 s. Distances from the operating deck to the dome were about 7-9 m in both facilities; hence mixing velocities of 5 m/s are of the right order of magnitude. However, individual measurements can be cited that suggest considerably higher or lower values, and it is also evident that the situation is much more complex than a simple uniform expansion of a heated plume.

Clearly there are substantial uncertainties in the appropriate value of v_{mix}, but the experiments suggest 5 m/s is most likely a reasonable order of magnitude and sensitivity studies have indicated results are not very sensitive to this value, within reasonable limits. This value is also approximately consistent with treatments used in older DCH calculations [Wil87, Wil88] in which nondefault input to the deflagration model was used to force unconditional hydrogen combustion. A flame speed of 5 m/s was employed there also, but in that approach, τ_{rx} would correspond to the time required for complete combustion.

Standard Prescription. The deflagration model parameters were left at default values in the standard prescription for the experimental analyses (see, however, Section 7.9). The DFB parameters are as in Table 3.2-1, other than those remaining at default values; however, caution is needed in analyses assessing the potential effects of co-dispersed water, and in Section 7.9, it is now recommended that no threshold temperatures for the DFB model be

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[*] *D. S. Stamps, Sandia National Laboratories, private communication; M. M. Pilch, Sandia National Laboratories, private communication.

used. The values of the BSR threshold temperature, 'srtemp' given in Table 3.2-1 were based upon applying the kinetics and scaling analyses noted above to the 1/10-scale Zion IET experiments. The same approach could be applied generally and defined as being the "standard prescription." However, the effort involved is not trivial and may not be justified, since there are insufficient experimental data available to validate this approach for DCH analysis.

It may be noted that application of this approach at NPP scale yields values of 'srtemp' only slightly higher than the default value, 773 K, and sensitivity studies with 'srtemp' at or near the default value resulted in only minor changes in the present experimental analyses provided the change did not result in crossing the threshold for BSR initiation in the dome. It is likely, but not proven, that application of the standard combustion prescription defined to include use of the default value of 'srtemp' will err on the side of conservatism if it is in error. Hence use of the default value in NPP calculations is judged to provide a reasonable starting point.

Two additional uncertainties in the use of the BSR model should be noted. First, strong thermal stratification was observed in at least some of the experiments, which could make the treatment tend to be conservative. On the other hand, BSR initiation by hot debris was suppressed by setting 'debconc' equal to 10^6 kg/m^3. Although the concept of hot debris favoring reaction is certainly a reasonable one, current information was judged inadequate to defend parameters defined for this model. This limitation could make the treatment nonconservative. Section 7.9 provides some additional guidance for use of the combustion models in NPP DCH analyses, including some suggested sensitivity studies and modifications to the parameters given in Table 3.2-1 based, in part, on lessons learned in the course of this work.

3.3.2 Atmosphere-Structure Radiation.3.2 Atmosphere-Structure Radiation.3.2 Atmosphere-Structure Radiation

At the high temperatures typical of DCH events, thermal radiation may be the dominant process contributing to atmosphere-structure heat transfer. CONTAIN has a reasonably sophisticated model for calculating the atmospheric emissivity associated with optically active gases which control emissivities during many non-DCH scenarios. However, in DCH events, dense aerosol clouds probably control emissivities. For example, in experiments in which hydrogen can burn, combustion always manifests itself as bright orange flames with the brilliance often being sufficient to cause white-out of the visual record [Bla94]. In a clean atmosphere, hydrogen flames would be almost invisible.

The CONTAIN model for aerosol emissivities is largely parametric and is believed to have some significant deficiencies, e.g., neglect of scattering (aerosols are "black" and absorb only). Hence, an option has been defined for use in DCH calculations in which the emissivity is explicitly set by the user. This is done by setting the parameter kmx (in the atmospheric radiation input block) equal to a negative value. The absolute magnitude of kmx is then taken to be the emissivity.

Standard Prescription. Emissivity = 0.8; i.e., kmx = -0.8. The value of 0.8 is taken as being typical of the oxides present in oxidized debris, whether core debris or thermite. (Pure alumina would have lower emissivities, but even small amounts of iron and chromium oxides would suppress the low emissivity of pure alumina.)

3.3.3 Convective Flow Velocities.3.3 Convective Flow Velocities.3.3 Convective Flow Velocities

In the CONTAIN atmosphere-structure heat transfer model, the convective heat transfer calculation includes evaluation of a correlation for forced flow across the various heat transfer structure surfaces defined in the problem (natural convection is also considered). For each structure, the forced flow velocity assumed is equal to an estimate of the volumetric flow rate of gas through the cell divided by the hydraulic area of the flow path, A_h. By default, $A_h = V_{cell}^{2/3}$; however, the user may also specify A_h for each structure.

The convective flow velocities have some additional uses in the DCH model. In evaluating the de-entrainment criterion for the first structure impact, the convective flow velocity calculated for the first structure (as defined in the CONTAIN input block for structures) is used if it is larger than the gas flow velocity based upon the incoming jet. Likewise, the gas velocity for the second impact de-entrainment criterion in the TOF/KU model is equal to the flow velocity calculated for the second structure in the cell, and the debris velocity assumed for the second impact is equal to this flow velocity divided by the slip factor specified for the cell. In addition, the gas convective flow velocity at the second structure is used to evaluate the flow velocity required to evaluate heat transfer and reaction rates for the trapped debris field when nonairborne interactions are being modeled.

The flow velocities can have significant effects upon the calculated results, which can therefore be sensitive to inappropriate specifications of A_h. If, for some reason, the A_h values thought to be appropriate for a DCH calculation differ from those considered appropriate for the heat transfer calculation, the user can introduce one or two dummy structures with infinitesimal surface areas as the first structures defined in a cell, in order to control the DCH velocities independently of those used for any "real" structure.

Standard Prescription. A_h is left equal to its default value except when the geometry is such that the cross section for flow clearly differs from that given by the $V_{cell}^{2/3}$ default. In the latter case, A_h values equal to the actual geometric cross section of the flow path are prescribed. In the present analyses, nondefault values were used only for the cavity (and chute where modeled) cells which have elongated geometries for which the flow cross sections are clearly less than what would be given by the default value. In all cases, the defaults were used in the subcompartments for the results presented in Section 4.

3.4 Nodalization.4 Nodalization.4 Nodalization

In any CONTAIN analysis, a task that always requires much judgment on the part of the analyst is deciding how to nodalize the containment. The nodalizations used in the present work will be briefly summarized here. Additional details are given in Appendix A.

For the Zion IET geometry experiments, a quite detailed 14-cell deck was used. This deck included one cell to represent the accumulator and a second cell to represent the melt generator (two cells were used because the flow resistance between the two can reduce blowdown rates when the melt generator hole size is large). Two more cells were used to represent the cavity and the chute. The dome was represented by two cells separated by a vertical boundary; the space between the crane wall and the Surtsey shell was represented by a cell; and the remaining 7 cells were used to represent the subcompartments. One of these cells represented the seal table room and the remainder of the subcompartment volume was subdivided into six cells. In defining the latter division, the guiding principle was a belief that it would be undesirable to have a single cell represent a volume within which conditions would vary greatly, and that cell dimensions therefore should not substantially exceed mean free paths for debris trajectories, especially close to the cavity chute. Detailed measurements from drawings were used to define structures and flow paths such that these representations are believed to be quite accurate. ANL/IET experiments were analyzed using a scaled-down version of the SNL/IET deck.

Setting up the detailed Zion IET deck proved quite tedious, and a similar level of detail was not attempted for any of the other analyses. Analyses of the Surry geometry IET experiments performed in the CTTF were carried out using an 8-cell deck that included the accumulator, melt generator, cavity, residual heat removal (RHR) platform, seal table room (STR), annulus between the crane wall and the containment shell, basement, and the dome. When referring to the "subcompartments" in this deck, all cells downstream of the cavity are included except the dome. Representation of structures and flow paths in this deck was much less detailed than in the 14-cell Zion deck.

SNL/LFP and SNL/WC experiments were analyzed using 5-cell decks consisting of the accumulator, melt generator, cavity, and two cells representing the Surtsey vessel. The latter were separated by a horizontal boundary at the level of the concrete slab used to limit the debris flight path as summarized in Section 2.1.

A 5-cell deck was also used to represent the Zion IET experiments in some sensitivity studies. This deck included the accumulator, melt generator, cavity (including the chute), a cell to represent the subcompartments, and a cell to represent the remainder of the Surtsey volume. Results obtained for ΔP and hydrogen production agreed well with the 14-cell deck, although there were some differences in the hydrogen combustion behavior at later times. Certain parameters in the trapping model are ambiguous when the subcompartments are collapsed to a single cell, and there was some sensitivity in the dome transport fraction, f_{dome}, to these parameters. Depending upon the parameters of the problem, DCH loads can be sensitive to the dome transport fraction, and the 14-cell representation was therefore preferred. However, errors in the trapping behavior calculated by the 5-cell deck tend toward being conservative, and it does appear that the simpler deck could be used in many cases provided care is taken to ensure that results are not overly sensitive to the calculated trapping behavior.

Late in this work, a few analyses were performed for the Surry IET experiments using a 12-cell deck derived from the 8-cell deck by dividing the crane wall annulus into four quadrants and the basement into two halves. Rather unexpectedly, the effect was to increase the calculated ΔP by up to 0.05 MPa. This result was traced to differences in the calculated gas flow and combustion behavior, not differences in debris transport and trapping (the latter differences were negligible). Many flow path and structure definition simplifications exist in both the 8-cell and the 12-cell decks and it is not certain that the 12-cell representation is necessarily giving more realistic results. This difference is interpreted as a measure of the variation that can result from uncertainty in how to define the containment nodalization. It should also be noted that it is not clear to what extent further refinement of the containment representation would improve results, since momentum-driven flow effects that CONTAIN cannot model may be involved. These results are discussed further in Section 6.6.3.

4 Principal Results of the CONTAIN Analyses4 Principal Results of the CONTAIN Analyses4 Principal Results of the CONTAIN Analyses

In this section, we summarize the most important findings of this study. Results obtained using the standard prescription are presented first, and are followed by the results of selected sensitivity studies and their interpretation. The sensitivity studies were performed after the standard prescription was defined and thus did not play a role in defining the standard prescription. A more complete description of the sensitivity studies performed for this work is given in Section 6. The information summarized in the present section may suffice for the needs of many readers, but cross-references to Section 6 are given in order to assist those requiring more detailed information.

The sensitivity studies performed include three cases that were run for all the experiments that were analyzed using the standard prescription.[*] These cases involve variations for two important parametric models, the nonairborne debris model described in Section 3.2.7 and the slip model described in Section 3.2.3. The complete set is included because both of these models involve a user-specified input parameter whose appropriate value cannot be fully established independently and that was, therefore, in part established by a comparison with experimental results, principally those of the SNL/IET-1 and -3 experiments. The ability to match the results of one experiment, or a few similar experiments, may be inconclusive in these models. It is only by determining whether more general trends can be reproduced that conclusions as to the usefulness of the models may be drawn. For each experiment, the following four cases were run:

Case 1. Standard prescription as described in Section 3.

Case 2. Case 1 except nonairborne debris interactions were modeled in the cavity only (not included in the subcompartments).

Case 3. As in Case 1 except no nonairborne debris interactions were modeled.

Case 4. As in Case 1 except that a slip factor, s_d, equal to 5 was specified for all the subcompartment cells.

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[*] *SNL/IET-5 was run with DFB parameters set to CONTAIN default values for reasons noted in Section 3.3.1.

Table 4-1 Integral Performance Statistics					
Quantity	Statistic	Case 1	Case 2	Case 3	Case 4
ΔP	R^2	0.89	0.74	0.53	0.94
	σ_e (MPa)	0.035	0.049	0.077	0.024
	δ_{bias} (MPa)	0.014	−0.012	−0.039	0.006

Discussion of results for Case 2 is deferred to Section 6.3, except to note that they tend to be intermediate between Cases 1 and 3 for the Zion-geometry experiments and more closely resembled Case 1 results for the other experiments.

Some statistical measures of performance for each of these cases are given in Table 4-1. Results are given for pressure rise due to DCH and for hydrogen produced by DCH. In order to facilitate comparison of the results of experiments performed at different scales, all hydrogen results are scaled up to NPP scale by dividing by S^3, where S is the linear scale factor. Quantities given are the fraction of the total variation in the experimental results that is explained by the model (R^2 value), the mean model bias (δ_{bias}), and the standard error of estimate, σ_e. The bias and errors of estimate are defined by

$$\delta_{bias} = \frac{\sum_{i=1}^{N_e} (y_{i'} - y_i)}{N_e}\ ; \text{ and } \sigma_e = \sqrt{\frac{\sum_{i=1}^{N_e} (y_{i'} - y_i)^2}{N_e}}\ ,$$

9 (4-1)

where y_i is the experimental value for the ith experiment, y_i' is the corresponding CONTAIN prediction, and N_e is the number of experiments.

4.1 Results for the Standard Prescription.1 Results for the Standard Prescription.1 Results for the Standard Prescription

4.1.1 Results for DCH-Induced Pressurization (∆P).1.1 Results for DCH-Induced Pressurization (∆P).1.1 Results for DCH-Induced Pressurization (∆P)

CONTAIN predictions for ∆P are plotted against the experimental values in Figure 4.1-1a. Plot symbols distinguish experiments performed in open geometry, the LFP series other than LFP-8A, the SNL/IET (Zion) experiments with hydrogen combustion and without hydrogen combustion, the ANL/IET experiments, and SNL/IET (Surry) experiments performed in CTTF.

In general, the CONTAIN results give a good account of the major trends in the data. Comparison of the ANL/IET results with the SNL/IET Zion results reveals no obvious scale distortion. The Surry-geometry IET results for ΔP line up well with the Zion IET results, despite the substantial differences in geometry, driving pressure, and atmospheric conditions within containment prior to the DCH event. Furthermore, the fairly substantial differences among the three Surry-geometry ΔP results are reproduced well.

Asterisk plot symbols give the results for the open-geometry experiments (WC series and LFP-8A). These points also fall in line reasonably well with the others, which is significant in that it indicates that, with the same standard prescription (including particle size distribution), the code is able to handle tests in which debris interacting directly with the containment atmosphere is important, as well as tests in which results are dominated by debris-steam interactions in the cavity and the subcompartments.

On the negative side, the results for four of the five LFP experiments that were performed in compartmentalized geometry are seen to be overpredicted by 35% to 75%. The reason is that the trapping and slip modeling in the standard prescription resulted in overprediction of the transport beyond the concrete slab limiting the flight path. The value of ΔP for the ANL/IET-1RR experiment is underpredicted by about 30%. The reason for this discrepancy has not been identified. All other calculated values agree with the experimental results to within 20%.

4.1.2 Hydrogen Production and Combustion.1.2 Hydrogen Production and Combustion.1.2 Hydrogen Production and Combustion

Interpretation of Hydrogen Data. The interpretation of the hydrogen data is not as straightforward as the interpretation of the ΔP results. Data for hydrogen produced and hydrogen burned are inferred from the results of analyzing the composition of gas grab samples taken before the test and at various times after the test. In all cases, the number of moles of hydrogen cited in this work have been calculated from the relationships

$$N_{H_2,burn} = 2\,(N^0_{O_2} - N_{f,O_2})$$
$$N_{H_2,prod} = N_{f,H_2} - N^0_{H_2} + N_{H_2,burn} .$$

10 (4.1-1)

Here, $N_{H2,burn}$ and $N_{H2,prod}$ are, respectively, the number of g-moles of hydrogen burned and produced; the superscript 0 refers to the number of moles present before the test; and the subscript f refers to the final number after the test. The gas analysis numbers themselves are believed to be quite accurate. However, in the tests considered here, the gas samples were taken at times ranging from 15 s to 30 minutes after the test, times which are long compared with the DCH time scale ($\leq$ 3 s, based upon the time required to reach peak pressure). Hence there is no assurance that the results calculated from Eq. (4.1-1) represent reactions that actually occurred during the DCH event. This question is revisited later in this section.

In Eq. (4.1-1), all reductions in atmospheric oxygen content are interpreted as representing hydrogen which is first produced and then burned. In reality, there may be some direct metal-oxygen reaction in both the experiment and the calculation. Since there is no unambiguous way of separating the two processes, and since they represent the same total energy release, both the experimental data and the CONTAIN results are represented using Eq. (4.1-1).

In the Surry-geometry experiments performed in CTTF, the pretest atmosphere included steam. The gas analysis, however, assayed only the noncondensible components, and the initial steam content of the atmosphere had to be inferred from measured temperatures and pressures and some additional analysis taking into account containment leakage [Bla94]. For these experiments, the gas numbers are estimated from the initial conditions and the posttest noncondensible ratios under the assumption that the number of moles of nitrogen does not change during the tests. The experimental hydrogen numbers used in the present work therefore differ somewhat from those in Reference Bla94, which utilized a different method and which furthermore incorporated estimates as to how much of the inferred changes in O_2 content of the atmosphere represented direct metal-oxygen reactions.* For all other tests, numbers cited in the experimental reports have been used directly.

Hydrogen Production Results. CONTAIN predictions are compared with experimental results for DCH-generated hydrogen in Figure 4.1-1b. Hydrogen results are plotted after scaling up to plant scale (i.e., by dividing by S^3), in order to facilitate comparison of experiments performed at different scales.

The hydrogen data in Figure 4.1-1b show more scatter than did the ΔP results, but the general trends are still reproduced reasonably well for both the hydrogen produced and the hydrogen burned. There may be some tendency to overpredict the hydrogen production for the small-scale ANL/IET experiments. One possible explanation is that the prescription used to scale the effective particle size, d_t, in the nonairborne model [Eq. (3.2-7) with m = 0.8] may yield a dependence of d_t upon scale that is somewhat too strong. If this is the case, it would overpredict interactions in the small-scale ANL/IET experiments but might underpredict interactions if extrapolated to NPP scale. Although the evidence is far from conclusive, it does illustrate the need for caution when applying this prescription to NPP analysis. Use of Eq. (3.2-7) with m = 1 is recommended in the User Guidance section, where sensitivity studies to investigate uncertainties are also strongly recommended.

Time Scale for Hydrogen Production. Experimental data on hydrogen production do not include sufficient time resolution to address the question of whether all the hydrogen was actually produced on the time scale of the DCH event. It has been suggested that chemical

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* *These analyses were performed at a time when only a review draft of [Bla94] was available. The final draft also included hydrogen results based upon the nitrogen ratio method that was used here.

reactions occurring after the DCH event might enhance the apparent hydrogen production results for cases that include cavity water and/or oxygen in the atmosphere, with the time scale for these late reactions being too long to contribute to DCH. It was therefore suggested that only cases with inert atmospheres and dry cavities should be included in the validation tests for hydrogen production during DCH. These dry and inert cases include the six LFP experiments and two of the three WC experiments.

If this hypothesis were correct, one would expect the ratio of predicted to experimental hydrogen production (P/E ratio) to be lower for the cases with water and/or oxygen atmospheres than for the dry and inert cases, because the CONTAIN analyses modeled no metal oxidation reactions occurring after the end of the accumulator blowdown. The actual P/E ratios with their standard deviations are 0.92 ± 0.16 for the dry and inert cases and 1.05 ± 0.27 for the other cases. The difference between the dry and inert cases and the others is small and, furthermore, the difference that does exist is in the opposite direction from that predicted. Hence the CONTAIN analyses do not support the hypothesis that only the dry and inert cases should be used, and all the hydrogen production data are accepted as valid for the purposes of this report.

<u>Hydrogen Combustion Results</u>. Figure 4.1-2 gives results for hydrogen burned in experiments for which any significant amounts could burn. Agreement is generally reasonable, though there is a tendency to overpredict hydrogen combustion somewhat in several cases. However, for two experiments (SNL/IET-6 and SNL/IET-7), combustion is underpredicted. These experiments included pre-existing hydrogen in the atmosphere, and the posttest gas analyses indicated that a significant fraction of it reacted. In the CONTAIN analyses, the maximum dome temperatures were under 700 K, well below the BSR threshold (848 K) prescribed, and most of the pre-existing hydrogen did not burn in the calculation. It is likely that some pre-existing hydrogen did react in these experiments, but the time scale was too slow to contribute substantially to the ΔP resulting from DCH [All94b].

Figure 4.1-2. CONTAIN predictions versus experimental results for scaled H_2 combustion for the standard input prescription.
6

4.2 Nonairborne Debris and Cavity Water.2 Nonairborne Debris and Cavity Water.2 Nonairborne Debris and Cavity Water

In the Case 3 analyses, only the interactions of airborne debris with blowdown steam and the containment atmosphere are modeled. Neither debris-water interactions nor nonairborne debris interactions are included. Results summarized in this section indicate that Case 3 is based upon an incomplete description of the processes that actually can contribute to DCH. We first summarize the trends observed for the Case 3 results (Section 4.2.1), and then consider the degree to which cavity water may be confounding the possible interpretations (Section 4.2.2). In Section 4.2.3, we consider further the implications of the Case 3 calculations for the Zion-geometry IET results, including the degree of certainty one should attach to these implications.

4.2.1 Effects of Nonairborne Debris in the Standard Prescription.2.1 Effects of Nonairborne Debris in the Standard Prescription.2.1 Effects of Nonairborne Debris in the Standard Prescription

Case 3 calculated results are compared with experimental results for ΔP and for hydrogen produced in Figures 4.2-1a and 4.2-1b, respectively. For the ΔP results, the magnitude of the effect of deleting the nonairborne interactions is quite different for different experiments. For the Zion-geometry experiments, the effect is large, with ΔP being underpredicted by about a factor of two for those SNL/IET Zion experiments in which hydrogen could burn.

The calculated △P values for the Surry IET experiments in Figure 4.2-1 are only moderately too low; the effect is evidently considerably less than in the Zion experiments. Even this comparison overstates the effect in the Surry geometry because, with the nonairborne debris interactions deleted, calculated dome temperatures in IET-10 and IET-11 did not quite reach the threshold for the BSR model and some of the reduction in △P is due to the failure to burn most of the pre-existing hydrogen. Deleting nonairborne debris interactions had very little impact upon the LFP and WC results for △P.

The hydrogen production results are even more sensitive to deleting the nonairborne debris interactions, with all the calculated results other than IET-9 being too low, including all the LFP and WC results. Indeed, with no nonairborne debris interactions, there is no significant correlation between predicted and measured hydrogen production ($R^2 = 0.09$ in Table 4-1). Most of the experiments other than the Zion IET cases included no water in the cavity, and the possible confounding effects of water to be discussed below for the Zion experiments are therefore absent in the other cases.

As was true of the △P results, the largest deficiencies in calculated hydrogen production are for the Zion-geometry IET experiments, for which hydrogen production is underpredicted by a factor of about two. One reason that the Zion experiments appear to be more sensitive to the nonairborne debris model than the other experiments may be that the cavity was connected to the Surtsey vessel by a relatively long chute, and the subcompartment volume is relatively small and includes complex internal structures. The surfaces of these structures may have enhanced the opportunity for debris films to interact with the noncoherent portion of the steam blowdown. However, it is now believed that the cavity water also played a role, and some of the effects attributed to nonairborne debris in the standard input prescription might actually be due to the water.

The metal content was high in all the DCH experiments analyzed here, and increased production and combustion of hydrogen is an important mechanism by which nonairborne debris is calculated to augment DCH loads. For melts with a low metallic content, these effects are expected to be smaller. This point is potentially significant because recent work has concluded that highly metallic melts are very unlikely for the scenarios that were considered [Pil94b].

4.2.2 Effects of Cavity Water.2.2 Effects of Cavity Water.2.2 Effects of Cavity Water

Zion IET Experiments. All the Zion IET experiments other than SNL/IET-8 had condensate levels of water (3.48 kg at 1/10-scale) in the cavity, and there are no dry-cavity cases available for determination of the effects of the water by direct comparison of

Table 4.2-1 SNL/IET-3 Sensitivity Studies Involving Nonairborne Debris and Cavity Water				
Case	Description	ΔP (MPa)	H_2 (moles)	
			Burned	Produced
	SNL/IET-3 Experimental	**0.246**	**190**	**227**

experimental results. Although the amount of water involved may seem small, it amounts to 193 g-moles, and efficient thermal and chemical interaction of this water with airborne debris would be sufficient to account for most or all of the discrepancy between the Case 3 calculations and the experimental results. This is illustrated in Table 4.2-1, which presents results for some sensitivity studies involving nonairborne debris and co-dispersed water in the SNL/IET-3 experiment.

In Case I3-4, no nonairborne debris interactions were modeled but the cavity water was assumed to interact with the debris. It is evident that much of the difference between the cases without nonairborne debris (Case I3-3) and the experimental results could be accounted for by interaction with the water, especially if one assumes that the debris-water interactions result in a smaller debris particle size (Case I3-5). Case I3-6 was run assuming that the water participated as in Case I3-4 and that nonairborne debris also participated but with an efficiency reduced by increasing d_t to 0.02 m. This case gives results very similar to the standard case. It is evident, therefore, that equivalent integral results can be obtained with a wide range of assumptions concerning the relative contributions of nonairborne debris and co-dispersed water.

Additional insight is provided by considering the pressure-time histories plotted in Figure (4.2-2) for the experimental results, the standard case, the case without nonairborne debris (NAD in the figure legend), and the various cases involving water. It is apparent that the pressure rise is too slow in the standard case and too rapid in the cases that include water but no nonairborne debris. The case that includes both nonairborne debris and water interactions provides the best agreement. Calculations corresponding to Cases I3-4 and I3-6 were run for the other six SNL/IET (Zion) cases that had condensate levels of water in the cavity. The behavior illustrated here was found to be general: on average, the agreement for integral ΔP and hydrogen results was as good in the cases including both nonairborne debris and water interactions as it was for the standard prescription (Section 6.4.4), and this case gave better agreement for the pressure-time history than either the standard case or the case with water only, although the agreement was not always as good as in Figure (4-3); see Section 6.5.1 for the detailed results. The preferred interpretation, therefore, is that both nonairborne debris and debris-water interactions contributed significantly to the Zion IET results.

Figure 4.2-2. Comparison of experimental and calculated pressure-time histories for the SNL/IET-3 experiment.

The SNL/IET-8B experiment had much larger amounts (62 kg) of water in the cavity than did the other Zion IET experiments. The experimental results implied that about 74% of the water was vaporized [All94b], suggesting that efficient debris-water interactions did occur. Some CONTAIN analyses of this experiment are summarized in Section 6.4.5. It was found that the CONTAIN model can yield nonconservative results when large amounts of water are involved and that sensitivity studies in which only a fraction of the water is assumed to participate are therefore recommended.

For compartmentalized geometries, the CONTAIN model indicates that it may be possible for moderate amounts of co-dispersed water to enhance DCH loads substantially under certain conditions (Section 6.4.5; see also References Wil87, Wil88). No experimental data permitting a clean test of this possibility are available, however. As in the case of the nonairborne debris interactions, an important effect in the calculations is enhanced hydrogen production and combustion when metal-steam reactions would be steam-limited without the water. For highly oxidic melts, such as those defined in Reference Pil94b, the potential for water to enhance DCH loads may be less.

Debris-Water Interactions in Other Containment Geometries. The WC-1 and WC-2 experiments were performed in an open containment geometry and were very similar except that WC-1 had a dry cavity while WC-2 had 11.76 kg of water in the cavity. Experimental results showed very little difference in ΔP while WC-2 yielded about 25% more hydrogen. Previous analyses [All92a] indicated that debris-water interactions were inefficient in this experiment and CONTAIN results summarized in Section 6.4.2 support this conclusion. The CONTAIN analyses predict no increase in ΔP due to the water in WC-2, whatever the efficiency of the cavity interaction. It appears, therefore, that the effects of water in compartmentalized geometries generally cannot be inferred from the results of experiments performed in open containment geometries; see Sections 6.4.2 and 6.4.4 for details.

The Zion-geometry experiments were the only cases analyzed with CONTAIN in which water was intentionally added to the cavity, but a small amount of condensate water is believed to have been present in the Surry-geometry experiment SNL/IET-9 [Bla94]. No water was modeled in any of the CONTAIN calculations. There is no evidence that either ΔP or hydrogen production is underpredicted as a result of neglecting the water in this experiment, suggesting that the water had little effect. It is possible that, even among compartmentalized geometries, the effect of water depends upon details of the geometry. Firm conclusions cannot be drawn, however, in part because the amount of water present in this test is not known.

4.2.3 Re-examination of the Case 3 Interpretations.2.3 Re-examination of the Case 3 Interpretations.2.3 Re-examination of the Case 3 Interpretations

Traditionally, DCH modeling has emphasized (often exclusively) the interactions between airborne debris and the containment atmosphere and/or blowdown steam, which are just the processes treated by the Case 3 analyses. The fact that Case 3 results for the Zion IET experiments underpredict the experimental results by a factor of about two implies that other processes are important in these experiments.

The "other processes" contributing to DCH that have been considered in the present work are the nonairborne debris and the debris-water interactions. Because these processes are not well understood and their representations in the CONTAIN code are parametric, there is a degree of uncertainty in the prediction of their effects on DCH calculations. Moreover, the results described above imply that the relative contribution of the various processes may be geometry-dependent, because the degree of underprediction in the Case 3 results for the Surry geometry is considerably less. The conclusions that debris-water interactions and/or nonairborne debris can augment DCH significantly are among the most important conclusions that have been drawn from the results presented in this report. Before accepting these conclusions, it would be well to examine possible alternative explanations for the failure of the Case 3 results to account for the observed ΔP and hydrogen measurements.

Bounding Analysis for the Airborne Debris Interactions. One possibility is that the CONTAIN model is underpredicting the efficiency of the airborne debris interactions. This possibility was addressed by running Case 3 for SNL/IET-3 and SNL/IET-6 with the particle size set to an unrealistically small value, 0.125 mm for all debris fields, in order to maximize the efficiency of the airborne debris interactions. Results given in Section 6.2.2 show that the calculated ΔP and hydrogen production were still only 50-67% of what was observed experimentally. Hence this explanation for the Case 3 results is considered to be implausible.

Independent Assessment of Mitigation Effects. A substantial mitigation effect in all the CONTAIN calculations in which hydrogen can burn is the combined effect of atmosphere-structure heat transfer together with incomplete or delayed combustion of hydrogen in temporarily oxygen-starved subcompartments. Sensitivity studies are given in Section 6.7 in which these effects were deleted from Case 3 analyses by setting structure areas to infinitesimal values and setting combustion parameters to ensure complete combustion. Eliminating these mitigation effects substantially reduced the difference between the Case 3 ΔP calculations and the experimental results, but it did little to improve agreement on hydrogen production numbers.

It is apparent, therefore, that the conclusions drawn from the Case 3 ΔP results depend to a considerable degree upon the validity of CONTAIN's treatment of the mitigation effects. As a check against the CONTAIN treatment, a simplified analytical calculation was performed as to the extent of mitigation that might be expected to result from the heat transfer and incomplete hydrogen burn effects. This analysis is given in Appendix C. The results agree reasonably well with the CONTAIN results for mitigation and support the belief that CONTAIN is treating the mitigation effects correctly.

Mutual Consistency of ΔP and H_2 Production Results. A more subtle check is provided by the observation that, in Table 4.2-2 and in Figures 4.1-1 and 4.2-1, the calculated ΔP values tend to agree with experimental results if and only if the calculated hydrogen production results agree, especially in the Zion experiments. Obtaining this result depends upon the balance between three processes: debris-gas heat transfer, debris-gas chemical reaction, and atmosphere-structure heat transfer. (Without the latter, ΔP values resulting from the hydrogen combustion calculated for Case 1 would be much greater than those observed.) The key point is that the parametric variations involved in deciding upon the prescription for the nonairborne model do not change the balance between these processes because the nonairborne model still uses the same basic heat/mass transfer analogy as is used elsewhere in CONTAIN; heat and mass transfer cannot be tuned separately. Likewise, varying the nonairborne model input does not affect the atmosphere-structure heat transfer model. Similar arguments apply to the simulation of debris-water interactions. Hence the fact that either ΔP and hydrogen results are both in reasonable agreement with experiment or neither are in agreement provides additional confirmation of the validity of the modeling; see Sections 6.4.4 and 6.7.3 for additional discussion.

Total Steam Correlation Versus Coherent Steam Correlation. Still another check is suggested by referring back to Section 2.2, where it was shown that the DCH ΔP data for experiments in compartmentalized geometries could be correlated quite well with the total steam in the accumulator together with allowing for the presence or absence of effective hydrogen combustion. If DCH loads were primarily governed by the interactions of airborne debris with coherent steam, one might expect to obtain an improved fit by correlating with the coherent portion of the blowdown instead of with the total steam.

Pilch [Pil94a] has made approximate estimates of the degree of coherence between the blowdown steam and debris dispersal for all the experiments in the data base. In order to test the coherence concept, Eq. (2.2-1) was re-evaluated as before except with N_{H2O} replaced by $f_{coh}N_{H2O}$, where f_{coh} is the fraction of the blowdown steam that is estimated to be coherent with debris dispersal. Results for the total steam and coherent steam correlations applied to the experiments in compartmentalized geometries are displayed in Figures 4.2-3a and 4.2-3b, respectively. Figure 4.2-3a is equivalent to Figure 2.2-1 with the open-geometry cases deleted for clarity. In the figure legend, S refers to the linear scale factor. 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. Furthermore, 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. 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.

Summary. Several convergent lines of evidence support the belief that the Zion IET DCH results cannot be explained in terms of interactions between airborne debris and coherent steam alone. Other processes must be contributing substantially to the observed DCH pressurization and hydrogen production in the Zion-geometry IET experiments. It is much less certain whether the dominant processes are those represented by CONTAIN's nonairborne debris model versus debris-water interactions. However, the pressure-time histories summarized previously suggest that the water does play a significant role, a fact that was less apparent at the time the standard prescription was defined and frozen for the current study.

4.3 Effect of Debris-Gas Slip in the Subcompartments.3 Effect of Debris-Gas Slip in the Subcompartments.3 Effect of Debris-Gas Slip in the Subcompartments

Case 4 was run for all experiments with the slip parameter, s_d, set equal to 5 in the subcompartment cells instead of being set equal to unity as in the other cases. Case 4 was otherwise identical to Case 1. The ΔP and hydrogen production results for Case 4 are presented in Figure 4.3-1. (Hydrogen combustion results differed little from Case 1 and are not presented.)

Comparison with Figure 4.1-1 indicates that there is little difference between Case 1 and Case 4 in terms of hydrogen production. For many of the experiments, there is also little difference in ΔP results. However, ΔP is reduced for the four LFP experiments that were overpredicted in Case 1, substantially improving agreement with experiment for these particular experiments. Thus, the overall ΔP validation plot is somewhat better for Case 4 than for Case 1; see also Table 4-1.

The principal effect of increasing s_d in the subcompartments is to reduce the fraction of the debris transported beyond the subcompartments, f_{dome}. Here we define f_{dome} as it is defined in the experimental reports:

$$f_{dome} = \frac{m_{d,dome}}{m_{d,sub} + m_{d,dome}},$$

11 (4.3-1)

where $m_{d,dome}$ and $m_{d,sub}$ are, respectively, the masses of debris located in the dome and in the subcompartments after the experiment. Calculated values of f_{dome} are plotted against the experimental values for Case 1 in the top half of Figure 4.3-2 and Case 4 in the bottom half.

It is apparent that f_{dome} for the LFP experiments is substantially overpredicted in Case 1, which is why ΔP is overpredicted for these experiments. On the other hand, f_{dome} is of the correct order of magnitude for both the Zion and Surry IET results in Case 1. There is considerable scatter in the experimental results for debris transport, as is indicated by the considerable range of results obtained in the Zion IET experiments, all of which were nominally the same in terms of parameters expected to govern debris transport. Evidently stochastic effects (e.g, resulting from FCIs) influence these results.

In Case 4, f_{dome} is considerably smaller than in Case 1, which yielded improved agreement for both f_{dome} and ΔP for the LFP experiments. For the IET experiments, f_{dome} is substantially underpredicted in Case 4, but this had little effect upon ΔP or hydrogen production because these experiments are heavily dominated by debris-steam interactions in the cavity and the subcompartments, and are much less sensitive to f_{dome}. Indeed, the increased s_d value in the subcompartments increased airborne residence times there somewhat, and the resulting increase in debris-steam interactions tended to compensate for whatever effect the reduced value of f_{dome} might otherwise have had.

In the LFP experiments, the cross sections for flow in the subcompartment were large and the steam blowdown rates were not very great, since driving pressures were relatively low. As discussed in Section 3.2, one would expect debris trajectories to largely decouple from the gas flow patterns under these conditions, an effect the CONTAIN model cannot take into account. Hence it is not surprising that the model yields poor results for these experiments.

The reason that Case 1 is preferred as the standard prescription has to do with possible behaviors when the model is extrapolated to scenarios more favorable to debris transport than those studied experimentally. Possible examples include scenarios with higher driving pressures and/or larger vessel failure sizes than those simulated in the experiments. In such cases, DCH loads could be more sensitive to f_{dome} than in the Zion and Surry-geometry experiments considered here, and the tendency of Case 4 to underpredict f_{dome} could then result in nonconservative predictions of ΔP.

In both the Zion and the Surry geometry, there exist momentum-driven transport paths through the seal table room (STR) to the dome, and CONTAIN cannot mechanistically model this momentum-driven transport. No effort was made to simulate this transport in the Zion-geometry analyses. Experimentally, momentum-driven transport deposited a relatively large amount of debris (~20%) in the STR, which was an order of magnitude greater than what CONTAIN calculated. However, there is some evidence that this transport path was not a major contributor to f_{dome} because the STR exit path was blocked by a concrete plug in one experiment (SNL/IET-3). The value of f_{dome} for this experiment (0.088) was in line with the values obtained for the other experiments (0.057-0.138), excluding two cases in which damage to subcompartment structures clearly enhanced transport. Hence, it is likely that the STR transport path did not dominate the f_{dome} results for the other experiments.

In the analysis of the Surry-geometry experiments, the momentum-driven transport was simulated nonmechanistically by introducing a fictitious flow path from the cavity cell to the seal table room. Dimensions of this path were based upon the geometries of the openings involved.

To sum up, it is obvious from Figure 4.3-2 that there is much scatter in the data and the correlation between predicted and observed values of f_{dome} is not very good. Even for Case 1, it is clear that considerable caution would be warranted in applying the model to scenarios involving large extrapolations from the present data base. On the other hand, the model does give the correct order of magnitude for f_{dome} in the IET experiments, and correctly predicts that the absolute magnitude of f_{dome} is small. As long as f_{dome} is not large in an absolute since, the calculated values of ΔP will not be very sensitive to substantial relative uncertainties in f_{dome}.

Table 4.4-1 Selected Sensitivity Studies				
Case	Description	ΔP (MPa)	H_2 (moles)	
			n_{burn}	n_{prod}
	IET-3 Experimental	**0.246**	**190**	**227**
I3-1	Standard	0.228	232	253
I3-7	No Trapping	0.372	317	427
I3-8	No Structures	0.401	256	261
I3-9	No Structures or Trapping	0.716	436	444
I3-10	Airborne Debris mmd = 0.5 mm	0.236	238	257
I3-11	5-Cell Nodalization	0.227	167	240
	IET-6 Experimental	**0.279**	**345**	**319**
I6-1	Standard (f_{coh} = 0.184)	0.248	256	240

4.4 Additional Model Sensitivities.4 Additional Model Sensitivities.4 Additional Model Sensitivities

In this section, we briefly discuss additional sensitivity study results for the CONTAIN DCH model. Some of the results to be considered are summarized in Table 4.4-1.

DCH Mitigation Processes. The principal processes that act to mitigate DCH are debris trapping, which slows or terminates debris interactions with the atmosphere, and atmospheric heat transfer to containment structures. Compartmentalization can enhance the effect of trapping by preventing most of the debris from ever reaching the dome. It can also enhance the heat transfer effects, in part because hydrogen hold-up in oxygen-starved subcompartments can delay hydrogen combustion and thus give heat transfer more time to be effective. One of the ways in which moderate amounts of co-dispersed water can enhance DCH loads is that the increased steam supply accelerates transport of energy and hydrogen to the dome, reducing this mitigation effect.

In Case I3-7, all trapping was turned off, allowing most of the debris to eventually reach the dome and substantially increasing ΔP. In Case I3-8, the usual trapping model was active but all heat transfer to structures was deleted, and it is apparent that this mitigation mechanism is as important as trapping. Deleting both mitigation processes results in a very large ΔP value (Case I3-9). Repeating these sensitivity cases for the IET-11 experiment resulted in the same general trends.

Additional sensitivity studies concerning the effect of atmosphere-structure heat transfer and hydrogen hold-up in the subcompartments are given in Section 6.7.3. The results indicate that, although the effects themselves are very important, the uncertainties in these effects are not large. Hence it is possible to take considerable credit for these mitigation effects even when a conservative calculation is desired.

Debris Source Characteristics. Case I3-10 was run with the airborne particle mmd decreased to 0.5 mm, which is seen to have only a small effect. One reason is that, in compartmentalized geometries, debris interactions with the coherent steam tend to be steam-limited and increasing the efficiency does not alter the limit set by the steam supply. For similar reasons, sensitivity studies for IET-3 and IET-10 in which the debris dispersed from the cavity was increased from the experimental values (60% and 73%, respectively) to 100% had only a small effect (<5% change in ΔP; see Section 6.3.2).

In the standard input prescription, the debris sources were always defined so as to match the experimental degree of coherence between debris dispersal and blowdown steam. Since this procedure is inapplicable for NPP analyses, it is of interest to determine the sensitivity to coherence. Sensitivity to coherence was checked for the SNL/IET-6 experiment, in which coherence was low ($f_{coh} \approx 0.184$), which would be expected to maximize sensitivity to f^{coh}. In Cases I6-2 and I6-3, the duration of the debris dispersal interval was lengthened while the blowdown time remained the same, thereby providing considerably larger values of f_{coh}. The resulting changes in ΔP were less than 10%, indicating that considerable uncertainty in coherence can be tolerated without producing large uncertainties in the calculated loads.

Hydrogen Combustion. In typical DCH calculations, the DFB model controls most of the combustion of DCH-produced hydrogen, while the BSR model controls combustion of pre-existing hydrogen. Detailed discussions of these models' performance are provided in Section 6.6.

The standard prescription assumes DFB will occur unless the atmosphere is almost totally inert, and it predicted the correct behavior for DCH-produced hydrogen in all cases except SNL/IET-5, in which the model erroneously predicted efficient combustion. This experiment had a containment atmosphere including 76 mole percent (m/o) CO_2 and only 4.35 m/o oxygen, which suppressed combustion. On the other hand, calculations with DFB parameters set to the standard CONTAIN default values, which are not based upon DCH conditions, underpredicted hydrogen combustion and ΔP for the IET-9 and IET-10 Surry- geometry experiments. The default is therefore potentially nonconservative and the standard DCH prescription is preferred. Although this prescription is potentially conservative with respect to the concentration thresholds, there is no evidence that it yields overly conservative results for those experiments in which the threshold was exceeded. The temperature threshold, however, should be reduced for cases involving large amounts of co-dispersed water (Sections 6.4.5, 7.8).

Calculations with the BSR threshold set to about 850 K correctly predicted that pre-existing hydrogen in the IET-6 and IET-7 experiments would not contribute significantly to DCH loads, while activating the BSR model by lowering the threshold to 600 K resulted in substantial overprediction of both ΔP and total hydrogen combustion (Case I6-4 in Table 4.4-1). For the Surry IET experiments, BSR was predicted to occur. Suppressing BSR reduced the calculated ΔP below the experimental values but the effect was quite small except for IET-11 (Case I11-2). Even for IET-11, the effect was no larger than the uncertainties associated with nodalization to be discussed next, and no conclusions could be drawn as to whether pre-existing hydrogen contributed significantly to DCH loads in these experiments.

<u>Nodalization Sensitivities</u>. A simple 5-cell deck was defined for the Zion IET experiments in which the Surtsey vessel was represented with just two cells, one for the subcompartment volumes and one for all volumes outside the subcompartments. Results for IET-3 (Case I3-11) revealed no major differences with respect to the 14-cell nodalization. However, certain parameters in the trapping model are ambiguous when the subcompartments are collapsed to a single cell as is discussed in Section 6.1.3, and there was some sensitivity in the dome transport fraction, f_{dome}, to these parameters. Depending upon the parameters of the problem, DCH loads can be sensitive to the dome transport fraction, and the 14-cell representation was therefore preferred.

A 12-cell deck for the Surry IET experiments was constructed by subdividing the subcompartment volume further. This resulted in an increase in the predicted ΔP values (Cases I11-3 and I11-4); additional details are given in Section 6.6.3. With the 12-cell nodalization, ΔP results agree better with the experimental results if BSR is suppressed in the dome. Some guidance on selecting an appropriate nodalization is given in Section 7.2.

Scale Dependencies. Comparisons between the ANL/IET and SNL/IET counterpart experiments reveal no dramatic overall scale effects or substantial overall scale distortion in the CONTAIN model. The absence of any strong overall dependence upon scale may reflect the cancellation of opposing effects, as there do appear to be significant scale effects in some specific phenomena. The experimental results and the CONTAIN analyses of the experiments, described in Section 6.8, tend to support the following conclusions:

- The degree of coherence between steam blowdown and debris dispersal is considerably greater in the small-scale ANL/IET experiments than in the larger-scale SNL/IET counterpart experiments, with the difference being about a factor of two. (This is an inference from the experiments, not a model prediction.)

- The model indicates that efficiency of interactions between airborne debris and gas can increase with increasing scale, but there is no direct experimental confirmation of this prediction.

- Experimentally, hydrogen combustion appears to be less efficient and less reproducible in the smaller-scale experiments, an effect that the CONTAIN model does not entirely capture.

- The CONTAIN nonairborne debris model gives interaction efficiencies that are approximately scale-independent if the parameter d_t is scaled using Eq. (3.2-7) with $m = 1$, and this choice yields reasonable agreement with the experimental results for the ANL/IET experiments. Hydrogen production is substantially underpredicted if d_t is not scaled at all.

- In Section 4.2.2, it was noted that a reasonable match to both ΔP and hydrogen production could be obtained by including debris-water interactions and increasing d_t to twice the standard value used without water (Case I3-6 in Table 4.2-1). This approach also yielded reasonable results for the ANL/IET-3 experiment; thus, its use does not appear to introduce any large scale distortions.

Although not all the scale-dependencies involved are completely understood, it is worth noting that the experiments analyzed in this work include linear scale factors ranging from 0.0255 to 1/5.75, a factor of about 6.8. This factor is actually slightly larger than the increase in scale in going from the Surry IET experiments in CTTF to full NPP scale. The fact that the results given in Figures 4.1-1 and 4.1-2 reveal no conspicuous scale distortions suggests that scale effects will not introduce gross error when the CONTAIN model is applied at full scale.

4.5 Observations Concerning DCH Analysis Uncertainties.5 Observations Concerning DCH Analysis Uncertainties.5 Observations Concerning DCH Analysis Uncertainties

Although numerous modeling uncertainties are identified in this report, it does not follow that DCH loads calculated by CONTAIN will be heavily affected by a large number of uncertainties. It is typical that the results for any given DCH scenario will be sensitive to at most a small number of the uncertain phenomena, although the identity of the more important uncertainties can be different for different DCH scenarios. For example, there are important uncertainties in the phenomena controlling debris trapping and transport, yet comparison of the Case 1 and Case 4 results for the Zion and Surry-geometry experiments shows them to be quite insensitive to these uncertainties. On the other hand, it is possible to identify DCH scenarios for which trapping and transport uncertainties can have larger effects upon the results. Since the intent of this report has been to take into account as wide a range of potential applications as is feasible, it has been considered necessary to address a substantially greater number of uncertainties than would be important for a more narrowly defined application.

Some sensitivity calculations are suggested in the User Guidance section of the report. These sensitivity studies are designed to provide the user with a reasonable measure of the uncertainty for the particular case at hand. This approach has been adopted because the impact of any given uncertainty upon the results of DCH calculations can depend strongly upon the initial and boundary conditions of the scenario of interest. It is therefore impossible to give a quantitative estimate of the magnitudes of these uncertainties that would be applicable to all DCH analyses.

5 Assessment of RPV and Cavity Models 5 Assessment of RPV and Cavity Models5 Assessment of RPV and Cavity Models

5.1 Introduction.1 Introduction.1 Introduction

The purpose of this section is to summarize the status of the assessment of the models for melt discharge from the RPV and debris entrainment and dispersal from the cavity. The original plan was to proceed in two stages:

1. Gain familiarity with the new models by exercising them on a selected experimental simulation (SNL/IET-3), and define a standardized prescription for their use, including specification of the "cavity constant" parameter, K_c [Gri94].

2. Using the standardized prescription, apply them to other experiments to determine the degree to which they can fit the experimental trends without retuning any parameters.

However, the first stage required more time than had been anticipated, as this effort was the first use (other than developmental testing [Gri94]) of these models in the integrated phenomenological environment of the CONTAIN code, and a number of unanticipated behaviors were encountered. Hence it was not feasible to proceed to the second stage within the scope of this work, and the present section should be viewed as more of a status report than a completed assessment.

The RPV models include ablation of the vessel hole, single-phase molten debris discharge, gas blowthrough, and two-phase debris/gas discharge. These models are described in more detail in References Gri94 and Pil92.

The cavity models include correlations for the entrainment rate of debris, for the total fraction of debris dispersed from the cavity, and a Weber break-up model for determining the size of entrained debris droplets. The assessment primarily focused on two of the entrainment rate models, the Whalley-Hewitt and Levy models. A previous assessment of the entrainment rate models using experimental results obtained with low-temperature simulants is described in Reference Wil96.

The cavity models include a number of user options. The present assessment has been limited to the most mechanistic option, in which the principal user-specified input includes the initial conditions, the entrainment correlation to be used, certain cavity geometric parameters, and a cavity constant, K_c, which is discussed below. The code then calculates the entrainment rate and takes into account the interactions between airborne and nonairborne debris and the cavity gas. The two-way coupling between debris entrainment and the entraining gas flow is therefore modeled, and the mass of debris dispersed from the cavity is simply the integral of the entrainment rate.

In other less mechanistic options, the user can specify the fraction dispersed, either directly or by specifying a dispersed fraction correlation which the code will first use to calculate the dispersed fraction. The code then calculates the entrainment rate in a side calculation using whatever correlation the user specifies, and normalizes this rate to obtain the predefined dispersed fraction. In effect, this side calculation generates debris source tables which are then input to the main calculation, much as if the user specified the sources directly. In the side calculation, debris-gas interactions are not modeled and there is no feedback or coupling between debris entrainment and the entraining gas flow. Instead, the user must define through input the conditions (e.g., pressure, gas density, molecular weight) expected to exist in the cavity during entrainment, and these conditions are held constant in the side calculation that generates the debris sources. These options have not been assessed in the present work.

The Weber model was not used in the present assessment, because the effects of the Weber model on the DCH cavity models have not been evaluated, and a stepwise approach to assessment was desired. The debris droplet size distribution was specified through input and was the same as in the standard prescription described in Section 3.2.2. Assessment of the Weber model is recommended as a future activity.

5.2 Initial Findings.2 Initial Findings.2 Initial Findings

5.2.1 CONTAIN Input Summary.2.1 CONTAIN Input Summary.2.1 CONTAIN Input Summary

The IET-3 test was modeled in CONTAIN with five computational cells instead of using the 14-cell deck employed elsewhere in this study. Sensitivity of the Zion IET analyses to nodalization is discussed in Section 6.1.3. In brief, some phenomena (notably debris trapping and transport in the subcompartments) are better represented with the more detailed nodalization, but the RPV and cavity entrainment modeling of interest here are not expected to be sensitive to the nodalization. The principal results of interest to the present study are the behavior of the RPV and cavity models, and these are insensitive to events downstream of the cavity exit. Since the 14-cell deck would have been awkward to use in the large number of exploratory runs that were required in this study, the 5-cell deck was adopted. The cells are defined as follows:

" Cell 1: Accumulator cell for steam blowdown.

" Cell 2: Melt generator, including pipe between melt generator and rupture disk. When the RPV model is to be used, debris is initially introduced into this cell at the start of the calculation.

" Cell 3: Cavity and chute.

" Cell 4: Subcompartment.

" Cell 5: Dome (main volume of the Surtsey DCH facility).

Except for the input required to use the RPV and cavity models, the deck used was equivalent to Case I3c547 of Section 6.1.3 and Table 6.1-4.

The melt generator hole size, d_h, was held fixed at 0.04 m. The ablation model was not used, since a graphite limiting plate (nominally nonablating) was used to determine the hole size in this experiment. Geometric parameters for the cavity were the recommended values given for Zion in Reference Gri94 (scaled to 1/10 linear scale). The various "standard values" required by the Levy model were also taken from Reference Gri94.

All the correlations available in the CONTAIN code for debris entrainment and dispersal require the user to specify a so-called "cavity coefficient," K_c, which must be determined by fitting to experimental results. Values of K_c obtained by fitting to the low-temperature simulant data base [Wil96] are summarized in Reference Gri94 and served as a starting point for the present investigation. However, there are large uncertainties involved in applying the results of the low-temperature, nonreactive simulant experiments to high-temperature chemically reactive melts. Hence it was not expected that the previous values would be immediately applicable to the present case. Model outputs as a function of K_c are discussed further in Section 5.3.

In terms of the RPV and cavity model assessment, the principal results of interest are the fraction of the total debris which is dispersed out of the cavity, f_{disp}, and the degree of coherence between the debris dispersal interval and the accumulator blowdown. For present purposes, the measure of coherence is taken to be f_{coh} as it was defined in Eq. (3.2-1). In evaluating f_{coh}, the time at which entrainment of debris from the cavity effectively ends was defined to be the time at which the mass dispersed from the cavity reaches 95% of its final value. The choice of 95% is partially arbitrary, although values either much larger or much smaller can be shown to be inappropriate. In any case, f_{coh} is only defined for the sake of convenience in comparing the degree of coherence obtained for various code calculations and/or experiments. These comparisons are not sensitive to how f_{coh} is defined, e.g., whether it is based upon a 90% or 95% dispersal point. No other result of interest (ΔP, H_2 generation, etc.) is affected by this choice.

5.2.2 Summary of Results of Exploratory Studies.2.2 Summary of Results of Exploratory Studies.2.2 Summary of Results of Exploratory Studies

The CONTAIN RPV and cavity models represent a first attempt to model classes of phenomena which have never been modeled before in the CONTAIN code, and a considerable familiarization effort was required. It would serve little purpose to detail every case that was run. Instead, we summarize some of the more important results, and give the prescription for use that was developed.

Timing of Gas Blowthrough. The model for gas blowthrough and two-phase discharge requires as input the diameter, D_{RPV}, of the RPV vessel (melt generator, in the experiment). This value is required in order to calculate the depth of the liquid and thus calculate the point at which gas blowthrough marks the onset of two-phase discharge. In addition, the depth at blowthrough is itself a function of the ratio D_{RPV}/d_h.

When the actual melt generator diameter (0.4 m) was specified, blowthrough was predicted to occur within the first 0.1 s following brass plug failure, in apparent disagreement with the experimental results. (Although one cannot precisely determine the moment of blowthrough in the experiments, the accumulator pressure-time curves show very little depressurization during the first few tenths of a second; see, for example, Figure 3.2-1.)

In developmental testing [Gri94], the tendency toward early blowthrough was reduced by setting D_{RPV} equal to a value considerably smaller (0.15 m) than the actual melt generator diameter, and this was done in some of the initial runs in the present study. However, both the blowthrough correlation and the correlation for discharge quality in the two-phase discharge stage depend explicitly upon the ratio D_{RPV}/d_h, in addition to the implicit dependence upon D_{RPV} (i.e., via the dependence of liquid depth upon D_{RPV}). Hence specifying a fictitious value of D_{RPV} would be expected to distort the model's dependence upon hole size, and this approach was abandoned.

Other RPV Ejection Issues. It would not be possible to match the experimental pressure-time histories for the accumulator simply by suppressing early blowthrough. If blowthrough were to be completely suppressed, a simple single-phase liquid ejection calculation shows that the melt would be ejected in about 0.25 s, assuming a liquid-phase discharge coefficient, $C_{d,liq}$ equal to 0.6. After this time, the melt generator orifice would then be completely unobstructed and single-phase blowdown would then proceed unencumbered by any liquid. The slope of the accumulator pressure-time curve would immediately reach its maximum at this point. Comparison with the experimental depressurization curves of Figure 3.2-1 shows that the curves do not actually reach their maximum slope until well after 0.5 s. Furthermore, the amount of depressurization that occurs by 0.25 s is typically less than the 4% which one would expect from ejecting only the melt, without even allowing for any steam blowdown.

The RPV two-phase discharge model is a simple separated-flow model, and it is apparent from the preceding that the model allows too rapid a rate of onset of the discharge process which could not be corrected by simply correcting the calculated time of blowthrough. The user can specify the discharge coefficient values used for both the liquid and gas phase, and these could probably be tuned to obtain better agreement with the early stage of the discharge process. However, there could be little confidence that the values used would give good results for other scenarios not studied. Furthermore, after approximately the first second, "normal" values [Sha53] of the gas discharge coefficient, 0.6-0.85, gave good results for the blowdown history. Hence, no effort was made to tune the discharge coefficients, and the values used were 0.6 for the liquid and 0.68 for the gas, with the latter value being the *vena contracta* factor specified for the CONTAIN choked flow model [Was91].

Once blowthrough occurs in the RPV model, the rate of liquid discharge rapidly decreases and steam blowdown rates rapidly accelerate. Taken together with the early blowthrough, this behavior means that the rate of discharge, rather than the rate of entrainment from the cavity, was found to determine the coherence factor, f_{coh}, when calculated entrainment rates were large. Although it has been conventional to assume that cavity entrainment processes, rather than RPV ejection processes, govern f_{coh}, there is no inherent reason why this must always be the case; note also that 5-10% of the melt remained in the melt generator in all the steam-driven Zion IET experiments. Thus, the behavior of the model in this regard is not necessarily unrealistic, at least in a qualitative sense.

There is some evidence, however, that the model is overestimating the degree to which the time required for melt ejection can increase f_{coh}, which is discussed further in Section 5.3. In other contexts, overpredicting f_{coh} tends to be conservative, and that may be the case here so long as melt ejection is complete well before blowdown is complete. However, in the present instance, no debris-steam interactions are normally modeled for melt remaining in the RPV. Furthermore, as d_h increases, the rate of steam blowdown in this model will increase considerably more rapidly than the rate of melt ejection. With a large hole size, there is a possibility that considerable melt could remain in the RPV until there is little or no blowdown steam left for it to interact with once it does leave the melt generator. (There are no experimental data to appeal to here, as all experiments with $d_h \geq 0.6$ m scaled equivalent have been performed in melt generators with a nonprototypical geometry having D_{RPV} much less than the prototypical scaled equivalent, which would suppress the effect of interest here.)

The nonairborne debris model can be activated in the RPV, and it could in principle be used to ensure that late ejection does not deprive the melt of all opportunity to interact with steam. Again, the concept is not inherently unreasonable (see Section 3.2.2), and some computational experiments were performed using the nonairborne model in the melt generator. Doing so resulted in the melt generator and accumulator pressures rising slightly until blowthrough occurred, and some numerical oscillations appeared. Although the latter were small in amplitude, they could be an indication that worse things could happen under other conditions. In addition, it was considered difficult to develop and validate a defensible "standard prescription" for the use of the nonairborne debris model in the RPV, something that was not envisioned when either the nonairborne model or the RPV model was developed. Hence this approach was not pursued further.

Initial Spike in Cavity Entrainment Rates. Initial experimentation with the RPV and cavity models was performed with the reduced value of D_{RPV} suppressing early blowthrough and without the nonairborne debris model being active. It was found that, immediately after blowthrough occurred, there would be a very sharp spike in the entrainment rate, which might disperse as much as 5-10% of the debris in about 0.01 s.

Experimental results show no sign of such behavior, and the reason for it in the calculation was found to be the fact that the RPV model calculates the rate of ejection but no actual ejection is modeled; the code simply performs a nonphysical transfer of debris from the RPV nonairborne debris field to the cavity nonairborne debris field. By the time blowthrough occurs, a large reservoir of debris may have accumulated in the cavity, yet the cavity atmosphere is still cold, a situation which is physically quite unrealistic. Once blowthrough occurs and entrainment starts, the cold cavity gas is rapidly heated, accelerating the flow out of the cavity, which accelerates entrainment, etc. The result is a "runaway" which terminates only as the cavity gas temperature approaches a steady-state value limited by the debris temperature.

In reality, the first debris ejected from the RPV heats the cavity atmosphere as it is ejected. Cavity pressure curves generally show a small initial pressure spike which is attributed to this process [All94b, Bla94]; note the small peaks during the first 0.05 s in Figure 3.2-2, prior to the main FCI peaks. This heating occurs as the first debris enters the cavity and is probably complete before any significant amount of debris accumulates in the cavity.

When this behavior of the model was identified, it was expected that use of the nonairborne model as in the standard prescription would pre-heat the cavity and yield a more realistic behavior, and the problem was initially believed to be of no great concern. This expectation was fulfilled so long as an artificially small value of D_{RPV} was used to suppress early blowthrough as described previously. However, when the correct value of D_{RPV} was used, the problem reappeared, although in a less extreme form. The reason was that, with the early blowthrough, the nonairborne debris no longer had time to heat the cavity atmosphere sufficiently to prevent the runaway effect at the onset of entrainment. One could still avoid the effect by specifying a reduced value of trapped debris field diameter, d_t, prior to blowthrough and then increase it to the desired (i.e., standard) value at or before blowthrough. Since the only available means of varying d_t in the nonairborne model is by explicit user specification, this approach requires foreknowledge (e.g., from a prior run) of when blowthrough occurs. It is not very amenable for use in a "standard prescription" and has not been pursued in this work.

An approach that was tried is specifying an initial temperature for the cavity atmosphere equal to the debris temperature. However, it was found that the cold cavity structures cooled that atmosphere so rapidly that the problem was only reduced, not eliminated. In addition, this approach represents a nonphysical perturbation of the mass and energy balance of the containment, albeit a very small one when the cavity volume is small, as is the case here. Hence the approach was not pursued further.

When the nonairborne debris model is used as in the standard prescription, it is likely that the problem considered here will only arise when blowthrough occurs soon after, but not at, the time of vessel breach. If the blowthrough is delayed, the nonairborne debris will heat the cavity gas as noted above. Although it has not been demonstrated, it is likely that the problem will not arise if blowthrough occurs immediately at the time of vessel breach, something which can easily happen if the initial value of d_h is large. The reason is that entrainment of debris should also start immediately, heating the cavity atmosphere before any significant reservoir of melt accumulates in the cavity.

The recommended procedure is therefore to attempt no a priori fixes, but to check the initial calculation for occurrence of this problem. If it does arise, the best approach is probably to specify a reduced value of d_t up to the time of blowthrough, when d_t should assume the value desired for the main calculation.

Debris-Water Interactions. When the cavity models were implemented, they were not designed for use with co-dispersed cavity water. There were several reasons for this limitation. One reason is that the assessment of candidate models against the data base obtained with low-temperature simulants provides no insights concerning FCI phenomena. Another is that the dry-cavity problem was considered to be complex enough for an initial implementation, without adding the further difficulty of debris-water interactions. A more physical reason, however, was a widespread belief that water may not play a very important role in DCH, on the grounds that the initial FCI may blow most of the water out of the cavity before it has any chance to interact with debris. Some experimental results, including the WC-2 results, have been cited to support this belief.

However, it is the present interpretation that results presented in Sections 6.4 and 6.5 justify reconsideration of the belief that water is unimportant, at least for the Zion-geometry experiments. As noted elsewhere (e.g., Section 3.2.8), CONTAIN's ability to model debris-water interactions is limited and parametric in key respects. The recommended procedure is to conduct parametric studies with water sourced into the calculation in parallel with the debris sources. Although parametric in terms of the amount of water assumed to participate, the approach does allow the user to investigate the potential consequences of debris-water interactions as a function of their efficiency in a controlled manner.

The point to be made here is that it may be difficult to investigate the potential effects of water when the cavity models are being used. In order to define an approach comparable to that recommended when user-defined sources are employed, the water and debris sources would be required to have the same time dependence. The water source is user-specified, but the debris source is generated by the code with a time dependence not known a priori. One cannot simply perform a preliminary run to determine the time dependence because introducing the water will have a large effect upon the gas flow velocities and densities that govern the entrainment rates and hence have a large effect upon the debris entrainment rates. Perhaps most important of all, even if one did match the time dependencies, the resulting debris source might be very unrealistic because the parallel-source approach with user-specified sources is an artifice designed to simulate other possible effects of debris-water interactions; it is not expected to yield a reasonable simulation of the relationship between cavity water and debris dispersal processes, even in a parametric sense, because the effect of water upon debris dispersal may be controlled by details of the actual FCI processes, which are not modeled.

At present, therefore, use of the cavity entrainment models with co-dispersed water sensitivity studies is not recommended, except in an experimental mode. This caveat may not apply to the less mechanistic modes in which the debris sources are generated in a side calculation, because the side calculation would not include the debris-water interaction.

Gas Velocity Modeling for Entrainment. In the entrainment models, the calculated entrainment rates are a strong function of the gas flow velocities through the cavity. In the default model, this flow velocity is based upon the average of the volumetric inflow and outflow rates divided by a cavity hydraulic area (specified as part of the geometric input [Gri94]), and calculations were initially performed using this option. If the keyword 'usevout' is specified, the velocity used will be based upon the volumetric outflow rate only. It was subsequently decided that this option is physically more reasonable in that the outflow rate is based upon cavity cell conditions (temperature, etc.) which, as always in CONTAIN, already represent an average for the conditions existing in the cell. Use of the default does no known harm, however; it can be compensated for by using larger values of K_c in order to obtain equivalent results.

Summary. To recapitulate, several possible problems with the behavior of the RPV and cavity models were identified. These include early blowthrough, discharge of melt too slowly relative to steam discharge rates, and an initial spike in the melt dispersal rate. Means of dealing with them were considered and appear to be useful if used with care based upon a consideration of the individual case at hand. However, we do not believe that any of them are sufficiently well justified that they can be recommended for incorporation into a standardized prescription for using these models.

The remainder of this assessment focused on studying dispersal behavior as a function of K_c and selecting values of K_c that yield reasonable results for the SNL/IET-3 experiment. With the exception of the choice of the 'usevout' option, model options selected are generally defaults, parameters based upon the actual geometry (including d_h and D_{RPV}), and "normal" values of the discharge coefficients (0.6 for the melt, 0.68 for the gas choked flow *vena contracta* factor). No special fixes for the potential problems discussed above are incorporated.

5.3 Discussion of Results with the Standard Input.3 Discussion of Results with the Standard Input.3 Discussion of Results with the Standard Input

The calculated results that are considered to be of greatest importance in assessing performance of the RPV and cavity models themselves are the dispersed debris fraction (f_{disp}) and the coherence fraction (f_{coh}). In addition, the sensitivities of the containment pressurization (ΔP) and hydrogen production ($N_{H2,prod}$) to the cavity model behavior are also of considerable interest, and these results will also be given.

An important result is that it is not, in general, possible to find values of K_c that permit a good match with the experiment results for both f_{disp} and f_{coh}. This result was also obtained when model options other than the standard options defined above were used; for example, it was also obtained when a reduced value of D_{RPV} was employed to suppress early blowthrough and when nonairborne debris interactions were not modeled.

Four cases of particular interest are summarized in the following discussion. These cases are defined as follows:

Case A: The Whalley-Hewitt entrainment rate model was used. The cavity coefficient, K_c, was varied until a match with the experimental data for the dispersed fraction (approximately 0.7) was obtained. The resulting value of K_c was 43.0.

Case B: As in Case A, except that K_c was increased to 300 in order to more nearly match the experimental value of the coherence fraction.

Case C: The Levy model was used to calculate the entrainment rate. The cavity coefficient, K_c, was varied until a match with the experimental data for the dispersed fraction was obtained, with a K_c value of 0.75 being obtained.

Table 5.3-1 Experimental and Analytical Results for SNL/IET-3					
Quantity	**SNL/IET-3 Experiment**	Case A	Case B	Case C	Case D
f_{disp}	~ **0.70**	0.687	1.000	0.678	0.987
f_{coh}	~ **0.25**	0.718	0.338	0.480	0.340
ΔP (MPa)	**0.246**	0.242	0.232	0.238	0.237
f_{dome}	**0.088**	0.081	0.114	0.107	0.155
$N_{f,H2}$ (g-moles)	**37**	95	49	82	49
$N_{H2,burn}$ (g-moles)	**190**	194	172	187	171
$N_{H2,prod}$ (g-moles)	**227**	288	221	269	220

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Case D: This case differs from Case C only in that the value of K_c was changed to 30.0 in order to more nearly match the coherence fraction.

The results are summarized in Table 5.3-1.

In Case A, using the Whalley-Hewitt entrainment rate model, a value of $K_c = 43.0$ produces a dispersed debris fraction of 0.687, which agrees with the experimental result of approximately 0.70. It is interesting (and perhaps surprising) to note that the Case A value of K_c agrees with the results of the assessment of the cavity models using the low-temperature simulant experiments, which also found that a value of 43 gave a reasonable fit for water dispersal fractions measured for the Zion cavity at 1/10-scale. However, the value of f_{coh} obtained for Case A, about 0.72, is much greater than the experimental value of about 0.25.[*] The containment pressure load due to DCH in Case A was 0.242 MPa, compared to 0.246 MPa from the IET-3 data.

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[*]*This value is slightly greater than the value of 0.23 cited for the SNL/IET-3 experiment elsewhere in this report because values in Section 5 were calculated in a way that permitted some perturbation due to oxygen uptake by nonairborne debris to increase the apparent value of f_{coh} to some degree, while this perturbation was largely or totally eliminated in the results cited in Sections 6 and 7. Comparisons of experimental and calculated f_{coh} values are not invalidated here as both were calculated in the same way.

K_c was set to 300 in Case B, producing a dispersed fraction of 1.0, but with a coherence fraction of 0.338, in better agreement with experiment. The pressure load on the containment due to DCH was 0.232 MPa. With the Whalley-Hewitt model, the coherence fraction becomes insensitive to K_c for $K_c > 300$, as illustrated in Figure 5.3-1. Therefore, the best value of the coherence fraction from the code simulation using the Whalley-Hewitt model is about 0.34, which is somewhat greater than the IET-3 experimental result. The reason that f_{coh} becomes insensitive to further increases in K_c is that the coherence is determined by the rate of ejection from the RPV rather than the entrainment rates when K_c is large, as was discussed in Section 5.2.2.

Examination of the details of the calculation indicated that about 28% of the steam had exited the accumulator at the time 95% of the debris had exited the melt generator. This means that an absolute lower bound to f_{coh} that the RPV model could give would be 0.28, even if one postulated instantaneous entrainment and instantaneous transport of entrained material out of the cavity. The fact that this lower bound to f_{coh} is still somewhat greater than the experimental f_{coh} indicates that the RPV model is overpredicting the role of RPV ejection in controlling f_{coh}, if such a role does exist at all.

Cases C and D use the Levy entrainment rate model. From the low-temperature simulant results, the recommended value of K_c is 0.0073, but this resulted in very little cavity dispersal being calculated ($f_{disp} \approx 0.04$). It was found that, for the Levy model, $K_c = 0.75$ results in a dispersed fraction of 0.680, while the coherence fraction is then 0.480. Note that this value of K_c is two orders of magnitude greater than that inferred from the low-temperature simulant experiments. Containment pressurization due to DCH was 0.238 MPa.

The desired coherence fraction was more closely approached by setting $K_c = 30$ (Case D), which yielded f_{coh} equal to 0.34, a dispersed fraction of 0.987 and a ΔP of 0.237 MPa. For $K_c > 30.0$, the coherence fraction does not change significantly, as shown in Figure 5.3-2. As with the Whalley-Hewitt model results, this limiting value is determined by the RPV ejection model and it is therefore essentially independent of the cavity model.

Table 5.3-1 summarizes the calculated values of f_{disp}, f_{coh}, and ΔP for these four cases and also gives the experimental results. Additional results given in the table include f_{dome} and results for the number of moles of hydrogen present at the end of the simulation ($N_{f,H2}$), the number of moles burned ($N_{H2,burn}$), and the number of moles produced ($N_{H2,prod}$). The inability to obtain good agreement with both f_{disp} and f_{coh} is evident from the table. The Levy model is somewhat superior to the Whalley-Hewitt model in this regard, in the sense that the value of f_{coh} obtained (0.48) when f_{disp} is matched (Case C) is smaller than the Whalley-Hewitt value (0.72) for Case A. This result is a consequence of the fact that the Levy model gives a more sharply peaked entrainment rate versus time curve.

For the most part, the Case A and Case C results are very similar to Case B and Case D results, respectively. This similarity supports the belief that results of interest are not very sensitive to details of the debris source time dependence so long the dispersal parameters f_{disp} and f_{coh} are reasonably similar. Note, however, that Case D does yield a higher value of f_{dome} than the others. This behavior reflects the more sharply peaked dispersal history calculated by the Levy model, plus the fact that the 'rhodg = mix' option of the TOF/KU trapping model is somewhat sensitive to high dispersal rates because it credits the debris momentum flux in evaluating the de-entrainment criteria (Section 3.2.4).

What may be somewhat more surprising is that all four cases are quite similar in terms of the hydrogen data and, especially, ΔP. There is also reasonably good agreement with experiment in all cases. To some extent, the similarity in the results reflects opposing effects as one goes from Case A to Case B, and from Case C to Case D. As f_{disp} increases, f_{coh} decreases.

Sensitivities to K_c are displayed graphically in Figures 5.3-1 through 5.3-10. In these figures, f_{coh}, f_{disp}, f_{dome}, ΔP, and $N_{H2,prod}$ are plotted against K_c for both the Whalley-Hewitt model and the Levy model. Again, sensitivity displayed by the ΔP and hydrogen production results is not large. As before, cancellation of opposing effects is a factor. However, it is also true that sensitivity studies varying f_{coh} and f_{disp} individually show that, with the standard prescription (including the nonairborne model), sensitivity to these parameters tends to be less than has often been assumed; see Section 6.3 for some of these results.

Figure 5.3-1. Coherent steam fraction as a function of the cavity coefficient, K_c, for the Whalley-Hewitt model.

Results given in Section 6.3 also show that sensitivity to f_{coh} and f_{disp} can be greater when the nonairborne model is not used, and that the experimental results for the Zion IET experiments tend to be underpredicted without the nonairborne model, even when both f_{disp} and f_{coh} are relatively large. Similar trends have been obtained when the cavity model is used without the nonairborne model; that is, there is greater sensitivity to f_{disp} and f_{coh} (and hence to K_c), and the experimental results are generally significantly underpredicted.

5.4 Summary, RPV and Cavity Assessment.4 Summary, RPV and Cavity Assessment.4 Summary, RPV and Cavity Assessment

The results of the assessment of the RPV and cavity models are encouraging in the sense that good agreement with the experimental results was obtained for the integral results of greatest interest (i.e., ΔP and hydrogen production), and this agreement did not appear to be very sensitive to uncertainties in the model.

An important qualification here is that the assessment has been limited to comparison with the results of a single experiment. It obviously would be desirable to extend the assessment to other experiments and, especially, to determine whether values of the cavity coefficient, K_c, which yield reasonable values of the dispersed fraction or the coherence factor continue to do so when applied to experiments for which the controlling parameters (driving pressure, vessel failure size, cavity geometry, and geometric scale) are different from those of the SNL/IET experiments. Note, however, that experiments with parameter combinations in the regime most likely to generate high containment loads (high driving pressure, large failure sizes, and in particular the combination of the two) are not available, especially in the case of the Zion geometry. This limitation applies to the entire assessment effort, however, and is hardly a reason for not proceeding further in the case of just the RPV and cavity models.

Another limitation of the assessment is that it has been limited to the most mechanistic of the options available. The various options that permit the user to exert more control over the entrainment and dispersal process have not been assessed.

The models have revealed some limitations which must be kept in mind and which would not be resolved by simply extending the assessment to include more experiments. These include the tendency toward early blowthrough, a possible tendency to eject melt too slowly in comparison with the rate of blowdown, an anomalous spike in the initial rate of entrainment from the cavity, and an inability to match both the dispersal fraction and the coherence factor with the same value of K_c. In addition, it is questionable whether the models will be useful in sensitivity studies involving debris-water interactions. (The latter limitation may not apply to the less mechanistic options.)

It is concluded, therefore, that use of these models can be recommended only in a "friendly user" mode. That is, they are recommended for use only by investigators knowledgeable about DCH phenomenology who are prepared to examine the results for unexpected or unreasonable behavior and to cope with it if it arises. Other users probably will be safer if they stay with the user-defined sources following the prescriptions given elsewhere (Sections 3.2.2 and 7.3) in this assessment report.

6 Detailed Assessments of Specific Model Features Detailed Assessments of Specific Model Features Detailed Assessments of Specific Model Features

In this section, a number of specific model features are assessed in more detail than was done in Sections 3 and 4. The assessment typically includes the results of sensitivity studies illustrating the effect of varying an appropriate parameter or modeling assumption. Most of the results will be summarized in tabular form. We also discuss the results of some experiments that have not been analyzed with CONTAIN when these results provide additional insights concerning the validity of the CONTAIN models.

In some cases, the sensitivity studies cited were performed prior to definition of the current standard prescription and/or prior to some relatively recent corrections to the coding of the slip and trapping models. These results are included here when subsequent changes have not invalidated the intended purpose of the comparisons. It would be tedious, and would serve little purpose, to detail every way in which each of these earlier studies deviates from the standard prescription. Hence, in the tables summarizing results, all cases which deviate from the standard prescription in ways not explicitly identified are marked with an asterisk (*). Comparisons between such cases should be limited to those discussed in the text since, in general, there may be differences between such cases other than those explicitly acknowledged. All cases not identified with an asterisk are run using the standard prescription except for those differences explicitly identified in the tables and the accompanying text. All these cases are therefore comparable with one another.

The large majority of all the sensitivity studies that involved the IET experimental series were performed for the SNL/IET series, and, for convenience, "SNL" will be omitted; it should be understood that "IET" refers to "SNL/IET" except where explicitly stated otherwise. The abbreviation "NAD" will be used to refer to the processes represented by the nonairborne debris model.

Format of Presentation of Results. In the course of this work, a large number of sensitivity studies were performed, not all of which will be discussed here. A tabulation of most of the results obtained after the standard prescription was defined is given in Appendix D, which also acknowledges some minor input errors that were subsequently discovered in some of the cases. (These errors are noted in the main text only if the effect on ΔP was $\geq 1\%$.) Most of the tables in the present section follow a standard format illustrated by Table 6.1-1 in the following subsection. An identifying case number is given first, followed by a brief description of the parameter or model variations defining the case and an asterisk if other differences with respect to the standard prescription exist. The first two or three characters of the case number are an abbreviation representing the experiment and are followed by a "c" and one or two digits designating the number of computational cells in the deck used. The last two digits are simply a serial number. For example, "L1ac501" represents a simulation of the LFP-1A experiment run on a 5-cell deck, "I6c1407" represents an IET-6 simulation run on the 14-cell deck, etc.

Subsequent columns in the tables give the pressure rise (△P) in MPa, the fraction transported beyond the subcompartments (f_{dome}) defined as in Eq. (4.3-1), the number of moles of hydrogen present at the end of the calculation ($N_{f,H2}$), the number of moles of hydrogen burned ($N_{H2,burn}$), and the number of moles of hydrogen produced ($N_{H2,prod}$). The last two quantities are defined as given in Eq. (4.1-1), which means that all oxygen consumption is treated as representing hydrogen which is first produced by metal-steam reactions and subsequently burned. For all quantities tabulated, the experimental results (where available) are given first in **bold** print.

6.1 Debris Trapping, Transport, and Nodalization.1 Debris Trapping, Transport, and Nodalization.1 Debris Trapping, Transport, and Nodalization

6.1.1 Open-Geometry Experiments.1.1 Open-Geometry Experiments.1.1 Open-Geometry Experiments

In the WC series and the LFP-8A experiment, the concrete slab which was used to limit the unobstructed flight path in the LFP experiments was 7.7 m above the cavity exit, and about 75% of the total Surtsey volume was below this slab. These experiments are therefore categorized as having an open or noncompartmentalized containment geometry. Sensitivity to trapping parameters was investigated for WC-1 and results are summarized in Table 6.1-1.

Table 6.1-1 Sensitivity to Trapping and Slip, Open Geometry (WC-1)						
Case	Description	ΔP (MPa)	f_{dome}	Hydrogen Data (g-moles)		
				$N_{f,H2}$	$N_{H2,burn}$	$N_{H2,prod}$
	WC-1 Experimental Results	**0.272**	**0.033**	**145**	**---**	**---**
W1c506	Standard Input	0.314	0.063	152	1.0	153
W1c510	No NAD	0.300	0.063	105	1.1	106
W1c505	L_1 = 6V/S (5.1 m)	0.277	0.048	145	1.0	146

The standard input prescription (Case W1c506) overpredicts ΔP by about 15% and gives a good result for hydrogen production. In the main containment volume (Cell 4), trapping in the TOF/KU model occurred on the first impact, which results in some sensitivity to L_1; reducing L_1 from 7.7 m (the actual cell height) to the value implied by the 6V/S rule (5.1 m) reduced ΔP by about 12%. On the other hand, specifying GFT trapping instead of TOF/KU trapping resulted in an increase in ΔP of about 13%.

As would be expected, totally eliminating trapping results in substantial additional increases in ΔP (Case W1c508). However, comparison with Case W1c514, in which both heat transfer to structures and trapping were deleted, shows that trapping is not the only mitigating effect; that is, even when there is no trapping, significant mitigation due to heat transfer to the structures is calculated to occur for the parameters of this particular scenario. Both Case W1c508 and Case W1c514 yield much greater hydrogen production than the cases with trapping because, without trapping, debris hangs in the air indefinitely and can eventually react with the blowdown steam even though the latter is greatly diluted by the inert containment atmosphere. With realistic trapping rates, little reaction can occur once the debris leaves the cavity and chute volume, due to the low steam concentrations.

Table 6.1-2 Trapping and Slip, Nonprototypic Compartmentalized Geometry (LFP-1A)						
Case	Description	ΔP (MPa)	f_{dome}	Hydrogen Data (g-moles)		
				$N_{f,H2}$	$N_{H2,burn}$	$N_{H2,prod}$
	LFP-1A Experimental Results	**0.117**	**0.026**	**235**	**---**	**---**
L1ac501	Standard Input	0.206	0.230	188	1.0	189
L1ac502	No NAD	0.198	0.240	158	1.1	159

In Case W1c515, the slip factor is set equal to 5 in the main containment volume. For this geometry, there is little effect. The fraction transported beyond the concrete slab (f_{dome}) is reduced; however, this fraction is unimportant in this case because f_{dome} is small even for s_d equal to unity and because most of the containment volume is below the slab.

6.1.2 Slip and Trapping in the LFP Experiments.1.2 Slip and Trapping in the LFP Experiments.1.2 Slip and Trapping in the LFP Experiments

Except for LFP-8A, the containment geometry in the LFP experiments may be characterized as compartmentalized but nonprototypic. In Section 4.3, it was noted that ΔP was overpredicted in these experiments, and the principal reason was that the fraction transported beyond the concrete slab limiting the flight path was substantially overpredicted. The overprediction of ΔP was largest for LFP-1A, and it was therefore selected for additional study.

Some results obtained for LFP-1A are summarized in Table 6.1-2. With the standard prescription, ΔP is substantially overpredicted while hydrogen production is somewhat underpredicted. Deleting the nonairborne debris interactions does not improve agreement because the effect upon ΔP is small while the tendency to underpredict hydrogen production is increased.

In Case L1ac508, s_d was set equal to 5 in the subcompartments (Cell 4), which substantially reduced f_{dome} and reduced ΔP, although both are still overpredicted somewhat. (Case L1ac508 is corresponds to the "Case 4" calculation of Section 4.3.) It is evident that overprediction of f_{dome} is the principal reason for the overprediction of ΔP when the standard input prescription is applied to this experiment. Since increasing s_d increases airborne residence time in the subcompartments for some of the debris fields, there is a slight increase in hydrogen production, relative to the standard case.

In the standard prescription, L_1 was taken to be the actual cell height, 0.91 m, since the debris enters the subcompartments via a vertical chute. L_2 was estimated to be 2.2 m using the 6V/S rule. These definitions are in accord with the general rules given in Section 3.2.4. However, the subcompartment in LFP-1A has a "pancake" geometry with the diameter (3.7 m) being about 4 times the cell height. It was conjectured that the cell height might be a better value for L_2 than the generic 6V/S value, and Case L1ac505 was therefore run with L_2 equal to 0.91 m. However, the improvement is seen to be minor. No doubt additional reductions in the trapping lengths would yield better results, but there would be no physical basis for such values and, hence, the results could not be used to develop a general rationale for defining the trapping lengths in other problems. Efforts to define "improved" trapping lengths were therefore abandoned.

Cases L1ac506 was run using the less conservative 'rhodg = gas' option; that is, only the gas momentum flux is credited when evaluating the Kutateladze number in Eq. (3.2-3). Results show a considerable reduction in f_{dome} and, hence, in ΔP, improving agreement with the experimental results. There is some reduction in hydrogen production, but the effect is not large. In this case, debris was calculated to de-entrain upon the first structure impact, which does not agree well with the experimental observation that only 7% of the dispersed debris was found to be adhering to the underside of the concrete slab; most was recovered from the floor of the Surtsey vessel. This experimental result agrees with the intuitive expectation that, with the first impact point less than a meter from the cavity exit, much of the debris would splash and remain airborne, with permanent de-entrainment requiring a second impact.

Case L1ac507 was run with 'vnost = cnvel', which had no effect. The 'vnost' option only has an effect when debris does not de-entrain on either the first or second impact, and debris evidently always de-entrained at either the first or second impact in this calculation.

It is believed that, in the LFP experiments, debris trajectories in the subcompartment largely decouple from the gas flow as was discussed in Sections 3.2 and 4.3. The trapping and transport modeling parameters seeming to give the best results for these experiments are believed to be potentially nonconservative if applied to analysis of other scenarios which may be of greater interest; i.e., more prototypic geometries and/or stronger driving forces for debris transport. Hence, it is not believed that the LFP results justify redefining the standard prescription.

The LFP-2A, LFP-2B, and LFP-2C experiments exhibited trends qualitatively similar to LFP-1A, but the effect of overpredicting f_{dome} was not as large. In LFP-1B, this effect was minor because only 20% of the debris was even dispersed from the cavity in this experiment and overpredicting f_{dome} for this relatively small amount of debris did not have a large effect. Sensitivity studies for these cases were limited to the four cases discussed in general terms in Section 4 and will not be discussed further here. Numerical results are included in the tables of Appendix D.

6.1.3 Slip, Trapping, and Nodalization in the IET Experiments.1.3 Slip, Trapping, and Nodalization in the IET Experiments.1.3 Slip, Trapping, and Nodalization in the IET Experiments

At the time the current assessment effort was initiated, most features of the standard prescription for trapping and slip had already been defined, based largely upon theoretical arguments and experience gained from earlier analyses. Some refinement and re-evaluation was required, however, in part due to recent corrections to the slip and trapping models that were made shortly before freezing the code for the present assessment. This re-evaluation was carried out by analyzing the IET-1 and IET-3 experiments, and the prescription was then frozen for the remainder of the study.

Nodalization, Zion-Geometry IET Experiments. When the present work was initiated, it was thought that a simple 5-cell deck might prove adequate. In this representation (see Appendix A), the subcompartments are represented by a single cell. However, it was found that the calculated result of greatest interest (f_{dome}) for assessing the transport and trapping models tended to be overpredicted unless subcompartment slip values significantly greater than unity were specified. Furthermore, f_{dome} proved somewhat sensitive to geometric parameters whose correct value was difficult to define based upon actual subcompartment geometry. There was also an unrealistic sensitivity to the differences between IET-1 and IET-3, which were quite similar in terms of parameters expected to govern f_{dome} and for which the experimental values of f_{dome} were found to be rather similar. We next discuss these findings in more detail, as they illustrate points that should be considered when defining the nodalization for CONTAIN DCH analyses and resulted in a decision to use the more detailed 14-cell deck developed previously for the IET-1 pretest analysis (see Appendix A).

One problem in the 5-cell deck is that the TOF/KU trapping model requires a flow velocity through the subcompartments to evaluate Ku at the second impact and to evaluate airborne residence times between the first and second impacts. This velocity is inversely proportional to the hydraulic area, A_h, for flow through the cell. With just one cell representing the entire

Table 6.1-3 Selected Sensitivity Studies for the Debris Trapping Model						
Description	IET-1			IET-3		
	ΔP (MPa)	f_{dome}	$N_{H2,prod}$	ΔP (MPa)	f_{dome}	$N_{H2,prod}$
Experimental Results	**0.098**	**0.116**	**233**	**0.246**	**0.088**	**224**
5-cell, default A_h (2.8 m^2) *	0.100	0.213	184	---	---	---
5-cell, A_h = 1.133 m^2 *	0.095	0.150	220	0.183	0.139	221
5-cell, A_h = 0.507 m^2 *	0.107	0.251	222	0.180	0.129	219

subcompartment volume, the default value of A_h (equal to $V_{cell}^{2/3}$) is equal to about 2.8 m^2. However, the subcompartments have a complex internal geometry with considerable internal structure, and the cross sections actually available for flow are considerably smaller than this default value. Use of the default value reduces flow rates and reduces debris transport velocities, which in turn acts to increase debris airborne residence times and transport beyond the subcompartments (f_{dome}) for the parameters of the Zion IET experiments.

Although a value of A_h appropriate to the subcompartments clearly should be less than the default value, any attempt to define a "correct" value appropriate for the entire subcompartment region is difficult to justify. Two values based upon the more detailed 14-cell representation were investigated. The first value, 0.507 m^2, was chosen based upon the default value (i.e., $V_{cell}^{2/3}$) of the first subcompartment cell downstream of the cavity exit in the 14-cell deck. The second value, 1.133 m^2, is equal to the sum of all the flow areas exiting the first subcompartment cell in the 14-cell deck. Some results obtained for IET-1 and IET-3 are summarized in Table 6.1-3, along with standard-prescription results using the 14-cell deck.

In the IET-1 analysis, f_{dome} first decreases as A_h is reduced and then increases as A_h is reduced further. The reason for the initial reduction is that, in the CONTAIN model, the fraction transported through a cell is approximately proportional to $\tau_{tr}/(s_d\tau_{fl}+\tau_{tr})$, where τ_{tr} is a characteristic time for trapping, τ_{fl} is a characteristic time for convective flow of the gas through the cell, and s_d is the slip factor specified for the cell (unity in the present instance). The characteristic time scale for trapping is based upon the trapping lengths divided by the corresponding debris velocities; since decreasing A_h increases the velocity between the first and second impacts, τ_{tr} is decreased. However, τ_{fl} is governed by the ratio $V_{cell}/_g$, where $_g$ is the volumetric flow rate of gas through the cell, which is not affected by varying A_h. Hence, reducing A_h tends to reduce calculated transport through the cell, provided the increased velocities do not result in major changes in the degree to which the various de-entrainment criteria based upon Ku are satisfied. However, when A_h was reduced to 0.507 m^2 in the IET-1 analysis, the criterion for de-entrainment on the second impact was no longer satisfied for part of the dispersal period, resulting in an increase in f_{dome}.

These results illustrate the potential sensitivity of the trapping model when the subcompartments are represented by a single cell. This sensitivity is further illustrated by the fact that similar behavior is not evident for the IET-3 analysis, in which conditions were slightly more favorable for de-entrainment on the second impact; no doubt f_{dome} would increase if A_h were reduced further. This sensitivity is believed to be unrealistic, in part because the abrupt threshold for de-entrainment is itself unrealistic and in part because the pathways for debris transport through the Zion subcompartments are somewhat tortuous, with several debris-structure impacts likely being required for any debris that is transported beyond the subcompartments.

Additional sensitivity studies for IET-1 (A_h = 1.133 m^2 case) indicated that f_{dome} was not significantly affected by specifying 'rhodg = gas' (note the contrast with LFP-1A) or specifying 'vnost = cnvel'. The calculated value of f_{dome} could be brought into approximate agreement with the experimental values by specifying s_d = 2, by arbitrarily multiplying trapping rates by a factor of 1.5, or by reducing L_2 and L_3 to 0.454 m, a factor of 1.5 smaller than the 6V/S standard prescription value (0.681 m). There is no good physical justification for any of these changes and, hence, it would be difficult to defend any claim that good results would be obtained for other scenarios involving differences likely to affect trapping.

In contrast with these results, the 14-cell deck gave reasonable values of f_{dome} for both IET-1 and IET-3 without any special tuning. The default values of A_h were used in all subcompartment cells and the trapping lengths were all set in accordance with the standard prescription of Section 3.2.4, with the 6V/S rule being used for L_2 in all subcompartment cells. In addition, f_{dome} values calculated using the 14-cell deck tended to be less sensitive to minor parameter variations, since transport through three cells (for the dominant flow paths) was required for debris to leave the subcompartments and results were not as heavily affected by any one de-entrainment threshold. In the present study, it was important that trapping behavior be reproduced as well as possible in order to minimize the impact of trapping uncertainties upon the assessment of sensitivity to other parts of the DCH model. Hence the decision was made that the 14-cell deck generally should be used for Zion IET analysis.

One reason for the relative success of the 14-cell deck is that, when it was originally designed, it was thought desirable that the nodalization within the subcompartments be sufficiently fine that actual conditions would not be expected to vary greatly within the region represented by a single cell. Among other things, this condition implies that cell dimensions should not be significantly larger than the mean unobstructed flight path for debris, since otherwise the amount of airborne debris is likely to vary substantially within the volume represented by the cell. (This condition was relaxed somewhat for parts of the subcompartment region further from the cavity exit.) Hence actual cell dimensions are of the same order of magnitude as the trapping lengths defined by the 6V/S rule, and the actual flow cross sections are of the same order of magnitude as the $V_{cell}^{2/3}$ default. The 14-cell deck therefore provides internally consistent geometric parameters to a degree that is not possible for the simpler representation.

Validation of 5-Cell Deck Use. Although the 14-cell deck was preferred for the present study, the price paid is that a deck as detailed as the 14-cell deck used here can be quite tedious to set up. To a lesser extent, its use also requires more computer time and user effort even after the deck itself has been developed. Depending upon the application, use of simpler decks may be justified. This possibility is illustrated by the last two cases tabulated for IET-1 and IET-3 in Table 6.1-3. In the first of these cases, the standard input prescription is used with the proviso that the value $A_h = 1.133\ m^2$ be accepted as "standard." Although f_{dome} is overpredicted, this overprediction did not have a large effect upon the ΔP or hydrogen production results. (There was a larger effect upon the amount of hydrogen burned for reasons unrelated to trapping; see Section 6.6.3 for details.) In the last case presented, the trapping lengths L_2 and L_3 are reduced by a factor of 1.5 from their standard values, which reduces the overprediction of f_{dome} but has only minor impacts upon ΔP and hydrogen production.

For this case, it is clear that any error in ΔP associated with the 5-cell deck is less than the uncertainties that generally must be allowed for in DCH analysis. In addition, the other results given in Table 6.1-3 support the belief that, when the 5-cell representation gives erroneous predictions of f_{dome}, the error tends to be in the conservative direction. Similar behavior is likely for any case in which f_{dome} is small and in which sensitivity calculations show that the results of greatest interest are not sensitive to reasonable variations in f_{dome}. If no detailed deck and/or no experimental results had been available, arriving at a suitable value of A_h would have posed more of a problem, however. Sensitivity to this parameter should be examined when less detailed representations are used without support from either detailed representations or experimental results.

Other Transport and Trapping Sensitivities. Some additional sensitivities to trapping and transport parameters are displayed in Table 6.1-4. The IET-1 cases tabulated are presented to illustrate the effect of the 'rhodg' and 'vnost' options discussed in Section 3.2.4 on this problem. (These cases were run before the standard prescription was defined and differ from the latter in ways not indicated in the table.) Specifying either 'rhodg = gas' or 'vnost = cnvel' reduces f_{dome} somewhat, but the effect is not large, especially for the 'vnost = cnvel' option. If 'rhodg = gas' is specified, the 'vnost' option has no effect, since it comes into play only if de-entrainment in a cell occurs on neither the first nor second impact, and this situation evidently did not arise when 'rhodg = gas' was specified. Although the effects observed here are small, one should not conclude that these modeling options make little difference in general; given a scenario in which large f_{dome} values are predicted for the standard prescription, the alternative options could make a much larger difference.

Table 6.1-4 Selected Sensitivity Studies for Debris Trapping and Transport Parameters						
Case	Description	ΔP (MPa)	f_{dome}	H_2 Data (g-moles)		
				$N_{f,H2}$	$N_{H2,burn}$	$N_{H2,prod}$
	IET-1 Experimental Results	**0.098**	**0.116**	**230**	**3**	**233**
I1c1403	No NAD*	0.072	0.118	130	0.7	131
I1c1404	No NAD, 'rhodg=gas' *	0.064	0.077	128	0.5	128
I1c1405	No NAD, 'vnost=cnvel' *	0.066	0.091	128	0.5	129
I1c1406	No NAD, 'rhodg=gas', 'vnost=gft' *	0.064	0.077	128	0.5	128
*Other differences with respect to the standard prescription exist.						
	IET-3 Experimental Results	**0.246**	**0.088**	**37**	**190**	**227**
I3c1407	Standard input prescription	0.228	0.101	21	232	253
I3c1412	Subcompartments s_d=5	0.235	0.032	20	241	261
I3c1406	Dome L_1=4.15 m (6V/S)	0.224	0.100	21	230	251

Case I3c1412 was run with s_d = 5 in the subcompartment cells and is part of the "Case 4" set summarized in Section 4.3; f_{dome} is substantially reduced but other results of interest are affected little. In Case I3c1406, L_1 in the dome is reduced to the 6V/S value, 4.15 m (the standard prescription here is the actual cell height, 7.5 m) and GFT trapping is used in the dome in Case I3c1408. Neither change had a significant effect. Relatively little debris is being transported to the dome and sensitivity to dome trapping parameters is therefore small.

The IET-10 cases given show that, in this Surry-geometry experiment, even the standard prescription underpredicts f_{dome} somewhat and the underprediction is again substantial if $s_d = 5$ is specified for the subcompartment cells. The 8-cell and 12-cell standard prescription cases (see Section 3.4 and Appendix A) gave very similar values of f_{dome}. The nodalization change resulted in a nontrivial effect upon ΔP for reasons related to hydrogen combustion; see Section 6.6.3.

Sensitivity to Slip in the Cavity and Chute. Calculations were run for SNL/IET-3 with $s_d = 1$ and $s_d = 10$ specified in the cavity and chute (Cases I3c1435 and I3c1436, respectively), and for SNL/IET-10 with $s_d = 1$ in the cavity (Case I10c833). Results given in Table 6.1-4 indicate that there is very little sensitivity in the calculated values of ΔP to s_d in the cavity and chute for these cases; f_{dome} and hydrogen production numbers show slightly more sensitivity but the effect is still quite small.

Cavity pressurization does show more sensitivity to s_d in the cavity and chute volumes. The calculations with $s_d = 5$ typically underestimate the maximum pressure differential between the cavity and the dome by factors of two to five. The IET-1, IET-3, IET-6, and IET-11 experiments were re-run with $s_d = 1$. Resulting values of net cavity pressurization (i.e., P_{cav}-P_{dome}) matched experimental values to within about 35%. The cavity pressurization results will not be discussed in detail here, as assessment of the CONTAIN code for predicting the extent of cavity pressurization would exceed the intended scope of this work. Available information indicates that more realistic results for cavity pressurization are obtained with $s_d = 1$ than with $s_d = 5$. Since the no-slip assumption ($s_d = 1$) is believed to be unrealistic, compensating effects may be involved and caution is warranted.

Observations on the Relation Between f_{dome} and ΔP. In general, f_{dome} is considered to be of interest because a large value of f_{dome} can increase loads, possibly substantially. Analysis of the IET experiments does not provide a very good opportunity to study this effect because the experimental values of f_{dome} are small, and the calculated values are also small if the calculation is at all realistic.

It is not true, however, that ΔP will always be sensitive to f_{dome}. In general, ΔP is expected to be sensitive to f_{dome} only if both the following conditions are met:

- Debris reaching the dome has not already lost most of its thermal and chemical energy (unreacted metal) before reaching the dome.
- Thermal and chemical interactions between the debris and the atmosphere are efficient once the debris does reach the dome.

In the present instance, it is likely that these conditions are not very well satisfied. The smallest particles largely react and transfer their thermal energy before reaching the dome, and it is these smaller particles which tend to dominate those that are transported as far as the dome. Furthermore, interactions may not be very efficient for whatever fraction of the larger particles does reach the dome.

The results given in Tables 6.3-3 and 6.3-4 suggest that sensitivity of ΔP to f_{dome} in these cases is small, even after taking into account the small magnitude of the variations in f_{dome}. As a further test, Case I3c1429 was run as in the standard case except specifying 'trapmul' to be 0.667 in all the subcompartment cells. (In the CONTAIN trapping input, 'trapmul' is a user-defined parameter with unit default value which permits the user to multiply all trapping rates by an arbitrary factor.) Comparison with Case I3c1407 indicates that f_{dome} was increased by about 40%, but other results of interest changed only slightly. If we divide the increase in ΔP by the change in f_{dome} to obtain a measure of the sensitivity, the result is [(0.233 - 0.228 MPa]/(0.143-0.101) = 0.12 MPa per unit change in f_{dome}, a rather small amount.

Experimentally, f_{dome} values in the SNL/IET Zion-geometry experiments ranged from 0.057 to 0.197, excluding the IET-8 cases. An attempt was made to correlate the measured ΔP with f_{dome}. No discernible correlation was identified. This result is consistent with the limited sensitivities found in the CONTAIN analyses discussed here.

It would be a mistake to assume that this limited sensitivity of ΔP to f_{dome} will always apply. For example, particle size sensitivities considered in Section 6.2 include cases in which all the particles are very small (0.125 mm). The extent of particle interaction in the cavity and subcompartments is then limited by the supply of coherent steam, and those particles which do reach the dome arrive still possessing much of their thermal and chemical energy. Once they reach the dome, their small size permits efficient interaction. Results to be cited in Section 6.2.2 for this small-particle case imply that the sensitivity of ΔP to f_{dome} is considerably greater, about 0.6 MPa per unit change in f_{dome}. Note that an increase of geometric scale (e.g., to NPP scale) can have effects qualitatively similar to a reduced particle size, in that both act to increase the ratio of the airborne residence time to the characteristic interaction time. At NPP scale, therefore, it is possible that sensitivity of the calculated loads to f_{dome} may be greater than sensitivity to f_{dome} at experimental scale.

6.2 Sensitivity to Particle Size.2 Sensitivity to Particle Size.2 Sensitivity to Particle Size

Particle size for airborne debris has long been recognized as a potentially important DCH parameter because it governs the characteristic time scales for thermal and chemical interactions with the atmosphere. If these time scales are long compared with those of certain competing processes (e.g., trapping), incomplete interaction may result in substantial mitigation of DCH loads. On the other hand, if particle sizes are sufficiently small that debris-gas interaction time scales are less than those of competing processes, further reductions in particle size may have little effect.

6.2.1 Particle Size Sensitivity in the Standard Prescription.2.1 Particle Size Sensitivity in the Standard Prescription.2.1 Particle Size Sensitivity in the Standard Prescription

Sensitivity in Open Geometries. Referring back to Table 6.1-1 in Section 6.1.1, the last entry in that table gives results calculated assuming a particle mass median diameter (mmd) of 1.45 mm. It may be recalled that 1.45 mm is the actual sieve mmd observed in this experiment, and that the standard value (1 mm) was based, in part, upon allowing for nonspherical and porous particles. Comparison with Case W1c506 shows that the increased particle size results in a 12% reduction in ΔP. Agreement with the experimental results is actually better for the larger particle size. However, the other uncertainties involved are sufficiently large that it would be risky to draw any firm conclusions from this result.

Compartmentalized Geometries: IET Results. Some particle size sensitivity studies for both the Zion and the Surry IET experiments are summarized in Table 6.2-1. Cases I3c1420 and I10c824, respectively, give results obtained for the IET-3 and IET-10 simulations, with the mass median diameter of the particle size distribution reduced from the standard value (1 mm) to 0.5 mm. All other parameters are left at their standard values. The size distribution is assumed to be lognormal with a geometric standard deviation, σ_g, of 4, as in the standard case.

Table 6.2-1 Sensitivity to Particle Size, SNL/IET Experiments						
Case	Description	△P (MPa)	f_{dome}	Hydrogen Data (moles)		
				$N_{f,H2}$	$N_{H2,burn}$	$N_{H2,prod}$
	IET-3 Experimental Results	**0.246**	**0.088**	**37**	**190**	**227**
I3c1407	Standard input prescription	0.228	0.101	21	232	253
I3c1420	Particle mmd=0.5 mm	0.236	0.120	21	238	259
I3c1410	No NAD	0.110	0.099	18	84	103
I3c1423	No NAD, d=0.125 mm (1 field)	0.175	0.153	26	127	153
I3c1428	I3c1423, 'trapmul'=1.5 in subcomp.	0.149	0.112	23	117	140

Sensitivity to the reductions in particle size below the standard value appears to be relatively small in both cases. There are probably several reasons for this result. One is that the broad size distribution tends to reduce sensitivity to particle size because the smallest sizes interact efficiently in both instances and the largest sizes are inefficient in both instances; it is only for the mid-range sizes that the sensitivity to particle size has a significant effect. In addition, the standard prescription already gives a fairly efficient interaction with the limited amount of coherent steam available, especially in IET-3, and a large increase is not possible. Furthermore, the fact that the nonairborne model is active in these cases can reduce sensitivity to airborne debris parameters because changes in the amount of steam that interacts with airborne debris tend to result in a compensating change in the amount that is available to interact with nonairborne debris (any given mole of steam can interact only once).

6.2.2 Small-Particle Limiting Case for Zion IET.2.2 Small-Particle Limiting Case for Zion IET.2.2 Small-Particle Limiting Case for Zion IET

If debris particles are sufficiently small, the debris thermal and chemical interactions will proceed until equilibrium is closely approached. In Table 6.2-1, Cases I3c1410, I3c1423, and I3c1428 explore this limiting scenario for IET-3, and Cases I6c1410 and I6c1415 examine it for IET-6. All these cases were run without nonairborne debris interactions, which is expected to maximize sensitivity to the airborne debris particle size. Another motivation for running these cases is that the inability of the calculation without NAD to reproduce experimental values of ΔP and H_2 production was the basis of the argument given in Section 4.2 for believing that NAD and/or cavity water must contribute substantially in the Zion-geometry IET experiments. It is therefore of interest to consider the maximum degree to which that argument could be compromised by any tendency of the standard prescription to underestimate the extent of interaction between airborne debris and coherent steam.

Cases I3c1410 and I6c1410 give results for the standard input except that no NAD is included (these correspond to the "Case 3" results of Section 4.2). In Case I3c1423 and I6c1415, the standard particle size distribution is replaced with a single debris field with particle diameter of 0.125 mm, which is sufficiently small to permit a close approach to debris-gas equilibrium. Significant increases in ΔP and H_2 production do result, but they still do not closely approach the experimental values. Furthermore, part of the increase in ΔP and H_2 production is due to the increased values of f_{dome} which are calculated for the small-particle case.

In order to evaluate the latter effect, Case I3c1423 was re-run with 'trapmul' set to 1.5, which reduces the transport to the dome (Case I3c1428). From the results, it may be inferred that at least half the difference in ΔP between Cases I3c1410 and I3c1423 is due to the increased transport to the dome, not the increased efficiency of debris interactions in the cavity and/or subcompartments. Evidently, if f_{dome} is constrained to be close to the correct value, even postulating very efficient interactions between airborne debris and coherent steam still leaves a substantial deficiency in the predicted ΔP and H_2 results.

6.3 Nonairborne Debris.3 Nonairborne Debris.3 Nonairborne Debris

An important finding of the present work is that calculations which include only the interactions of airborne debris with coherent steam underpredict DCH loads and hydrogen production, and other processes must also contribute. One class of "other processes" consists of those represented by the so-called nonairborne debris model in CONTAIN. As was discussed in Section 3.2.7, the term "nonairborne" only means that the processes involved are simulated by allowing debris in CONTAIN's trapped debris field to interact with blowdown steam and the containment atmosphere. It should not be interpreted as implying any particular geometric configuration for the debris-gas interactions, as a variety of processes may be involved and the actual geometry is not known.

The choice of d_t = 0.01 m for the 1/10-scale experiments was first used during developmental testing of the nonairborne model on the LFP and WC experiments; the model underwent significant modification subsequent to this testing. After the model development was completed, it was found that d_t = 0.01 m gave reasonable results for the IET-1 and IET-3 experiments provided NAD is also included in the subcompartments as described below. The prescription was frozen before analyzing the other IET experiments, and the LFP and WC experiments were also re-analyzed with the final version of the model. Subsequent to this empirical determination of d_t, an analytical model was developed based upon general heat and mass transfer correlations. This model does not involve fitting to any of the DCH experimental results. The model is described in Appendix B and it also predicts that a value of $d_t \approx 0.01$ m should be appropriate.

Two other questions requiring attention when using the NAD model are:

- Determining which locations should include modeling of NAD interactions; and

- Flow area A_h to be used in evaluating the gas flow velocity which is required for evaluating the NAD Nusselt and Sherwood numbers.

The first question was initially addressed in analyses of the IET-1 and IET-3 experiments, with the suitability of the resulting prescription being confirmed by sensitivity studies which were performed for the complete set of experiments analyzed. These studies were summarized in Section 4 as "Case 1" (NAD in both cavity and subcompartments), "Case 2" (NAD in cavity only), and "Case 3" (no NAD). The flow area, A_h, in the cavity was set equal to the estimated geometric cross section while the default value ($V_{cell}^{2/3}$) was used in all subcompartment cells except when the five-cell Zion deck was used, for which A_h was set equal to 1.133 m^2 (see Section 6.1.3). Thus, A_h is based upon the actual geometry and it is not an additional free parameter.

Some results illustrating the trends obtained are summarized in Section 6.3.1, and sensitivity to d_t is considered briefly. In Sections 6.3.2 and 6.3.3, respectively, consideration is given to the sensitivity of the results to the fraction of the debris dispersed from the cavity and to the coherence between debris dispersal and blowdown steam. The influence that the NAD model has upon these sensitivities is also evaluated. In Section 6.3.4, the rationale for defining the use of the NAD model in the standard prescription is summarized. One of the most important caveats concerning the use of the standard prescription is the potential confounding effect of cavity water in the Zion IET experiments. Since the potential impact of water is a major topic in its own right, its discussion is deferred to Section 6.4. In the meantime, the reader should remember that none of the results discussed in this section include any allowance for this water.

6.3.1 Effect of NAD in the Cavity and the Subcompartments.3.1 Effect of NAD in the Cavity and the Subcompartments.3.1 Effect of NAD in the Cavity and the Subcompartments

Open-Geometry Results. Results for the WC-1 experiment with and without NAD in the cavity were given in Table 6.1-1 of Section 6.1.1, and results for the other three open-geometry experiments considered are given in Appendix D. In all cases, including NAD made only a small difference in the calculated ΔP. In these experiments, direct interaction between airborne debris and the main containment atmospheric volume is responsible for much of the pressurization. Hence, the airborne debris interactions are not limited by the coherent steam supply, and adding the nonairborne interactions with the noncoherent blowdown steam does not make a large difference. The importance of the NAD contributions is also limited by the relatively low driving pressure in these experiments; that is, the steam remaining in the accumulator after dispersal from the cavity ends is limited, which reduces the potential importance of the nonairborne interactions.

The hydrogen results for the open-geometry experiments show a larger effect than the ΔP results, but the contribution is less than one third of the total in all cases. Note also that the containment atmosphere was inert in all the open-geometry experiments, which means debris dispersed into the containment would have little opportunity to generate hydrogen once it exits the cavity chute. In more realistic, steam-rich containment atmospheres, hydrogen production might be dominated by interactions between airborne debris and the main containment atmospheric volume, and the relative importance of NAD could again be reduced.

While the contributions of NAD clearly should not be neglected, it does seem likely that NAD interactions are not a dominant effect in open-geometry containments with realistic atmospheric compositions. This conclusion is limited to scenarios in which substantial fractions of the debris are dispersed into the main containment volume. If most of the debris is not dispersed from the cavity, NAD interactions in the cavity could dominate the overall result.

LFP Results. The effects of the nonairborne debris interactions upon the LFP analyses are illustrated by the results for LFP-2A given in Table 6.3-1. The effect of NAD upon ΔP is minor and the effect upon hydrogen production is larger but it is not a dominant effect. Including NAD in the subcompartment makes very little difference; evidently, the combination of a limited steam supply (i.e., low accumulator pressure) and relatively large

Table 6.3-1 Selected Sensitivity Studies for the Nonairborne Debris Model						
Case	Description	△P (MPa)	f_{dome}	H_2 Data (g-moles)		
				$N_{f,H2}$	$N_{H2,burn}$	$N_{H2,prod}$
	LFP-2A Experimental Result	**0.102**	**0.069**	**151**	**---**	**---**
L2ac501	Standard input prescription	0.138	0.175	148	0.6	148
L2ac502	No NAD	0.127	0.183	98	0.6	98
L2ac503	NAD in cavity only	0.133	0.172	147	0.6	148
	IET-1 Experimental Results	**0.098**	**0.116**	**230**	**3**	**233**
I1c1408	Standard input prescription	0.115	0.107	271	0.5	271
I1c1409	NAD in cavity only	0.093	0.108	216	0.5	216
I1c1410	No NAD	0.076	0.117	130	0.8	131
	IET-1R Experimental Results	**0.110**	**0.105**	**238**	**11**	**248**
I1c1407	Standard input prescription	0.101	0.096	248	0.6	247
I1c1409	NAD in cavity only	0.083	0.096	199	0.5	198
I1c1410	No NAD	0.063	0.095	100	0.5	99
	IET-3 Experimental Results	**0.246**	**0.088**	**37**	**190**	**227**
I3c1407	Standard input prescription	0.228	0.101	21	232	253

subcompartment volume keeps steam concentrations sufficiently low to preclude a significant amount of hydrogen generation from NAD in the subcompartment. The other LFP analyses exhibited similar trends.

IET Results (Zion Geometry). The IET-1R experiment was performed as a replicate of IET-1 in order to study reproducibility; they are the only replicate pair in the data base analyzed in this work. Results are given for both cases in Table 6.3-1, as well as results for IET-3. Both IET-1 and IET-1R had a containment atmosphere that was inert (N_2) except for unavoidable residual traces of oxygen ($\leq$ 0.2%).

In contrast with the open-geometry cases and the LFP experiments, NAD makes a significant contribution even to ΔP, and it is a dominant contributor to hydrogen production in the sense that the cases without NAD yield only 40-50% as much hydrogen as the standard prescription. In addition, NAD in the subcompartments is a significant contributor in the standard prescription.

These differences with respect to the open-geometry and LFP results are not difficult to understand. The Zion-geometry IET experiments were characterized by rapid debris ejection from the cavity, with limited coherence between debris dispersal and the blowdown; as much as 75% of the total blowdown occurred after dispersal was essentially complete. Hence, interactions of the airborne debris are limited by the restricted supply of coherent steam. On the other hand, the supply of noncoherent steam was considerably larger than in the previous cases, due to the combination of low coherence and a larger total steam supply (i.e., higher driving pressure in the accumulator). The potential for a significant NAD contribution is therefore increased. Furthermore, high steam concentrations can develop in the Zion subcompartments due to their relatively small volume and the larger steam supply, which provides a potential for NAD interactions to continue in the subcompartments.

Calculations with NAD modeled in the cavity only were run for all the experiments analyzed in this work and are compared with the experimental results in Figure 6.3-1. Comparison of this figure with the results for the standard prescription (Figure 4.1-1) shows that omitting NAD interactions in the subcompartments had little impact for many of the experiments, but it did result in underpredicting hydrogen production and ΔP for most of the SNL/IET Zion experiments. Partial exceptions are IET-1 and, for hydrogen production, IET-3.

In Cases I3c1417 and I3c1418, the nonairborne field diameter, d_t, was reduced from the standard value (0.01 m) to 0.005 m in order to examine sensitivity of the nonairborne model to this parameter. Comparison with Cases I3c1407 and I3c1409, respectively, shows significant increases in both ΔP and hydrogen production. With this smaller value of d_t, the case with NAD in only the cavity clearly agrees better with the experimental results. Thus, one cannot conclude from these results alone that NAD in the subcompartments is necessarily contributing. Even if one repeated the analysis of the complete data set, including NAD in the cavity only with a smaller value of d_t, the results might well prove inconclusive. However, comparisons between the WC experiments and the Zion IET experiments do suggest that processes of some kind in the subcompartments are contributing (see Section 4.2).

<u>IET Results (Surry Geometry)</u>. Surry-geometry results are illustrated for the IET-10 experiment by the last four cases given in Table 6.3-1. Deleting NAD in the subcompartments had only a relatively small effect, < 10% for both ΔP and hydrogen production. Deleting NAD in the cavity (Case I10c815) appears to have a somewhat larger effect upon ΔP, but part of this difference results from the dome temperature staying slightly below the BSR threshold (840 K) in this case, while the threshold was exceeded in the other two calculations. In order to separate the two effects, Case I10c821 was run with the BSR threshold, 'srtemp', reduced to 780 K, which yielded BSR behavior comparable to the standard case. When this is done, it is seen that total elimination of all NAD reduces ΔP by only about 15%, with a somewhat larger effect upon hydrogen production.

Rather similar results were obtained for sensitivity studies performed for IET-9 and IET-11 (Appendix D). In view of all the uncertainties involved, it is doubtful that a strong case could be made for the potential importance of NAD based upon the Surry-geometry results alone. It appears that the importance of NAD can depend upon the geometry.

6.3.2 NAD and the Dependence of Loads Upon Debris Fraction Dispersed.3.2 NAD and the Dependence of Loads Upon Debris Fraction Dispersed.3.2 NAD and the Dependence of Loads Upon Debris Fraction Dispersed

The fraction of the debris which is dispersed from the cavity has long been considered a very important DCH parameter. The usual supposition has been that DCH loads monotonically increase with increasing dispersal, and that postulating total dispersal provides a conservative bound. This supposition, however, is based upon the assumption that DCH is governed by the interactions of airborne debris with blowdown steam and/or the containment atmosphere, and that nonairborne debris may be neglected. The situation becomes more complicated when processes represented by the CONTAIN NAD model are allowed for.

Table 6.3-2 Selected Sensitivity Studies for the Nonairborne Debris Model						
Case	Description	ΔP (MPa)	f_{dome}	H_2 Data (g-moles)		
				$N_{f,H2}$	$N_{H2,burn}$	$N_{H2,prod}$
	IET-3 Experimental Results	**0.246**	**0.088**	**37**	**190**	**227**
I3c1407	Standard input prescription	0.228	0.101	21	232	253
I3c1413	100% dispersal from cavity	0.218	0.092	16	193	208
I3c1410	No NAD	0.110	0.099	18	84	103
I3c1415	No NAD, 100% dispersal	0.133	0.092	24	102	126
I3c1409	NAD in cavity only	0.186	0.102	19	192	211
I3c1414	NAD in cavity only, 100% dispersal	0.133	0.092	24	102	125

The standard IET-3 and IET-10 cases were rerun with airborne debris sources renormalized to correspond to the total thermite mass initially present in the melt generator, rather than to just the fraction ejected from the cavity (60% and 73% for IET-3 and IET-10, respectively). The time dependence of the debris sources was not changed. The results are summarized in Table 6.3-2, which also includes the experimental results and the results obtained in the standard analyses with the dispersed fraction equal to the experimental result.

It is apparent that the effects of postulating 100% dispersal are quite small and, furthermore, in IET-3 the effect is negative. When no NAD interactions are modeled, the effect of assuming 100% dispersal is, as expected, to increase ΔP and hydrogen production somewhat, but the effect is not large. In IET-3, the limited amount of coherent steam available interacts fairly efficiently even in the 60%-dispersal case, and there is not much room for increased interaction even when 100% debris dispersal is assumed. In the IET-10 experiment, the debris-steam coherence is considerably greater, but even in this case, increasing dispersal from 73% to 100% does not have a large effect. (Note that the comparison is based upon the no-NAD case with reduced BSR threshold, Case I10c821, in order to avoid having the comparison affected by the BSR threshold.)

In the IET-3 experiment, the case with NAD modeled only in the cavity yields a quite significant decrease in both ΔP and hydrogen production when 100% dispersal is postulated. Although this result may seem surprising, it is entirely reasonable in terms of the model being used here. Postulating 100% dispersal cannot substantially increase the extent of debris interaction with the coherent portion of the blowdown, and 100% dispersal eliminates the possibility of debris interactions with the noncoherent portion of the blowdown. Note that this negative dependence would be even stronger if one specified a smaller value of d_t in order to obtain a better agreement with the experimental result for the 60%-dispersal case with cavity NAD only.

In the IET-10 analysis with NAD in the cavity only, the 73% and 100% dispersal cases yield almost identical results. There is a greater degree of debris-steam coherence than in IET-3 while the contribution from NAD is smaller; the opposing effects of dispersing 100% of the debris cancel in this instance.

Experimental Correlation with Dispersed Fraction. In view of the various possible dependencies upon dispersed fraction discussed above, it is of some interest to determine whether a correlation with the fraction dispersed can be detected in the Zion SNL/IET results. The search for a correlation is complicated by the fact that the dispersed fraction varied over only a limited range, about 60-80%, and only the IET-1 and IET-1R experiments were replicates of each other. However, of the experimental variables studied, only variations in atmospheric composition that determined whether DCH-produced hydrogen could burn had a large effect. The impact of the other variables studied (water on the subcompartment floor, pre-existing hydrogen) turned out to be relatively minor.

In order to put the burn and no-burn results on a common basis, the experimental ΔP values for the cases with burns were normalized by dividing by the average for the four cases in which hydrogen did burn effectively, and the no-burn cases were normalized by dividing their ΔP values by the average for the three no-burn cases (which were considered to include IET-5). This procedure could distort presentation of results if the average fractions dispersed differed substantially for the experiments with and without hydrogen combustion, but the mean dispersal fractions were actually quite similar (0.683 vs 0.669, respectively).

Since the initial mass of thermite in the melt generator is the same in all the experiments, the amount of debris that exits the cavity is proportional to $f_{eject}*f_{disp}$. (Here, f_{eject} and f_{disp} are, respectively, the fraction ejected from the melt generator and the fraction of what enters the cavity which is subsequently dispersed from the cavity.) The normalized ΔP values are plotted against $f_{eject}*f_{disp}$ in Figure 6.3-2, and a least-squares fit is also shown. There is no discernible dependence upon the dispersed fraction, which is in agreement with the expectations based upon the standard prescription that includes NAD in both the cavity and subcompartments. The test is not very sensitive because of the limited range of values in the dispersed fractions. On the other hand, the scatter in the normalized ΔP values is small and it would seem that any very strong dependence upon dispersed fraction should be revealed.

Figure 6.3-2. Normalized experimental ΔP values plotted against debris fractions dispersed from the cavity for the SNL/IET Zion experiments.

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6.3.3 NAD and the Dependence of Loads Upon Coherence.3.3 NAD and the Dependence of Loads Upon Coherence.3.3 NAD and the Dependence of Loads Upon Coherence

In Section 3.2.2, the concept of "coherence" was introduced as a potentially important DCH parameter. By "coherence" is meant the extent to which the blowdown of steam from the RPV is simultaneous with the dispersal of debris from the reactor cavity. In experiments performed in compartmentalized geometries, relatively little debris is transported beyond the subcompartments, which limits the interactions between airborne debris and the containment atmosphere. Since de-entrainment of airborne debris in the subcompartments is rapid (at least in the CONTAIN model), there is also little opportunity for airborne debris to interact with that part of the blowdown steam which does not enter the containment until after debris dispersal from the cavity is largely complete. Insofar as the airborne debris is concerned, therefore, the contribution to DCH may be largely limited to its interaction with that part of the steam which enters the containment during the time that debris is being dispersed from the cavity. This steam is referred to as the "coherent" steam.

Just as the modeling of nonairborne debris interactions can reduce the sensitivity of DCH loads to f_{disp} by providing an alternate path for debris-steam interactions to occur, it can also reduce the sensitivity to coherence. Here we examine the sensitivity to coherence for the SNL/IET-6 experiment. It is chosen for study because f_{disp} was relatively large (0.83) for this experiment and it exhibited a sharply peaked cavity pressurization history (Figure 3.3-2) which shows that dispersal was largely complete by ~0.85 s. The accumulator had depressurized by less than 25% at this time (Figure 3.2-1), implying low coherence. This combination of a high dispersal fraction and low coherence is expected to maximize sensitivity to increases in the degree of coherence.

Since debris dispersal from the cavity tails off gradually, without an abrupt end, "coherence" is not a precisely defined concept. For present purposes, we define the coherent steam fraction, f_{coh}, to be the fraction of the steam which has left the accumulator at the time debris dispersal is 95% complete, as was done in Section 5. More precisely, the 95% point was taken to be the time that the Al_2O_3 dispersed from the cavity reached 95% of its final value, since the use of alumina as the measure of dispersal avoids complications associated with debris weight gains due to oxygen uptake. (Aluminum oxide produced by reaction of aluminum metal is given a different name in the calculation and thus causes no confusion.) The coherent steam fraction, f_{coh}, is then calculated from Eq. (3.2-1) as before.

In sensitivity studies varying f_{coh}, debris sources with a simple trapezoidal time dependence were defined in which the source rate was set equal to zero prior to t_0, increased linearly to its maximum value at a time equal to $t_0 + \Delta t_1$, held constant for a second time interval of duration Δt_2, and then decreased linearly for a third time interval of the same duration as the second, i.e., also equal to Δt_2. Three trapezoidal source time dependencies were so defined that they would integrate to the same mass of debris dispersed but have different values of f_{coh}. These source rates are plotted in Figure 6.3-3 along with the source time dependence derived from the cavity pressurization history. Also shown is the calculated accumulator pressure history, which is the same in all the cases.

Figure 6.3-3 Debris source time dependencies (left axis) and accumulator blowdown history (right axis) used in the coherence sensitivity study based upon the SNL/IET-6 experiment.

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Table 6.3-3 Sensitivity to Coherence						
Case	Description	ΔP (MPa)	f_{dome}	Hydrogen Data (moles)		
				$N_{f,H2}$	$N_{H2,burn}$	$N_{H2,prod}$
	IET-6 Experimental Results	**0.279**	**0.138**	**154**	**345**	**319**
I6c1407	Standard prescription (f_{coh}=0.184)	0.248	0.085	165	256	240
I6c1410	No NAD (f_{coh}=0.184)	0.127	0.086	191	98	108
I6c1419	Trapez. $S_d(t)$, $\Delta t_2=\Delta t_1$ (f_{coh}=0.19)	0.248	0.083	165	257	241

In all three of the trapezoidal source time dependencies, t_0 was taken to be equal to 0.45 s and Δt_1 was taken to be equal to 0.1333 s, while three values of Δt_2 were used: $\Delta t_2 = \Delta t_1$, $\Delta t_2 = 3\Delta t_1$, and $\Delta t_2 = 5\Delta t_1$. The parameters for the first of these three cases were chosen to give a simple approximation to the time dependence specified in the standard prescription in order to test the belief that sensitivity to the details of the time dependence is not large so long as a reasonable match to the coherence is obtained. The other two time histories were defined to investigate sensitivity to the coherence.

All four of the sources plotted in Figure 6.3-3 were run with and without the nonairborne interactions being modeled, making eight calculations in all. The results are summarized in Table 6.3-3. For each case, the column in the table headed "Description" includes the value of f_{coh}, which was obtained as defined above.

Results for Cases I6c1419 and I6c1420 agree well with the results of Cases I6c1407 and I6c1410, respectively. This agreement supports the belief that the CONTAIN model is not sensitive to details of the time dependence of the source, provided that the dispersed fraction and the degree of coherence are reasonably well matched.

The results for the other four cases with the simple trapezoidal time dependencies show that ΔP and hydrogen production do increase with increasing f_{coh}, but the sensitivity is not very great for the cases with the NAD interactions modeled. The sensitivity to f_{coh} is somewhat greater for the cases without NAD. Some caution is needed in generalizing these results, since sensitivity to coherence can depend upon other parameters of the problem.

Nonetheless, the results do illustrate the fact that significant uncertainty may exist in f_{coh} without resulting in a large amount of uncertainty in the principal results of interest.

6.3.4 Rationale for the Standard Prescription.3.4 Rationale for the Standard Prescription.3.4 Rationale for the Standard Prescription

The general results summarized in this section tend to favor the present prescription with NAD modeled in both the cavity and the subcompartments, as opposed to a prescription with NAD modeled in the cavity only but with a smaller value of d_t. Not the least of the disadvantages of the latter is the possibility of a negative dependence upon dispersed fraction, which could be a potential pitfall for the unwary user convinced that it is always conservative to specify 100% debris dispersal. Of course, a negative dependence can also arise even for the present standard prescription, but it is less likely to be a large effect when NAD is modeled in the subcompartments also.

There is no justification other than simplicity for assuming that, if NAD is modeled in both the subcompartments and the cavity, the values of d_t assumed must be the same in both locations. Allowing two (or more) different values in two (or more) different locations would turn a one-parameter problem into a multiparameter problem. Since neither independent physical reasoning nor fitting to the data are adequate to justify more than an approximate value for the single-parameter version, attempting to fit a multiparameter model to the data is not justified.

Except for the increase in d_t used to shut off NAD interactions at late times described in Section 3.2.7, the present standard prescription provides a time-independent value of d_t. There are both theoretical arguments (Appendix B) and experimental evidence (Section 6.5) that this prescription over emphasizes interactions that occur late in the blowdown relative to those occurring earlier. A more realistic time dependence for the NAD interactions might be obtained by starting with a smaller value of d_t and allowing it to increase as the blowdown proceeds. Physical understanding of the processes involved is not adequate to provide a convincing prescription for what this time dependence should be. In the absence of such understanding, attempting to fit a time dependence for d_t to the experimental data is not justified, since there would be little confidence that it would be applicable to scenarios other than the experiments used in the fitting process. (It might, however, be possible to alter the model to give a qualitatively more reasonable behavior, although important uncertainties would remain; see Appendix B for a brief discussion.)

6.4 Effects of Cavity Water.4 Effects of Cavity Water.4 Effects of Cavity Water

6.4.1 Introduction.4.1 Introduction.4.1 Introduction

The most important limitation of the standard prescription may be that it attributes all the differences between experiment and the "Case 3" results of Section 4.2 to the effects of nonairborne debris interactions. It is now believed that debris-water interactions also played a significant role in the Zion-geometry IET experiments. The possible effects of debris-water interactions upon the integral ΔP and hydrogen results are considered in this section, while insights concerning the role of water obtained from the containment pressure-time histories are discussed in Section 6.5.1.

In all the Zion-geometry IET experiments analyzed here, there was 3.48 kg of water in the cavity (scaled amounts in ANL/IET), and some of the experiments had much larger amounts (71.1 kg) on the subcompartment floor, which represents the floor of the basement of the Zion containment building. In addition, one of the WC experiments (WC-2) had 11.76 kg of water in the cavity.

In Section 3.2.8, the degree to which CONTAIN can model interactions between core debris and cavity water was discussed, and it was acknowledged that the treatment is not sufficient to justify a claim that the code can provide a mechanistic prediction of what the actual effects of cavity water will be. One of the limitations of the analysis is that there is no way to predict the amounts of water which will actually interact effectively with the debris. If, for example, some of the water is blown out of the cavity without interacting, the amount that actually interacts may be less than that which is initially present. In compartmentalized geometries, however, this effect may be countered by interactions between the dispersed water and dispersed debris that can continue to occur in the subcompartments. In open containment geometries, debris and water likely have little opportunity to undergo further interaction after dispersal from the cavity.

In all calculations involving water, the water was introduced as a source with the same time dependence as the airborne debris source. As was discussed in Section 3.2.8, this treatment maximizes the opportunity for debris-water interactions to occur in the sense that it maximizes temporal coherence, but it does not necessarily provide a true bound on the potential effect.

The cavity pressure histories (e.g., Figure 3.2-2) indicate that FCI-related pressure peaks occur prior to the debris entrainment and dispersal period, and introducing the water and the debris in parallel obviously does not capture this effect. However, attempting to obtain a more realistic timing with the current CONTAIN model would introduce additional complexity and potential variability into the problem (e.g., how to define the time-dependent interaction rate and how much debris dispersal to allow during the FCI interaction). The treatment adopted here has the virtue of simplicity and reduces the number of free parameters to one, i.e., the amount of water postulated to interact.

A more physically based reason for introducing the water in parallel with the airborne debris is that this time dependence is more nearly correct if the actual interactions largely occur in the subcompartments.

Analysis of the open-geometry experiment, WC-2, is discussed in Section 6.4.2. Calculations attempting to include the water that was on the basement floor at the start of some of the Zion IET experiments were not performed, but experimental results indicating that this water did not play an important role are summarized in Section 6.4.3. The analysis of the potential effects of condensate levels of water in the Zion-geometry IET experiments is discussed in Section 6.4.4. Exploratory analyses of the IET-8B experiment, in which the amounts of cavity water were much larger (62 kg), are summarized in Section 6.4.5.

6.4.2 Cavity Water Effects with Open Containment Geometries.4.2 Cavity Water Effects with Open Containment Geometries.4.2 Cavity Water Effects with Open Containment Geometries

The WC-1 and WC-2 experiments were very similar except that WC-2 included 11.76 kg of water in the cavity while WC-1 was dry, and thus these experiments provide a matched pair permitting direct comparison of cases with and without water. Some results obtained analyzing these experiments are summarized in Table 6.4-1. WC-1 results are presented first, and are followed by the corresponding results obtained for WC-2. The standard prescription does not include water and the results calculated for WC-2 are very similar to those calculated for WC-1, illustrating the similarity between these experiments in terms of parameters other than the water.

Table 6.4-1
Effects of Water in Open Containment Geometry Experiments: WC-1 and WC-2

Case	Description	ΔP (MPa)	f_{dome}	Hydrogen Data (moles)		
				$N_{f,H2}$	$N_{H2,burn}$	$N_{H2,prod}$
	WC-1 Experimental Results	**0.272**	**0.033**	**145**	**---**	**---**
W1c506	Standard input prescription	0.314	0.063	152	1.0	153
W1c510	No NAD	0.300	0.063	105	1.1	106
	WC-2 Experimental Results	**0.286**	**.052**	**179**	**---**	**---**
W2c504	Standard input prescription	0.317	0.064	143	3.8"	147
W2c505	No NAD	0.302	0.064	102	1.1	103
W2c501	15% co-dispersed water	0.306	0.055	208	0.9	209

The similarity of the CONTAIN results calculated for WC-1 and WC-2 without water supports the intuitively reasonable interpretation that any differences between the experimental results are attributable to the water. The experimental results then suggest that there was only a slight increase in ΔP (which may well be within the experimental reproducibility), while there was approximately a 25% increase in hydrogen production.

In Reference All92a, CONTAIN analyses were used to argue that approximately 15% of the cavity water interacted in WC-2. Those analyses included some features now considered obsolete, but they were used as a starting point for sensitivity studies in this work. Cases W2c504 and W2c505 were run with 15% co-dispersed water with and without NAD, respectively, and comparison with Cases W2c501 and W2c502, respectively shows that the effects are qualitatively in agreement with the experimental observations; i.e., there is little effect upon ΔP while hydrogen production is increased.

Quantitatively, the effect is overpredicted somewhat. The predicted increase due to the water is about 55-60 g-moles, compared with a difference between the WC-2 and WC-1 experimental results of 34 g-moles. The amount of water included in the calculation corresponds to 98 g-moles, which is significantly more than the increase in hydrogen production due to adding the water. Since there is a large excess of metal available, these results show that the interaction is not calculated to proceed to completion, due to the rate limitations calculated by the CONTAIN chemistry model.

In Cases W2c507 and W2c508, 100% of the cavity water is assumed to be co-dispersed. Hydrogen production is now grossly overpredicted even in the case without NAD. The increase in hydrogen production in the case with NAD is still larger because, in the model as applied here, the steam generated by vaporizing the water can interact with the nonairborne field as well as the airborne fields.

Despite the large hydrogen increases, the calculated ΔP is not increased; in fact, it is reduced slightly relative to the 15% case and the latter shows a slight reduction in calculated ΔP relative to the dry-cavity case. One reason is that energy transferred from the debris to vaporize water comes at the expense of energy which, with an open containment geometry, otherwise could have been transferred to the containment atmosphere after the debris is dispersed. The debris fields with the smallest particle sizes are the ones that are most effective in transferring their energy to the water, and these are also the debris fields that would have been most effective in transferring their energy to the containment atmosphere in the absence of water. As will be seen Section 6.4.4, the situation can be quite different in compartmentalized geometries.

Cases W2c509 and W2c510 were run with the chemical reaction threshold reduced from the standard value of 1200 K to 900 K in order to test whether quenching of chemical reaction was a factor in the calculations with 100% co-dispersed water. This check is always recommended when analyzing scenarios involving significant water. In the present instance, the results are not being affected by quenching of the chemical reaction.

It might be supposed that, given a prototypical atmosphere in which hydrogen could burn, the increased hydrogen generation due to water would increase ΔP. However, this may not be the case in open-geometry containments, for the same reason that water did not increase ΔP in the open-geometry experiment. That is, hydrogen generation due to debris-water interactions occurring in the cavity may take place at the expense of debris-steam (or debris-oxygen) interactions that would otherwise occur in the containment atmosphere. Without more study, it is not clear what the net effect would be.

Table 6.4-2
Results of IET Experiments Relevant to Subcompartment Water

Experiment	Water Mass (kg)		ΔP (MPa)	$N_{H2,prod}$ (g-moles)
	Cavity	Subcomp.		
IET-3	3.48	0	0.246	227

6.4.3 Effects of Water on the Subcompartment Floor.4.3 Effects of Water on the Subcompartment Floor.4.3 Effects of Water on the Subcompartment Floor

Experiments IET-3 and IET-6 were similar to IET-4 and IET-7, respectively, except that the second two had 71.1 kg of water on the subcompartment floor at the onset of the experiment, while the subcompartment floor was dry in the first two cases. Results for ΔP and hydrogen production are summarized in Table 6.4-2. A comparison between IET-3 and IET-4 would support the hypothesis that the subcompartment water increased hydrogen production somewhat, while a comparison between IET-6 and IET-7 would not. The principal difference between IET-3 and IET-4 versus IET-6 and IET-7, respectively, was that the last two included some pre-existing hydrogen in the atmosphere, and the first two did not. There is no obvious reason why this difference should alter the effect of subcompartment water on hydrogen production. Hence, it is plausible that the lower hydrogen production in IET-3 is the result of chance variation rather than the result of the dry subcompartment floor.

Another piece of evidence against a large amount of interaction with the subcompartment water is provided by comparisons between the temperature rise and the pressure rise in the main volume of the Surtsey vessel [All94b]. From these comparisons, it may be inferred that the subcompartment water did not result in a large increase in the total number of moles of gas in the containment atmosphere, such as would have resulted if much of the subcompartment water had been vaporized.

Any attempt to model debris interactions with the subcompartment water in CONTAIN would be largely parametric, and the effects upon the results would be qualitatively similar to the effects of cavity water. In view of the experimental evidence that the effect of the subcompartment water was at most limited, it was not included in any of the CONTAIN simulations of the IET experiments.

Surry Geometry. In the Surry-geometry experiments, IET-9 and IET-11 had water on the basement floor, while IET-10 (and IET-12) did not. There were sufficient differences between these experiments in addition to the water that one cannot infer the presence or absence of an effect from direct comparisons of the experimental results. However, the ability of the CONTAIN simulation to reproduce the experimental trends did not show any discrepancies that might reasonably be attributed to the failure of the simulations to treat subcompartment water. Again, the evidence is that the water did not have a large impact.

6.4.4 Analysis of Cavity Water in the IET Experiments.4.4 Analysis of Cavity Water in the IET Experiments.4.4 Analysis of Cavity Water in the IET Experiments

The standard prescription for the nonairborne debris model was developed and assessed largely by comparing calculated and measured results for the IET experiments under the assumption that water does not contribute. It follows, therefore, that adding any significant interaction of water to the standard prescription would tend to overpredict the experimental results for hydrogen production and ΔP. The approach adopted here was to investigate the degree to which water could provide an alternative (i.e., to NAD) interpretation of the large discrepancies between the "Case 3" results of Section 4.2 and the experimental results for the Zion IET experiments. In this approach, no NAD interactions were modeled and, instead, water sources were introduced in parallel with the debris sources as described previously. Some results that include both NAD and water are given at the close of this section.

Even without running any calculations, it is clear that water cannot be a very important contributor unless its interaction is considerably more efficient than appears to be the case in WC-2. In the IET analyses, the discrepancies in hydrogen production between the calculations without NAD and the experimental results ranges from about 100 to 200 g-moles. If only 15% of the cavity water in the IET experiments is assumed to interact with debris, it could contribute less than 30 g-moles even if it reacted with 100% efficiency. The difference between the WC-2 and WC-1 experimental hydrogen results (34 g-moles) is also much less than the discrepancy of interest, despite the larger amount of water present in WC-2. Hence, the calculations investigating potential effects of water in the IET experiments were run with 100% of the water being co-dispersed with the debris.

Before giving results, it should be noted that there are no apparent reasons for debris-water interactions in the cavity in the IET experiments to be much more efficient than debris-water interactions in the cavity in WC-2. Hence, if water is a major contributor in the IET experiments, it is likely that much of the interaction must actually occur in the subcompartments. The fact that water initially present in the subcompartments did not play a major role does not necessarily imply that cavity water and debris cannot interact after both enter the subcompartments. If blown out of the cavity by the initial FCI, the cavity water will impact upon, and coat, the subcompartment structures, and/or and splash or drip from them. A fraction of a second later, the dispersed debris will impact the same structures and undergo very similar processes. It seems quite plausible that the opportunity for debris interactions with the dispersed cavity water in the subcompartments will be much greater than is the case for debris interactions with water that is lying quietly on the subcompartment floor at the start of the event.

All of the SNL/IET experiments were analyzed assuming no NAD and with 100% co-dispersed water, with all other input left at the standard values. Results for IET-1, IET-1R, IET-3, and IET-6 are summarized in Table 6.4-3, and Appendix D gives all the results.

Table 6.4-3 Potential Effects of Co-Dispersed Water, Zion IET Experiments						
Case	Description	ΔP (MPa)	f_{dome}	Hydrogen Data (moles)		
				$N_{f,H2}$	$N_{H2,burn}$	$N_{H2,prod}$
	IET-1 Experimental Results	**0.098**	**0.116**	**230**	**3**	**233**
I1c1410	No NAD	0.076	0.117	130	0.8	131
I1c1412	100% co-dispersed water, no NAD	0.111	0.227	216	1.6	217
	IET-1R Experimental Results	**0.110**	**0.105**	**238**	**11**	**248**
I1rc1410	No NAD	0.063	0.096	80	0.5	79
I1rc1413	No NAD, 100% co-dispersed water	0.083	0.122	187	0.23	185
I1rc1414	100% water, NAD d_t=0.02 m	0.109	0.122	250	0.3	249
	IET-3 Experimental Results	**0.246**	**0.088**	**37**	**190**	**227**
I3c1410	No NAD	0.110	0.099	18	84	103

Considering first the IET-1 and IET-1R results, there is some increase in ΔP and a large increase in hydrogen production when the water is included. Some of the increase in ΔP in IET-1 is probably due to the increase in the calculated value of f_{dome} that results from the increased steam flow rates generated by the vaporizing water. No other experiment analyzed showed an effect upon f_{dome} this large. For IET-1R, but not IET-1, ΔP and hydrogen production are underpredicted significantly even with the water. The IET-1R response was more typical of the other cases studied than was the IET-1 response.

In the experiments in which hydrogen could burn, adding water to the no-NAD cases also substantially increased ΔP and H_2 production, but both are still significantly underpredicted. Similar results were obtained for IET-4 and IET-7 (Appendix D). Reducing the particle size by a factor of two (Cases I3c1424 and I6c1416) further reduces the discrepancy with the experimental results and suggests that one could probably explain most or all of the difference between the no-NAD results and the experimental results as being due to the water rather than being due to NAD, as is assumed in the standard prescription. However, the dry-cavity experiments (LFP, WC other than WC-2) show that it is difficult to account for the observed hydrogen production without some contribution from the nonairborne debris processes, and it would be unreasonable to assume they make no contribution to the IET results.

Cases with Both NAD and Water. Since the WC-2 results also indicate that there is at least some contribution from water, it is likely that both water and nonairborne debris are significant contributors. For example, the combination of 100% co-dispersed water and NAD with a d_t value double the standard value reproduces the data reasonably well (Cases I1rc1414, I3c1425 and I6c1418). There would be any number of combinations of NAD and water contributions capable of providing a reasonable match to the data, and it is not possible to resolve the effects of the two on the basis of integral data alone.

The cases with co-dispersed water and NAD $d_t = 0.02$ m were originally run primarily to make the point that one can define many combinations of water and nonairborne debris interactions that fit the integral data reasonably well. However, when detailed comparisons of calculated and experimental pressure-time histories were made (Section 6.5), it was found that this case sometimes matched the experimental pressure histories better than did either the standard prescription or a simulation that included only co-dispersed water. This case was therefore run for all the other Zion SNL/IET cases. Predicted ΔP values for the SNL/IET Zion experiments are plotted against experimental values in Figure 6.4-1a for the standard prescription (which includes NAD but no water), the case with co-dispersed water and no NAD, and the case for co-dispersed water and NAD only. The predicted versus experimental values for hydrogen production are plotted in Figure 6.4-1b.

Figure 6.4-1. CONTAIN predictions versus SNL/IET Zion experimental results for (a) ΔP and (b) hydrogen production, for alternative assumptions concerning

The case with water but no NAD is underpredicts the data, but it could no doubt be improved by specifying a smaller particle size. There is little to choose between the standard prescription and the case with both co-dispersed water and NAD with $d_t = 0.02$ m. Another interesting feature is that none of the model variations show any ability at all to correlate the hydrogen production data. To be sure, these experiments did not involve large variations in parameters affecting hydrogen production and the range of experimental values is not large. It is, however, significantly larger than the range in the calculated values. It should be recalled that the calculations do take into account experimental variations in accumulator steam supply, blowdown rate, dispersed fraction, and debris-steam coherence. None of these seem to account for the variation in the experimental results, at least according to the CONTAIN model. Stochastic effects associated with the FCI behavior may be involved.

The seemingly remarkable inability to use either the ΔP results or the hydrogen results to choose between a wide range of relative NAD versus water contributions is actually a consequence of the fact that both interactions are still controlled by the CONTAIN heat/mass transfer analogy, and the ratio of heat to mass transfer is not a free parameter. Hence, if one is matched, the other is matched provided the degree of mitigation due to atmosphere-structure heat transfer is being calculated approximately correctly. As will be shown in Section 6.7.2, very different results are expected if the calculation of this mitigation effect is in serious error.

Although it is clearly not possible to use the integral results to choose between the various possible mixes of NAD and water contributions, our current "best estimate" for the Zion SNL/IET experiments does correspond to a mix of water and NAD contributions roughly equivalent to the case with 100% co-dispersed water and NAD $d_t = 0.02$ m, with perhaps a larger contribution from water in those experiments which had a vigorous FCI. The reasons for this choice have to do with the implications of the SNL/IET-8B experiment, discussed in the next subsection, and comparisons of the experimental and calculated pressure-time histories, described in Section 6.5.

6.4.5 Analysis of the IET-8B Experiment.4.5 Analysis of the IET-8B Experiment.4.5 Analysis of the IET-8B Experiment

In two of the SNL/IET Zion-geometry experiments, IET-8A and IET-8B, the cavity contained a much larger amount of water, 62 kg. Originally, neither was analyzed as part of the present effort, but some exploratory calculations were subsequently performed for IET-8B and some of the results obtained will be summarized here. In IET-8A, the steam accumulator did not open to the melt generator and only a relatively small amount of nitrogen was available to eject the melt; this experiment has not been analyzed with CONTAIN. It is worth noting, however, that hydrogen combustion and production in IET-8A were only 55-60% as great as in

IET-8B, and containment pressurization in IET-8A was only 0.087 MPa versus 0.244 MPa in IET-8B. Dispersal of debris from the cavity was also much more nearly complete in IET-8B than in IET-8A. It is evident that the large amount of water in the cavity did not completely suppress DCH-like behavior in IET-8B.

Energy Balance for IET-8B. Before discussing the results of the CONTAIN calculations, it is worth considering some insights that may be inferred from this experiment using simple energy balances. In Reference All94b, experimentally measured temperatures and pressures were used together with the ideal gas law to infer that about 3100 g-moles of steam were added to the containment atmosphere during the experiment, of which 550 g-moles came from the accumulator; hence, it was estimated that about 2550 g-moles of water, or 75% of that originally present in the cavity, had been vaporized. As is noted in the reference, there is some evidence that much of the debris interaction with the cavity water actually occurred in the subcompartments rather than in the cavity. It was also estimated that the energy required to vaporize this much water corresponds to about 84% of the total energy potentially available from the debris ejected from the melt generator (101 MJ thermal energy plus 25 MJ metal oxidation energy). This estimate assumes that none of the vaporization energy was supplied by hydrogen combustion.

The 3100 g-moles of steam added to the containment atmosphere correspond to a steam partial pressure of 0.108 MPa at the saturation temperature (~375 K). Thus about 44% of the containment pressurization observed in this experiment can be attributed to addition of steam moles to the atmosphere, with the remainder being due to the addition of sensible heat. In terms of energy, conversion of 2550 g-moles of water at the initial temperature of 321 K to saturated steam required 114 MJ, heating the noncondensible gases from their initial temperatures to the peak containment atmosphere temperature observed in the experiment (462 K) required about 25 MJ, and heating the steam from saturation to 462 K required 7 MJ, for a total sensible heat addition of 32 MJ. Thus, most of the energy did go into vaporizing water rather than adding sensible heat even though the sensible heat addition was responsible for over half the ΔP. This disparity simply reflects the fact that the pressurization resulting from adding sensible heat to the atmosphere is 4-5 times as great as when the same energy goes into vaporizing water and adding the steam to the atmosphere.

Based upon the above, the total energy released to water and the atmosphere must have been at least 114 + 32 = 146 MJ. Of this, combustion of 281 g-moles of hydrogen as observed in the experiment would have supplied about 67 MJ, with the remainder (~79 MJ) coming from the debris, which corresponds to about 62% of the total potentially available. Thus transfer of energy from the debris must have been rather efficient. Note that this estimate neglects energy losses due to atmosphere-structure heat transfer, and therefore is a minimum estimate. Atmosphere-structure heat transfer is very important to the CONTAIN calculations of the other IET experiments (Section 6.7.3). Temperatures in IET-8B were lower than in the other experiments, which would have reduced this effect.

It is interesting to note that the estimated hydrogen combustion energy is about twice the estimated addition of sensible heat to the atmosphere in the preceding analysis. This suggests some hydrogen burn energy may have gone into vaporizing water. Since most hydrogen combustion occurs in the dome, this would imply that significant amounts of water were carried to the dome as aerosol or a fine spray and were available in the atmosphere to absorb some of the burn energy. Video pictures of the event do show white clouds (presumably condensing steam or water spray) entering the dome immediately prior to the appearance of the hydrogen flames, but it is difficult to draw quantitative conclusions from the video. This observation is consistent with the argument that water carried to the dome can contribute to quenching of DCH energy releases, but the argument is weakened by the fact that the simple analysis given above does not take into account atmosphere-structure heat transfer. If these energy losses could be included, it might be found that little of the hydrogen burn energy would be available for vaporizing water.

CONTAIN Analysis of IET-8B. In Section 3.3.1, it was noted that the fundamental "standard prescription" for the DFB model is to set the burn parameters to ensure that most of the DCH-produced hydrogen will burn; the specific values chosen in the analysis of the other experiments were expected to be appropriate for events with no water or small amounts of water. The temperature thresholds involved were not expected to be suitable for analysis of events involving large amounts of water, where gas temperatures can be much lower. Hence the DFB threshold temperature was reset to 300 K for analysis of SNL/IET-8B. Since the justification for using the high value (20.0) of the maximum diluent/combustible mole ratio ('shratio') in the subcompartments was the high temperature threshold specified for the "dry" parameter set, 'shratio' was reset to its default value (9.0) in these analyses. In addition, d_t was set equal to 0.02 m, as suggested by the results discussed in Section 6.4.4.

Airborne debris sources were not derived from the cavity pressurization histories because it appeared that the cavity pressurization was dominated by the debris-water interaction, not by debris entrainment and dispersal, as in the other experiments analyzed in this work. Hence the debris source was represented with a simple trapezoidal time dependence using the procedures described in Section 7.3.

Some results are summarized in Table 6.4-4. The base case defined above gave about the correct amount of hydrogen production and combustion, and the final steam mole fraction in the containment (0.29) agreed reasonably well with the value (0.31) inferred from the steam addition to the containment. However, the calculated ΔP value is substantially underpredicted, and the dome temperature (370 K) is equal to the saturation temperature, which is in

Table 6.4-4 Analysis of the SNL/IET-8B Experiment						
Case	Description	ΔP (MPa)	f_{dome}	Hydrogen Data (moles)		
				$N_{f,H2}$	$N_{H2,burn}$	$N_{H2,prod}$
	IET-8b Experimental Results	**0.244**	**(0.37)[a]**	**306**	**281**	**299**
I8B-1	Base Case (dftemp=300, shratio=9, d_t=0.02 m)	0.146	0.110	259	322	292
I8B-2	"Dry Standard" DFB parameters	0.086	0.129	536	40	288
I8B-3	'shratio'=20	0.155	0.103	211	370	293
I8B-4	'thresh'=300 K	0.160	0.127	253	374	339
I8B-5	No water aerosol in cavity, chute	0.436	0.069	240	560	508
I8B-6	46.5 kg water (75%)	0.210	0.120	265	332	309

disagreement with the experimental results. Performing an energy balance on the CONTAIN results analogous to that performed for the experimental results indicates that about 119 MJ were transferred to the water and the atmosphere, of which only 12 MJ represents sensible heat added to the atmosphere. In the calculation, water not vaporized in the cavity is assumed to condense as water aerosol, most of which is subsequently calculated to transport to the dome where it is available to quench the hydrogen burn energy. In reality, much more water may de-entrain in the subcompartments than the aerosol model calculates.

Since the hydrogen burn energy in the calculation is actually slightly larger than the experimental result, the shortfall in total energy transfer in the calculation must represent insufficient transfer of thermal energy from the debris. Based upon the amount of energy remaining in the trapped debris at the end of the calculation, about 40% was transferred, compared with the minimum of 62% estimated above for the experiment. Among other things, the shortfall implies that the close correspondence between the heat transfer and the mass transfer controlling chemical reaction appears to break down in this analysis. If, for example, the debris particle size was to be reduced to increase heat transfer, the hydrogen production would be overpredicted.

There are at least two possible explanations for this result. In the experiment, FCIs caused heavy damage to subcompartment structures, which allowed the debris transport fraction to the dome to be much higher (0.37) than that observed in previous experiments. No attempt was made to model this damage in CONTAIN. This transport might have enhanced direct heating of the dome atmosphere, although it is possible that this debris would have lost much of its energy to the water before reaching the dome.

The second possibility is that direct debris-water contact results in enhanced heat transfer due to effects such as direct debris-water contact that are not modeled in CONTAIN, as was discussed in Section 3.2.8. That is, the situation might correspond to that diagrammed in Figure 3.2-4b, rather than to that represented by Figures 3.2-3 and 3.2-4a. Since the CONTAIN heat/mass transfer analogy applies only to gas-phase transfers, it does not apply to the processes represented by $R_{hx,3}$ and $R_{mx,3}$ in Figure 3.2-4b and it would not be surprising if the calculated heat/mass transfer ratios are incorrect in this instance.

Case I8B-2 was run with the DFB standard prescription parameters that had been used for the other experimental analyses, with the result that hydrogen combustion was almost totally quenched. The reason is that flows entering the dome were calculated to be below the threshold specified, 400 K. The latter result agrees with the experimental measurements, which were also below 400 K [All94b]. Since the DCH-produced hydrogen clearly did burn, the temperature threshold should not be used.

Case I8B-3 tests the sensitivity to the assumption that airborne debris entrained in the steam-hydrogen mixture may promote combustion even if the steam/hydrogen ratio is very high. This sensitivity is found to be minor.

In Section 3.2.8, it was noted that the CONTAIN model can artificially quench chemical reaction because it mixes hot, fresh debris with older, cooler debris. In Case I8B-4, sensitivity to this effect was examined by setting the threshold to 300 K. Differences with respect to the base case are not large. Debris trapping, not quenching, is the principal effect limiting the extent of reaction in these calculations. In NPP calculations, however, this artificial quenching is more likely to arise because the airborne residence times increase, permitting more aged debris to be mixed with the fresh debris. Hence the reduced threshold is recommended for NPP calculations involving substantial amounts of water.

In reality, quenching of chemical reactions is a legitimate possibility. A separate-effects calculation using the CONTAIN modeling indicated that all the energy-generating metals (e.g., chromium) must react before significant cooling can occur, but that cooling would start once iron is the only remaining metal, since the iron-steam reaction generates little energy. However, by the time the temperature reached the iron solidification point (~1800 K), 80-90% of the iron was calculated to react. The calculation was performed assuming co-dispersed water kept the steam-hydrogen mixture at the saturation temperature. Only debris-atmosphere heat transfer was modeled in the analysis. Direct debris-water heat transfer might enhance the tendency to quench debris prior to complete reaction.

Case I8B-5 was run to illustrate a peculiarity of the CONTAIN model that can give unphysical results if water aerosol formation is not modeled. In the IET-8B calculations, water was introduced into the cavity much faster than debris-gas heat transfer could supply the energy needed to vaporize it, and the water normally condenses as water aerosol. In Case I8B-5, water aerosol formation in the cavity and chute was artificially suppressed. When this is done, CONTAIN still applies a two-phase equation of state for steam thermodynamics, but liquid and vapor phases are not differentiated and the chemical reaction model erroneously interprets the very high total water concentration as representing a very high steam density. Hence reaction rates are greatly overpredicted. The result is calculation of excessive hydrogen production and combustion, and an excessively high ΔP value.

The remaining cases in the table were run to illustrate the sensitivity to the amount of water assumed to actually interact with the debris. Note that sensitivity to whether the "wet" or "dry" DFB parameters are used is slight for the cases with 20 kg of water, and it would also be slight for lesser amounts of water. If the range of results obtained by varying the amount of water is interpreted as an uncertainty range for the effects of the water, it obviously does encompass the experimental results. This range is undesirably large for the present case, in which the amount of water is known. In NPP analysis, however, the amount of water may not be known, and a wide range of water quantities might have to be considered in any case.

These results also suggest that intermediate amounts of water might yield higher DCH loads than either the very small amounts present in the other Zion IET experiments or the large amount present in IET-8B. No experimental data are available for testing this hypothesis, however. Note also that, as in the case of NAD interactions, the potential for water to augment DCH loads is partly due to increased hydrogen production when metal-steam reactions would otherwise be steam-limited, and this potential may be less if the melt is highly oxidic.

6.5 Pressure-Time and Temperature-Time Histories (Zion IET).5 Pressure-Time and Temperature-Time Histories (Zion IET).5 Pressure-Time and Temperature-Time Histories (Zion IET)

Results in Sections 6.3 and 6.4 show that the ability to use the integral results (ΔP and hydrogen production) to sort out the phenomena governing the Zion-geometry IET experiments is limited. In particular, the results provide strong evidence that the data cannot be explained in terms of the interactions of airborne debris and blowdown steam alone, but they do not provide much guidance as to whether the dominant effect is nonairborne debris, debris-water interactions, or a combination of the two.

In principle, pressure-time histories and temperature-time histories provide more detailed information which might be useful for this purpose. Some comparisons with measured pressure-time and temperature-time histories will be presented here, as they do provide some additional insights into the physical processes involved as well as insights concerning the capabilities and limitations of the CONTAIN model.

Since the shapes of pressure-time histories are sensitive to rates of energy input, comparisons given here emphasize four experiments (IET-1R, IET-3, IET-4, and IET-6) for which it is believed that the blowdown rates and debris source rates derived from the experimental accumulator and cavity pressure histories (Section 3.2.2) are reasonably reliable. In IET-1, accumulator pressure increased after the accumulator was opened to the melt generator, whereas normally it decreases due to the increase in free volume, and this anomaly casts doubt upon the estimated number of steam moles initially in the accumulator. In IET-5 and IET-7, the cavity pressure histories were sufficiently anomalous that there may be more uncertainty in the time dependence of the debris sources than in the other cases. The latter three experiments will also be included, however.

6.5.1 Pressure-Time Histories in the Containment.5.1 Pressure-Time Histories in the Containment.5.1 Pressure-Time Histories in the Containment

The time required for pressure equilibration within the containment (including the subcompartments but not the cavity) is short compared with DCH time scales. Hence, the rate of pressure rise is a reasonable measure of the rate of total energy input to the containment atmosphere, without strong sensitivity to the location of the energy input (subcompartments versus dome, etc.). Comparing experimental and calculated pressure-time histories can therefore provide some insight as to the dominant physical processes involved.

In Figure 6.5-1a, the IET-3 experimental pressure-time history for the Surtsey dome is compared with calculated results for the standard input prescription and the various IET-3 cases that were tabulated in Table 6.4-3. The solid curve without plot symbols gives the experimental results. One feature of interest is that there is a significant rise in containment pressure even before the onset of debris entrainment, which begins at about 0.5 s (see Figure 3.2-2). This initial rise in pressure presumably represents the effects of the debris-water interactions which are believed to cause the cavity pressure peaks at times earlier than 0.5 s in these experiments. In the CONTAIN calculations, the water is introduced in parallel with the airborne debris source that represents entrainment (Section 3.2.8). None of the calculations attempt to capture debris-water interactions prior to the onset of debris entrainment, and hence none can reproduce the initial rise in containment pressure.

Figure 6.5-1. Experimental and calculated dome pressure-time histories for (a) SNL/IET-3 and

After the initial rise attributed to the FCI, the experimental curve shows a more rapid rise between 0.5 and 1.0 s, and then continues to rise more slowly. The curve calculated for the standard prescription shows a qualitatively similar behavior. Quantitatively, however, the initial rapid rise is too small and the contribution of the slow rise after 1 s is too large and persists too late into the event. This result is consistent with the expectation that, in the standard prescription, the nonairborne model overemphasizes interactions occurring late in the blowdown. There are several possible reasons for this tendency:

- The efficiency of the interaction may not scale correctly as a function of steam flow rates (Appendix B)

- The model neglects heat transfer from debris to structures.

- Processes represented by the "nonairborne" model may include splashing and dripping effects that prolong de-entrainment in the subcompartments beyond what is allowed for by the trapping model for airborne debris, but which may diminish considerably more rapidly than allowed for by the nonairborne model standard prescription (see Section 3.2.7).

Another likely reason for the difference in shape between the experimental and the standard prescription curves is the effects of the cavity water. The dashed curves in the figure give results calculated for no NAD and no water (Case I3c1410 in Table 6.4-3), no NAD and 100% co-dispersed water (Case I3c1422), and no NAD and 100% co-dispersed water and reduced particle size (Case I3c1424). Except for their amplitude, these three curves have a similar shape, characterized by a very rapid rise during and immediately after the dispersal interval followed by a rapid flattening. These curves are more squared off than the experimental results, suggesting that there is some later-time contribution from nonairborne debris effects, even if it is less than implied by the standard prescription.

The case that includes both water and NAD with $d_t = 0.02$ m turns out to give a rather good agreement with the experimental pressure-time history. The principal qualification is that some of the debris-water interaction should actually be credited during the first 0.5 s rather than all being concentrated during the interval of debris dispersal.

Figure 6.5-1b presents equivalent results for the IET-6 experiment, which reveals some distinct differences. In terms of shape, agreement with the standard prescription curve is noticeably poorer than in IET-3, while the agreement with the curves that include co-dispersed water but no NAD is somewhat better than in IET-3. The curve calculated for the case including both water and NAD with $d_t = 0.02$ agrees with the experimental curve as well as any, but the agreement is not as good as it is for IET-3. The contribution of NAD appears to be too large, or at least it persists too late into the event. A careful examination of the curves shows that most of the differences noted actually reflect differences in the two experimental curves; the calculated curves for corresponding analyses of the two experiments are quite similar.

These results can be interpreted as indicating that debris-water interactions were more important in IET-6 than in IET-3, with the difference being partially compensated for by increased NAD interactions in IET-3. This interpretation is consistent with the observation that IET-6 had a strong FCI with explosive characteristics and a cavity pressure rise of 2.2 MPa, while IET-3 had a relatively weak FCI, with a nonexplosive cavity pressure rise of only 0.25 MPa (see Figure 3.2-2). The containment ΔP in IET-6, 0.279 MPa, was also somewhat greater than in IET-3, 0.246 MPa. (It should be recalled here that pre-existing hydrogen was included in IET-6 but not in IET-3, although any contribution of this hydrogen to ΔP in IET-6 is believed to be minor; see Section 6.6.3.)

In Figure 6.5-2a, similar results are given for IET-4 except that no case with a particle mmd of 0.5 mm was run. Results are intermediate between those obtained for IET-3 and IET-6. FCI behavior (Figure 6.5-2b) and containment ΔP (0.262 MPa) were also intermediate between those of IET-3 and IET-6.

Also shown in the figure is a "limiting NAD" case, in which no debris dispersal from the cavity was allowed but the trapped field diameter, d_t, was set to a sufficiently small value (0.002 m) that blowdown steam came to a good approximation of thermal and chemical equilibrium with the debris in the cavity, converting the steam into very hot hydrogen which burned upon entering the containment. This case therefore represents the maximum possible rate of energy input to the containment atmosphere provided energy transport rates are limited to that which can be transported by blowdown steam. Though this case included no airborne debris, including it does not alter the steam limit; airborne debris can increase total energy transfer rates only insofar as it can interact with something in addition to blowdown steam. (Note that curves for both the no-NAD case and the standard prescription are enveloped by the limiting-NAD curve at all times.) The interesting point is that this limiting NAD case shows an initial rate of pressure rise that is slower than what was observed, even though the final ΔP calculated was higher than that observed. Additional steam provided by vaporization of cavity water appears to be the most plausible candidate for the additional interactions required to explain the rapid pressure rise, since compartmentalization limits direct interaction between airborne debris and the containment atmosphere.

<ins>Pressure-Time Histories with an Inert Atmosphere</ins>. Much of the energy input to the containment atmosphere in the experiments discussed above resulted from hydrogen combustion, and the calculated pressure-time histories could therefore be affected by any uncertainties in the calculated hydrogen combustion rates. However, this is not an issue when the containment atmosphere is inert. In Figure 6.5-3a, pressure-time histories are compared for IET-1R as in the previous series. Except for the much lower amplitude of the curves, results are similar to those given previously, especially the IET-3 case, with the curve including both water and NAD giving relatively good agreement with experiment. It is likely, therefore, that the previous results are not being heavily distorted by uncertainties in the rate of hydrogen combustion.

The FCI signature in IET-1R (Figure 6.5-3b) is nonexplosive with a maximum cavity pressurization of about 0.32 MPa, and thus resembles IET-3 more nearly than it does IET-4 or IET-6. This result continues the apparent correlation between shape of the pressure-time history with FCI strengths; i.e., the cases with weak nonexplosive FCIs yield pressure-time histories in reasonable agreement with the calculation including both water and NAD with d_t = 0.02 m, while the cases with stronger FCIs yield a more rapidly rising pressure-time history. This apparent correlation was not anticipated and seems somewhat surprising since the comparisons discussed are based upon the main pressure rise during and immediately after debris entrainment and dispersal, while the FCIs occur earlier, during the first few tenths of a second of the event. If the correlation is real, it presumably reflects the effect of the FCI upon subsequent events.

Other SNL/IET Zion Cases. The calculated and experimental pressure-time histories are compared for IET-1 in Figure 6.5-4a and the FCI signature is reproduced in Figure 6.5-4b. All cases except the no-NAD, no-water case overpredict the peak pressure, which is not what would be expected based upon previous trends, in view of the relatively strong FCI. Figure 6.5-5 gives equivalent results for IET-5. Note that the cavity pressure curve in Figure 6.5-5b never converges to the containment curve due to an experimental difficulty; for this reason, the time dependence of the debris source for this case is suspect. However, hydrogen combustion may be the reason the experimental ΔP results are underpredicted. Experimentally, 53 g-moles of hydrogen were estimated to burn, while only 10-20 g-moles burned in the calculations. This difference is enough to account for the differences in ΔP.

Results for IET-7 are given in Figure 6.5-6. Note that the cavity pressurization curve is considerably broader and lower than those obtained for the previous experiments. Careful examination of the experimental pressure-time history for IET-7 indicates that its rate of rise during the debris dispersal interval is somewhat slower and longer in duration than that of the other cases in which hydrogen burned, as would be expected from a slower and longer debris dispersal history. Hence the difference in the cavity pressurization history is probably real, not an experimental problem. The calculation with co-dispersed water and NAD d_t equal to 0.02 m gives a good account of the containment pressure-time history.

6.5.2 Cavity Pressure-Time Histories.5.2 Cavity Pressure-Time Histories.5.2 Cavity Pressure-Time Histories

Experimental pressure-time histories for the dome and the cavity for SNL/IET-3 are given in Figure 6.5-7a, which also includes the corresponding pressure-time histories for the standard input prescription (Case I3c1407). The net cavity pressurization associated with the debris entrainment interval is significantly underpredicted in the calculation, but the shape and timing of the net cavity pressurization peak is similar to that experimentally observed. Of course, the significance of the similarity in shape is limited because the cavity pressure-time histories were used to derive the debris sources in the first place. The fact that the code then regenerates a similar pressure-time history does mean that the assumptions used in defining the sources from the experimental pressure-time history are consistent with the model, and the treatment is therefore internally consistent.

Figure 6.5-7. SNL/IET-3 experimental and calculated cavity pressurization histories, with

It may be noted that, in the calculation, the cavity pressure curve does not return as rapidly to the containment pressure curve as in the experimental histories. In the calculation, the persistence in cavity pressurization is associated with the rapid flow of steam out the cavity exit chute as the blowdown continues, which results in some cavity pressurization even after dispersal terminates. There are probably several reasons why the effect is overestimated in the calculation, and one of them is the tendency of the standard prescription to overestimate the degree of steam heating by nonairborne debris at late times.

In Figure 6.5-7b, similar comparisons are made for Case I3c1425 (co-dispersed water, NAD $d_t = 0.02$ m). Here even the absolute magnitude of the net cavity pressurization, as well as the shape, agrees well with the experimental result. In some degree, this agreement is probably coincidence. However, it is likely that some of the water dispersed by the FCI initially wets the cavity and chute surfaces; indeed, the entire cavity water inventory could be accommodated by a film only 1 mm thick on these surfaces. As debris exits the cavity, any such water could hardly escape vaporization and the additional steam generated would add to the cavity pressurization in a manner qualitatively consistent with the calculated effects.

Comparisons between calculated and experimental cavity pressurization curves are difficult to interpret, in view of the possible impact upon cavity pressures of some of the limitations of the modeling used. Relatively little effort has been spent on making such comparisons. The most important result is probably the fidelity with which the code reconstructs the shape of the pressure-time history, which demonstrates the internal consistency of the approach being used here to define the debris sources.

6.5.3 Subcompartment Temperature-Time Histories.5.3 Subcompartment Temperature-Time Histories.5.3 Subcompartment Temperature-Time Histories

Temperature-time histories are more difficult to interpret than pressure-time histories because they represent conditions at a single location rather than integral values (temperature equilibration times within the containment are not short compared with DCH time scales), and the measurements themselves are extremely difficult to perform reliably in the intensely hostile DCH environment. Furthermore, CONTAIN can calculate only average temperatures for any one cell. No attempt to calculate temperature distributions in the dome was made.

Of the measurements taken in the subcompartments, the most useful for purposes of comparing with CONTAIN calculations appear to be the results cited in Reference All94b for temperatures of gases exiting the subcompartments through the RCP 1A vent space, located above one of the reactor coolant pumps on the same side of the refueling canal as the cavity exit. Experimental data obtained for this location appeared to be of good quality except for two cases (IET-1 and IET-3) in which it is known that damage to the thermocouples perturbed the measurement [All94b]. The temperature histories measured at this location for the other experiments were all rather similar except in IET-8, for which temperatures were much lower, presumably reflecting the quenching effect of the large amount of cavity water.

The most nearly comparable CONTAIN temperature would be the temperature calculated for Cell 11 of the 14-cell deck (Appendix A), which represents the pump deck level on the cavity exit side of the refueling canal. Experimental and calculated temperature histories are compared for IET-6 and IET-1R in Figures 6.5-8a and 6.5-8b, respectively. Corresponding curves for the two experiments are rather similar, with IET-6 yielding somewhat higher temperatures due to hydrogen combustion. However, the differences between the two experiments are not large, indicating that hydrogen combustion did not greatly affect either the measurements or the calculations. The reason is that the subcompartment oxygen supply is quickly consumed, and most hydrogen combustion evidently occurred in the dome at an elevation above the location of the thermocouples in the RCP 1A vent.

Figure 6.5-8. Comparison of temperature-time histories calculated for the pump deck cell

Trends exhibited by the later portions of the temperature-time histories are somewhat as might be expected from the previous pressure-time comparisons. The standard prescription overpredicts the late-time temperatures, the cases with no NAD underpredict these temperatures, and the case with both water and NAD interactions with d_t = 0.02 m gives the most reasonable results.

At early times, all the calculated curves show a much higher and sharper temperature excursion than do the experimental curves. The calculated temperature excursions are due to the interactions of the airborne debris with steam and with the subcompartment atmosphere. These airborne interactions are generally considered to be the best-understood processes contributing to DCH, and are the processes modeled in the most detail in CONTAIN. Hence, this discrepancy might be considered surprising if one could be certain that the measurements were capable of following the rapid temperature excursions involved. The thermocouple time constant quoted by the manufacturer, 0.3 s [All94b], is at best borderline in this regard; however, the manufacturer's calibration was for a nitrogen atmosphere and it is possible that the higher thermal conductivity of the steam-hydrogen mixture could give a more rapid response in the DCH environment.

If the early temperature discrepancy is viewed as real, one conceivable explanation that was considered prior to the start of the present assessment effort was the possibility that the airborne interactions are actually relatively inefficient and the NAD interactions dominate. In this event, one would expect the time-temperature histories to be less sharply peaked, which is in qualitative agreement with the experimental results. It was also found that simple correlations based upon debris films on structures (basically similar to correlations discussed in Appendix B) could actually correlate the complete DCH data base for compartmentalized geometries fairly well. However, it is now believed that this agreement principally reflects the simplicity of the data base systematics, which can also be correlated fairly well merely by considering the total accumulator steam inventory together with allowing for whether hydrogen can burn (Section 2.2). This extreme form of the nonairborne model also appears to be incompatible with some of the CONTAIN results. For example, even the "limiting NAD" case run with d_t = 0.002 m yielded too slow a pressure rise (Figure 6.5-2a), and a model based upon more realistic estimates of NAD interaction efficiencies would yield even slower rises.

Since there is some doubt as to whether the measurements were capable of following the rapid temperature excursions predicted,* additional comparisons of temperature-time histories will not be considered here. Further examination of this question might be justified if it can be

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

established that the measurements should have been able to follow the excursion and that the discrepancy is therefore real.

6.6 Hydrogen Combustion Models.6 Hydrogen Combustion Models.6 Hydrogen Combustion Models

In this subsection we consider what may be learned concerning the performance of the CONTAIN hydrogen combustion models in a DCH event. In all the calculations, the deflagration model parameters were left at their standard values. Although small deflagrations were sometimes calculated to occur in some of the subcompartment cells, the conditions were such that they would have little effect upon the calculation and no effort was made to assess the deflagration model in this work. In plant calculations, there are certain pitfalls potentially associated with the deflagration model which will be discussed in connection with user guidance in Section 7.

6.6.1 Diffusion-Flame Burn (DFB) Model.6.1 Diffusion-Flame Burn (DFB) Model.6.1 Diffusion-Flame Burn (DFB) Model

The diffusion-flame burn model was responsible for most of the combustion of DCH-produced hydrogen that was calculated to occur in the IET experiments (especially the Zion-geometry cases). For reasons discussed later, it was accepted that the threshold for DFB initiation could not be accurately reproduced by the simple concentration and temperature criteria available in the model. Hence assessment was limited to showing that the results are not sensitive to DFB parameters when the changes do not result in crossing combustion thresholds, and to illustrating results when the thresholds are crossed.

Some results of interest are tabulated in Table 6.6-1. For all experiments except SNL/IET-6 and SNL/IET-7, the first two cases tabulated are the standard prescription cases followed by a case with all DFB concentration parameters left at their default values. The latter are much less conservative: 55 mole-percent (m/o) versus 95 m/o for the steam inerting threshold, 5 m/o versus 1 m/o for the minimum oxygen concentration in the receiving cell, and 9 versus 20 (in the subcompartments) for maximum diluent/combustible mole ratio in the incoming gas. The temperature threshold was left as in the standard prescription.

Table 6.6-1
Results for DFB and BSR Model Assessment

Case	Description	ΔP (MPa)	f_{dome}	Hydrogen Data (moles)		
				$N_{f,H2}$	$N_{H2,burn}$	$N_{H2,prod}$
	SNL/IET-3 Experimental Results	**0.246**	**0.088**	**37**	**190**	**227**
I3c1407	Standard input prescription	0.228	0.101	21	232	253
I3c1430	Default DFB concentration limits	0.232	0.102	10	242	253
	SNL/IET-5 Experimental Results	**0.103**	**0.057**	**468**	**53**	**319**
I5c1412	Standard input prescription	0.212	0.084	140	310	247
I5c1407	Default DFB concentration limits	0.085	0.102	430	18	245
	ANL/IET-6 Experimental Results	**0.250**	**0.138**	**2.95**	**4.22**	**4.89**
A6c1402	Standard input prescription	0.260	0.067	3.15	4.58	5.43
A6c1406	Default DFB concentration limits	0.321	0.066	0.91	6.78	5.38
	SNL/IET-6 Experimental Results	**0.279**	**0.138**	**154**	**345**	**319**
I6c1407	Standard input prescription	0.248	0.085	165	256	240
I6c1412	Dome 'srtemp' = 600 K	0.365	0.085	19	401	239
	SNL/IET-7 Experimental Results	**0.271**	**0.074**	**234**	**323**	**274**
I7c1407	Standard input prescription	0.244	0.057	243	296	255

Table 6.6-1 (Continued) Results for DFB and BSR Model Assessment						
Case	Description	ΔP (MPa)	f_{dome}	Hydrogen Data (moles)		
				$N_{f,H2}$	$N_{H2,burn}$	$N_{H2,prod}$
	SNL/IET-11 Experimental Results	**0.430**	**0.240**	**137**	**1828**	**1517**
I11c801	Standard input prescription[a]	0.437	0.262	9	1902	1462
I11c821	Default DFB concentration limits[a]	0.449	0.260	9	1887	1447
I11c802	Dome 'srtemp' = 2000 K[a]	0.372	0.263	373	1540	1464
I11c809	Reduced 'srtemp' by 100 K[a]	0.437	0.261	5	1908	1465
I11c811	As I11c809, 'srrate' 2 x standard[a]	0.444	0.260	5	1912	1468

For IET-3, the large difference in the burn thresholds made essentially no difference; the DFB model was able to operate effectively with default parameters because most of the hydrogen combustion occurred as the flow entered the dome and oxygen depletion was insufficient to drop below even the default limits. In IET-5 (heavily inerted with 75.8% CO_2 and only 4.35% O_2), the standard prescription erroneously allowed extensive hydrogen combustion and hence overpredicted ΔP substantially, while the default values yielded more realistic behavior.

The IET-9, IET-10, and IET-11 experiments illustrate the motivation for defining the more conservative standard prescription. These experiments provide a graded series with respect to the chemical reactivity of the atmosphere in that steam concentrations are 67.24%, 48.2%, and 32.25% respectively, while oxygen concentrations are 6.14%, 10.17%, 13.66% respectively. In IET-9, the default DFB parameters totally suppress this combustion mode, while they would do so only after substantial oxygen depletion in IET-11. IET-10 presents an intermediate case, initially noninert with the default parameters but with inerting developing relatively quickly as the atmosphere is vitiated.

Results are in accord with expectations in that the difference between the standard prescription and the default settings are greatest for IET-9 and least for IET-11. In all cases, the standard prescription gives better agreement with experiment although it is a little too efficient in cleaning out the residual hydrogen in IET-10. The IET-9 results show that the default settings can be very nonconservative for the DCH environment, and also suggest that, for a realistic degree of containment inerting, the potential for excess conservatism in the standard prescription may not be of practical import because actual containments are not likely to be more heavily inerted than was the atmosphere in this event.

Although the standard prescription for DFB parameters may result in overly complete hydrogen combustion, the extra combustion predicted probably occurs late in the event with little or no contribution to ΔP. (The BSR model is also involved in the overprediction of the late combustion, however, and the effect of the two cannot always be cleanly separated; the code does not separately keep track of how much hydrogen each model burns.) However, there is little evidence that the standard prescription DFB parameters result in overpredicting ΔP except in those cases for which the acknowledged excessive conservatism with respect to thresholds results in the model predicting combustion where in fact relatively little combustion occurs, as in IET-5.

Observations on Thresholds for the DFB Model. The first observation is that the concept of a distinct "threshold" may not be fully applicable to DCH scenarios, in which the hydrogen-containing gases may enter the oxygen-containing volume at extreme temperatures. As the first oxygen-containing gas is entrained into the hydrogen jet or plume, the high temperature probably ensures that at least some reaction occurs. If the oxygen concentration is sufficiently low, the energy release will not be sufficient to heat the entrained diluent that accompanies the oxygen, and the reaction will snuff out before enough oxygen is entrained to burn most of the hydrogen entering the cell. The best a "threshold" model can hope to do is provide an approximate representation of this effect. Some reaction is still expected to occur even on the "inert" side of the threshold, but the expectation is that this combustion will be insufficient to contribute substantially to ΔP.

Results summarized below for the ANL/IET-8, SNL/IET-5, and SNL/IET-12 experiments all illustrate the expected behavior, in that a limited amount of hydrogen did burn but the containment pressurization resulting was much more in line with the totally inert cases than with the cases in which combustion of DCH-produced hydrogen appeared to be quite efficient. Nonetheless, in SNL/IET-5, significantly more hydrogen did burn than is predicted by the default model, which is in agreement with the expectation that the CONTAIN models will give too sharp a threshold behavior.

From the IET-9 results, it is clear that the default DFB parameters could be very nonconservative for DCH conditions. The IET-5 event was more heavily inerted than IET-9 and it is possible that a DFB parameter set giving good results for both experiments could be found. However, a search for such parameters is not recommended because examination of the complete data base, including experiments not analyzed with the CONTAIN code, shows that it will not be possible to find parameters that give the correct result in every case. This evidence will be discussed next.

Experimental data of possible interest to the question of concentration thresholds are summarized in Table 6.6-2. The ANL/IET-8 and SNL/IET-12 experiments are included even though they have not been analyzed with CONTAIN because they provide insights as to the variations in combustion behavior that can arise. The first four columns give the experiment number, the identity of the diluent gas, the diluent mole fraction (expressed as excess over air when N_2 is the diluent), and the oxygen mole fraction. The last four columns give results for ΔP, hydrogen moles burned and moles produced, and f_{trans}. The last quantity is the fraction of the initial thermite mass transported beyond the subcompartments and is equal to $f_{eject}*f_{disp}*f_{dome}$, in the notation used in Section 6.3.2. Parameters not listed in the table, but which are possibly relevant, include the presence of pre-existing hydrogen in ANL/IET-6, SNL/IET-9, SNL/IET-10, and SNL/IET-12; the fact that the last three were in Surry geometry while the others are Zion; and the small scale (approximately 1:40) of the ANL/IET experiments.

Table 6.6-2 Data of Interest to Assessing DFB Threshold Concentrations							
Experiment	Diluent		O_2 Mole Frac.	ΔP (MPa)	H_2 Data (g-moles)		f_{trans}
	Type	Mole Frac.			$N_{H2,burn}$	$N_{H2,prod}$	
ANL/IET-1RR	N_2	> 0.99	0.0012	0.150	~0	4.00	0.123
ANL/IET-3	N_2	0.48	0.108	0.190	3.50	4.65	0.040
ANL/IET-6	N_2	0.50	0.099	0.250	4.22	4.89	0.093
ANL/IET-8	Steam	0.51	0.077	0.133	1.0	5.6	>0.029
SNL/IET-1	N_2	>0.99	0.0003	0.098	(~3)	233	0.089

The following points should be kept in mind when evaluating the results given in the table:

- When comparing results for experiments involving different diluents, N_2 is expected to be less effective in suppressing combustion than either steam or CO_2. An approximate representation of this effect is included in the CONTAIN model [Mur95].

- Large scale is expected to favor combustion because one factor determining whether the reaction can be self-sustaining is the competition between energy release by chemical reaction versus the energy losses due to various processes tending to cool the reacting system. Within certain limits, the time scales for the chemical kinetics factors controlling reaction rates tend to be approximately scale-independent while the time scales of the cooling processes tend to increase with scale. No scale effect is modeled by the code.

- It is not known whether the geometry differences (i.e., Zion versus Surry) could have a significant impact upon the effective threshold values.

If one were to attempt to correlate combustion behavior with concentration limits alone, the following anomalies would be apparent:

1. Although most DCH-produced hydrogen did burn in ANL/IET-3, comparison with the ANL/IET-1RR ΔP shows that its contribution to containment pressurization was considerably less efficient than for either ANL/IET-6 or SNL/IET-3.

2. There was little hydrogen combustion in ANL/IET-8 even though its degree of inerting was substantially less than that of SNL/IET-9, which did burn hydrogen.

3. Hydrogen combustion contributed relatively little to the SNL/IET-12 event while it contributed effectively in SNL/IET-9, even though the latter had significantly higher steam concentrations and lower oxygen concentrations.

The difference between ANL/IET-3 and SNL/IET-3 probably represents the effect of scale, and the same may be true of the failure of significant hydrogen combustion to occur in ANL/IET-8. The reason for the difference between ANL/IET3 and ANL/IET-6 is less immediately clear. Although the latter did include pre-existing hydrogen, there is little evidence that pre-existing hydrogen contributed significantly to ΔP even in the larger-scale SNL/IET-6 and SNL/IET-7 experiments. The clearest anomaly, however, is the failure to burn hydrogen effectively in SNL/IET-12. Although this event was 1/10-scale while SNL/IET-9 was 1/5.75-scale, this relatively small difference in scale is unlikely to account for the difference in behaviors.

We believe that one plausible explanation is that the efficiency of hydrogen combustion in marginal cases may be affected by the amount of hot debris accompanying the hydrogen stream. For all the pairwise comparisons which are otherwise difficult to explain, the values of f_{trans} in the case which did not burn hydrogen effectively are substantially lower than in the case in which hydrogen combustion was more effective. The low value of f_{trans} in SNL/IET-12 versus the much higher value in SNL/IET-9 is especially noteworthy.

Even in cases that are otherwise explainable, the value of f_{trans} may have played a contributing role. Thus, SNL/IET-5 has a low value of f_{trans}. The same may have been true of ANL/IET-8; however, an unknown amount of debris was lost during the recovery procedure for this experiment and the value of f_{trans} tabulated is only a lower limit.

Summary, DFB Model Assessment. The CONTAIN DFB model does not take into account any effect of debris mixed with the hydrogen flow entering a cell, and it does not include any allowance for the effect of scale. Hence it is not expected that the model will reproduce threshold effects in borderline cases, whatever choices are made for the DFB parameters. The standard prescription, it is to be recalled, is not based upon a claim that the parameters chosen are the correct values; rather the prescription is intended to ensure that, in scenarios not involving large amounts of water, most DCH-produced hydrogen will burn except when oxygen is almost completely absent. Based, in part, upon the IET-9 result, it appears that this assumption will be correct for most NPP DCH scenarios; when it is not correct, the prescription errs on the side of caution, as was intended. While the prescription is deliberately conservative with respect to some of the thresholds involved, it is not excessively conservative with respect to the consequences when the thresholds are exceeded. That is, given that the thresholds are exceeded, there is no evidence that the standard prescription yields overly conservative results. The standard prescription is therefore judged suitable as given for NPP DCH scenarios that do not involve large amounts of water.

In scenarios that do involve substantial water, the standard prescription temperature thresholds are potentially nonconservative and should be lowered or eliminated. Additional user guidance for this situation is given in Sections 7.8 and 7.9.

6.6.2 Bulk Spontaneous Reaction (BSR) Model.6.2 Bulk Spontaneous Reaction (BSR) Model.6.2 Bulk Spontaneous Reaction (BSR) Model

In CONTAIN DCH calculations, the BSR model provides the usual mechanism by which most of the pre-existing hydrogen can burn. Although some pre-existing hydrogen will burn in the subcompartments, and pre-existing hydrogen entrained into a diffusion flame is also assumed to burn in the DFB model, combustion of most of the pre-existing hydrogen usually will not occur unless temperatures in the main volume of the containment dome exceed the threshold temperature, 'srtemp'. In all the Zion-geometry calculations, calculated dome temperatures were of the order of 700 K or less, which is well below the value that was specified in the calculation (848 K) or even the default value (773 K). On the other hand, the specified value (840 K) in the Surry-geometry CTTF experiments was always exceeded in the standard prescription cases, and the pre-existing hydrogen therefore burned.

Sensitivity to assuming that the pre-existing hydrogen could burn in the Zion-geometry experiments was investigated by setting 'srtemp' to 600 K, and results are given in Table 6.6-1. In all three cases, ΔP and hydrogen combustion are substantially overpredicted while the hydrogen remaining unburned is substantially underpredicted. It is apparent, therefore, that the pre-existing hydrogen did not contribute appreciably to ΔP.

In ANL/IET-6, the hydrogen consumed was less than that produced. In the larger-scale SNL/IET-6 and SNL/IET-7 experiments, however, the hydrogen burned exceeds that produced. The results are consistent with the hypothesis that, in the SNL experiments, significant reaction of pre-existing hydrogen did occur but on a time scale too slow to contribute substantially to ΔP. Even some contribution to ΔP cannot be ruled out, as these experiments yielded ΔP values slightly higher than did either the standard-prescription calculation or the experimental values for IET-4 and, especially, IET-3. However, the differences are too small to be at all convincing and could easily reflect chance variables. Indeed, the apparent correlations with FCI characteristics (discussed in Section 6.5.1) suggest that the stochastic variability of FCI behavior could have been a more important factor.

The difference between the amount of hydrogen combustion in ANL/IET-6 versus the SNL cases is large enough to be at least suggestive, especially in view of fact that the difference is in the direction of the expected scale effect. Hence it might be premature to assume that the pre-existing hydrogen could not contribute to ΔP in an NPP-scale event. Furthermore, if the reaction rates are controlled by chemical kinetics, only a moderate increase in dome temperature would be required to accelerate the rates by orders of magnitude, increasing the likelihood that a significant contribution to ΔP might be expected. A more vigorous DCH event could provide higher temperatures, as would more prototypic initial containment temperatures, which were only ~300 K in the experiments. On the other hand, if factors such as gas mixing rates are controlling the reaction rate for pre-existing hydrogen, combustion of this hydrogen might be ineffective even in a more severe event.

The code calculations themselves suggest an alternative explanation which has different implications when extrapolated to NPP scale and/or more severe DCH scenarios. Inspection of the hydrogen production and combustion numbers in Table 6.6-1 shows that the standard prescription results are actually quite faithful to the trends noted above; i.e., hydrogen combustion calculated for ANL/IET-6 is less than that produced while combustion exceeds production for SNL/IET-6 and, especially, SNL/IET-7. The reason is that some pre-existing hydrogen is calculated to burn as containment gases recirculate back into the still-hot subcompartments after the blowdown is complete. Additional discussion of this result is given in Section 6.6.3.

Surry-Geometry CTTF Results. Table 6.6-1 also gives results for IET-9, IET-10, and IET-11 in which 'srtemp' in the dome was set to 2000 K in order to suppress combustion of pre-existing hydrogen in the dome. In IET-9, there was a negligible effect upon ΔP and the effect upon hydrogen combustion was not large because, in both calculations, most of the unburned hydrogen was DCH-produced hydrogen which remained in oxygen-starved subcompartment volumes. In IET-10, suppressing BSR in the dome did result in considerably more hydrogen being left unburned, but the effect upon ΔP was still minor. Experimentally, the amount of unburned hydrogen left was intermediate between the two calculations and does indicate that some pre-existing hydrogen reacted. There is no way of knowing whether it did so sufficiently rapidly to contribute to ΔP. The reason for the small effects of the pre-existing hydrogen in the calculations is that the amounts were small, corresponding to oxidation of only ~15% of the Zr clad.

In IET-11, the amount of pre-existing hydrogen was somewhat larger, corresponding to about 24% Zr oxidation, and allowing it to burn made a somewhat larger difference in ΔP, about 0.06 MPa. The standard prescription result is considerably closer to the experimental result than is the case with BSR suppressed in the dome. It was originally thought that this result was sufficient to establish a preference for the hypothesis that pre-existing hydrogen did contribute to ΔP and that values of 'srtemp' significantly higher than what was assumed here might not be defensible. However, it was later discovered that analysis of the Surry- geometry experiments was sensitive to nodalization in a way not anticipated from the Zion-geometry results, and further discussion of whether pre-existing hydrogen contributed will be deferred until the nodalization sensitivity is discussed in Section 6.6.3.

In Case I11c809 of Table 6.6-1, the threshold temperatures for the BSR model were reduced by 100 K in all cells, with negligible differences resulting. In Case I11c811, the temperature thresholds were reduced as I11c809 and, in addition, the reaction rates were increased a factor of two in all cells, with the effect again being minor. These results illustrate a common observation with BSR use, that the most important question is typically whether the dome threshold temperature is or is not exceeded. If it is exceeded, it usually matters less as to what the exact threshold is or what the reaction rates are, unless the latter are significantly longer than the standard values. Of course, exceptions can arise, and it must be expected that sensitivities will be larger when the amounts of pre-existing hydrogen are larger.

6.6.3 Sensitivity to Containment Nodalization.6.3 Sensitivity to Containment Nodalization.6.3 Sensitivity to Containment Nodalization

Zion Geometry. In Table 6.1-3 of Section 6.1, results were presented for a 5-cell calculation (Case I3c557) in which it was found that the ΔP value calculated using the 5-cell representation (0.226 MPa) was in good agreement with the 14-cell results (0.228 MPa). There is, however, a larger difference in the amount of hydrogen burned, with the 5-cell deck giving 167 g-moles burned while 232 g-moles were burned in the 14-cell calculation. Most of this difference was due to differences in the amount left unburned (72 g-moles versus 21 g-moles, respectively) rather than differences in the amount produced. Experimentally, the amount left unburned (37 g-moles) lies between the two calculated values and is closer to the 14-cell result.

The differences in hydrogen burned, 65 g-moles, in the two decks is not entirely trivial: if we attribute the difference between the experimental IET-1 and IET-3 ΔP values, 0.148 MPa, to the 190 g-moles observed to have burned in the experiment, one might expect burning an extra 65 g-moles in the 14-cell deck to contribute about 0.05 MPa. The reason the actual impact upon ΔP was much smaller is illustrated in Figure 6.6-1. In this figure, the pressure-time histories calculated for both decks are plotted (left-hand axis). The total hydrogen burned, and also the hydrogen burned in the subcompartments, is plotted against the right-hand axis. The curves are very similar for both decks until about the time the blowdown is complete, by which time the peak pressure has been reached. At later times, the curves diverge, but only at times too late to affect the peak pressure; only the rate of pressure decay is affected.

Figure 6.6-1. SNL/IET-3 experimental and calculated pressure-time histories and calculated cumulative hydrogen combustion, comparing calculations for 5-cell and 14-cell decks.

This behavior can be understood in terms of the Zion subcompartment geometry. The volume of the subcompartments is relatively small (~ 5% of the total Surtsey free volume) and quickly becomes oxygen-starved. Relatively little hydrogen combustion can occur at early times in the subcompartments and results are not sensitive to the details of how it is modeled. During most of the time of interest, combustion occurs principally as the continuing blowdown sweeps hydrogen from the subcompartments to the main dome volume. The latter never approaches oxygen starvation, and the rate of flow through the subcompartments is controlled by the blowdown; hence the processes involved are not sensitive to nodalization.

After blowdown is complete, combustion of hydrogen remaining in the subcompartments can occur only insofar as convective flows bring oxygen into the subcompartments and/or permit hydrogen to leave the subcompartments. In the 5-cell deck, in which the entire subcompartment volume is lumped into one cell, the parameters controlling combustion drop below the governing thresholds sooner than they do in those parts of the 14-cell representation in which the combustion is occurring. Thus more hydrogen burns in the 14-cell deck, but it occurs too late to affect ΔP. The behavior calculated with the 14-cell deck seems reasonable and this calculation gives better agreement with experiment as to the amount of unburned hydrogen; however, the curves in Figure 6.6-1 show that the slope of the experimental pressure decay curve is actually reproduced better in the 5-cell deck. Thus it is not clear that the 14-cell calculation provides the most realistic behavior.

In SNL/IET-6 and SNL/IET-7, the same process was calculated to occur and, in addition, the pre-existing hydrogen in containment gases burned after re-entering the still-hot subcompartments. The additional energy release associated with this hydrogen also kept the process going somewhat longer in the IET-7 analysis. Consideration of the scale dependencies involved shows that increasing scale would be expected to favor this process and hence it is reasonable that, in ANL/IET-6, it did not occur to any obvious extent. The CONTAIN calculations also reflect this difference. Even at NPP scale, the process is unlikely to be sufficiently rapid to contribute to the DCH ΔP (at least in Zion geometry), especially since it cannot even begin until the blowdown is almost complete. It is also a process that will not accelerate rapidly as the severity of a DCH event increases.

One cannot accept this explanation as proven, but the results obtained with the 14-cell deck are certainly suggestive. However, the pressure-time histories for these cases, as in Figure 6.6-1, also exhibited a delay in the onset of pressure decay that was not in complete agreement with experiment. Partly for this reason, the proposed explanation for the observed results is considered tentative. Although this late hydrogen combustion, if real, is irrelevant to the calculated ΔP, its explanation is not irrelevant to the interpretation of the experiment and this interpretation can have important implications for ΔP in other DCH scenarios. If the partial combustion of pre-existing hydrogen is interpreted as representing the onset of kinetics-controlled bulk reaction, a much more energetic response might require only a moderately more severe stimulus, while the CONTAIN-based interpretation involves a process with little potential to ever be very threatening.

<u>Surry Geometry</u>. The subcompartment geometry in the Surry experiments is very different from that of Zion. The volumes considered to be the "subcompartment" are considerably

larger, about 30% of the total containment free volume. Most of this is in the basement and the annulus between the crane wall and the containment shell, with the annulus including about two thirds of the total. Thus the "subcompartment" is not a compact, well-enclosed volume as in Zion; instead it is spread out across the entire bottom of the containment (the basement) and around most of the outer periphery (the annulus). Furthermore, flow connections with the dome are large compared with those connecting the Zion subcompartments with the dome.

During the DCH event, gas jets exiting the cavity will impact the ceiling of the RHR platform area, which is also the structure forming the floor of the seal table room. Owing to its momentum, some debris can enter the seal table room if the seal table is displaced, but the opening is too small for much gas flow to pass that way; most gas is deflected radially outward where it exits the RHR platform and enters either the annulus or the outer part of the basement. Gas jets entering the annulus strike the containment shell (as does much debris) and can be deflected sideways or downward but cannot flow directly upward because the floor of the seal table room extends outward to the containment wall at this point. This structure, called the seal table shelf, blocks flow directly upward from the RHR platform exit. Azimuthally, it does not extend significantly beyond the RHR platform in either direction and the annulus is elsewhere open in the upward direction.

In the 8-cell deck, the first volumes downstream of the cavity are the RHR platform and the seal table room; based upon the Zion experience with the trapping models, it was thought desirable to model these small volumes explicitly as separate cells. The annulus and the basement were each modeled as a single cell. A number of simplifications were made in representing the various structures and flow paths elsewhere in the containment.

When the calculated pressure-time histories were examined, it was observed that the rate of pressurization was excessive. The reason was thought to be that treating the basement and, especially, the annulus as single well-mixed volumes was unrealistic and allowed hydrogen entering these volumes to burn immediately in the DFB model as long as oxygen concentrations exceed the 0.01 limit specified in the standard prescription. In reality, one would expect oxygen depletion in the vicinity of the RHR platform exit to slow combustion.

It was not expected that this effect would have an important impact upon the calculated ΔP (if anything, overprediction of ΔP was expected to result from overpredicting the burn rates), and investigating it further was not assigned a high priority. Late in the assessment effort, a 12-cell deck was constructed by dividing the annulus into four quadrants and the basement into two sections. No other refinements to the 8-cell deck were made.

As expected, there was little change in the calculated values of f_{dome} (see Table 6.6-1); debris transport was not sensitive to the change in nodalization. The impact upon containment pressure-time histories is displayed in Figure 6.6-2 (left-hand axis). The cases plotted are Case I11c818 and I11c1206 in Table 6.6-1. The initial rate of rise calculated with the 12-cell deck is somewhat smaller, as anticipated, but the difference is not large. What was unexpected is that the total pressurization calculated by the 12-cell representation was significantly higher, by about 0.05 MPa. This difference does not reflect differences in total hydrogen combustion, as these differences are trivial (Table 6.6-1).

Figure 6.6-2. SNL/IET-11 experimental and calculated pressure-time histories and calculated

The dotted curves and right-hand axis give total hydrogen burned as a function of time. These results do not explain the pressure differences, as the differences in hydrogen burned are either too small or in the wrong direction for all times of interest. The dashed curves show hydrogen burned in the subcompartments and illustrate the considerably greater initial combustion in the subcompartments for the 8-cell deck. Thus, the distribution of combustion is different.

What appears to be the crucial difference is shown in the lower half of the figure, where cumulative hydrogen combustion in the dome is plotted. The 12-cell deck gives larger values at all times. The reason is that the annulus quadrant adjacent to the RHR platform quickly becomes oxygen starved. Subsequently, hydrogen combustion occurs as it flows into adjacent cells, one of which is the dome. In the 8-cell deck, the delay in oxygen starvation in the annulus cell reduces the flow of hydrogen into the dome. Hydrogen burned in the dome contributes to containment pressurization more effectively because the calculated subcompartment temperatures become extremely high and surface/volume ratios are high; hence, energy loss rates are very high. Dome temperatures and surface/volume ratios are substantially lower, which makes the dome a better accumulator for energy.

At this point, no judgment is offered as to which deck gives more accurate results. Although the 12-cell deck does reduce the lack of realism in modeling the annulus as a single well-mixed volume, it also may overpredict the upward flow of hydrogen because it does not model the horizontal deflecting action of the seal table room shelf. If momentum-governed effects dominate the flow patterns, CONTAIN cannot model these phenomena even if more detail is introduced into the representation of flow paths and structures.

At present, no preference will be expressed for either the 8-cell or the 12-cell representation over the other, and the difference in results is accepted as a measure of the uncertainty associated with nodalization. This difference is about equal to the difference in ΔP which results when BSR is suppressed in the dome. Furthermore, reanalyzing IET-9 and IET-10 with 12-cell decks (see appendix D for the numerical results) did not clarify this situation: while the 8-cell deck gives a good reproduction of the trends for these three experiments provided BSR is allowed to occur in the dome (see Section 4.1), the 12-cell representation gave equally good results provided BSR was not allowed to occur in the dome. Hence, no conclusion can be drawn as to whether combustion of pre-existing hydrogen contributed significantly to ΔP in any of the three experiments.

In IET-9, the 12-cell deck did tend to overpredict hydrogen combustion (underpredict hydrogen left unburned) somewhat. Since burn completeness is sensitive to the various burn parameters specified, this result is not very conclusive.

It is interesting to compare the effects of nodalization in the Zion versus Surry geometries. In the Zion geometry, the simpler representation was seen to give an inferior treatment of trapping; ΔP was insensitive to the nodalization provided f_{dome} was predicted about right; and total hydrogen combustion was greater in the 14-cell deck due to differences in late-time combustion effects. In Surry geometry, the nodalization sensitivities observed were almost exactly the reverse: sensitivity of f_{dome} was negligible; ΔP was sensitive to nodalization even though total hydrogen combustion was not; and the difference in ΔP turned out to be due to differences in the <u>location</u> of the <u>early-time</u> combustion.

Before leaving this subject, it is appropriate to provide some perspective on the nodalization sensitivity considered here. The ~0.05 MPa difference obtained for the 8- versus 12-cell IET-11 analysis is only somewhat more than 10% of the IET-11 ΔP, and it cannot be considered a dominant effect. Furthermore, an 8-cell calculation for IET-11 with all mitigation due to atmosphere-structure heat transfer eliminated (Section 6.7.3) yielded a ΔP of 0.693 MPa, more than 0.25 MPa higher than the standard prescription. Hence the uncertainty in mitigation associated with the nodalization difference is only 20% of the total mitigation effect associated with heat transfer. While not trivial, this uncertainty is far from being fatal to the utility of the analysis.

6.7 Mitigation Processes.7 Mitigation Processes.7 Mitigation Processes

6.7.1 Mitigation Processes and the Definition of "Conservatism".7.1 Mitigation Processes and the Definition of "Conservatism".7.1 Mitigation Processes and the Definition of "Conservatism"

Early scoping analyses of DCH [NRC85] came up with excessively high estimates of DCH loads because the simple models used were unable to take credit for mitigation processes that can be very important to the outcome. In this section, we examine the impact of mitigation processes upon the assessment, focusing attention upon IET-11 (Surry geometry) and IET-3 and IET-4 (Zion geometry). Of the experiments in which hydrogen could burn, these span the range in terms of potential severity; i.e., IET-11 gave the highest value of ΔP ever measured in a DCH experiment while IET-3 and IET-4 were at the low end of the range in terms of potential energy input, because they lacked pre-existing hydrogen.

"Mitigation effects" includes a variety of complex and coupled phenomena, but for present purposes it is convenient to group them in terms of just two categories:

- Trapping effects; and

" Atmosphere-structure heat transfer together with incomplete and/or delayed hydrogen combustion.

The importance of mitigation effects is easily illustrated by some of the calculated results for IET-11 and IET-3 in Table 6.7-1. For each experiment, the first case is the standard prescription and the second is a case calculated with trapping deleted (by setting 'trapmul' to 10^{-10}) and heat transfer to structures deleted (by setting all structure areas equal to 10^{-20} m^2). If one adds the initial pressures (0.22 MPa and 0.188 MPa for IET-11 and IET-3, respectively), these results correspond to maximum containment pressures of 1.14 MPa and 0.90 MPa, respectively. Without the mitigation effects, even the "mild" IET-3 event has the potential to generate containment-threatening loads. Obviously, the mitigation effects cannot be treated as secondary concerns, and any DCH calculation will only be as accurate as its treatment of the mitigation processes.

Table 6.7-1
Selected Sensitivity Studies for Mitigation Effect Assessment

Case	Description	△P (MPa)	f_{dome}	H_2 Data (g-moles) $N_{f,H2}$	$N_{H2,burn}$	$N_{H2,prod}$
	IET-11 Experimental Results	**0.430**	**0.307**	**137**	**1828**	**1517**
I11c801	Standard input prescription	0.437	0.262	9	1902	1462
I11c820	No trapping, no hx to structures	0.918	0.714	5	2774	2330
I11c819	No trapping	0.567	0.635	13	2772	2336
I11c808	No heat transfer to structures	0.693	0.272	4	1942	1497
	IET-3 Experimental Results	**0.246**	**0.088**	**37**	**190**	**227**
I3c1407	Standard input prescription	0.228	0.101	21	232	253
I3c1432	No trapping, no hx to structures	0.716	0.946	8	436	444
I3c1431	No trapping	0.372	0.720	107	317	427
I3c1415	No heat transfer to structures	0.401	0.116	5	256	261
I3c1410	No NAD	0.110	0.099	18	84	103
I3c1427	No NAD, no struc., 'srtemp'=300 K	0.183	0.116	0	104	104
	IET-4 Experimental Results	**0.262**	**0.197**[a]	**63**	**240**	**303**

It might be supposed that underpredicting the mitigation effects would at least have the virtue of conservatism, and this is generally true when analyzing NPP scenarios. However, the present exercise is concerned with assessing the code against the experimental data base. In this context underpredicting the mitigation effects is likely to result in a nonconservative assessment. The reason is that, if mitigation effects are being underpredicted, yet the code matches the data reasonably well, it necessarily follows that some other processes that add to DCH loads are being underpredicted or missed altogether, and that the agreement with the experimental results obtained represents a fortuitous cancellation of opposing effects. (The simplicity of the DCH systematics reviewed in Section 2.2 implies that it is not difficult for this cancellation to arise.) However, when the code is applied to other scenarios, there is little reason to suppose that this cancellation will continue in all cases. In particular, it is likely that the code would then underpredict the loads when analyzing scenarios for which the mitigating effects are less important, since the code would be underpredicting the impact of the reduction in mitigation.

6.7.2 Mitigation by Trapping.7.2 Mitigation by Trapping.7.2 Mitigation by Trapping

Cases I11c819 and I3c1431 in Table 6.7-1 were run to illustrate the mitigating effect of trapping in IET-11 and IET-3, respectively. In both these runs, trapping was effectively turned off. The calculated ΔP values substantially exceed either the standard prescription results or the experimental values, but they are much less than was obtained in the previous cases in which both trapping and heat transfer to structures were turned off. Even elimination of trapping does not completely eliminate some of the mitigating effects of compartmentalization because the amount of debris-gas interaction that can initially occur is limited by the supply of steam and gas available in the subcompartments.

Eventually, most of the debris reaches the dome in this calculation but, by this time, much energy has been lost to the structures. Physically, these results are of limited significance because, in reality, any process capable of permitting such large amounts of debris to reach the dome would probably permit it to do so much more rapidly, with less time for mitigation by heat transfer. Nonetheless, the calculation does illustrate the point that the compartmentalized calculation without trapping is not equivalent to an open, noncompartmentalized geometry.

Although predictions of trapping may have larger uncertainties for any NPP scenarios differing substantially from those that have been simulated experimentally, it does not appear that limitations of the trapping model are distorting the assessment of other DCH model features in the sense discussed at the close of the preceding subsection. The principal result of practical interest for trapping is f_{dome}, and direct comparisons with experimental results are available for this quantity. The comparisons with experiment together with the sensitivity studies given previously (Section 6.2) indicate that errors in the trapping model are not distorting other results of interest sufficiently to be of concern.

6.7.3 Mitigation by Heat Transfer and Incomplete or Delayed Hydrogen Combustion.7.3 Mitigation by Heat Transfer and Incomplete or Delayed Hydrogen Combustion.7.3 Mitigation by Heat Transfer and Incomplete or Delayed Hydrogen Combustion

Mitigation effects associated with atmosphere-structure heat transfer were investigated by running Cases I11c808 and I3c1415 with all structure areas set to 10^{-20} m^2 and other input left as in the standard prescription. The ΔP values are increased over the standard prescription values by 0.256 MPa and 0.173 MPa in IET-11 and IET-3, respectively. These increases are actually larger than those that resulted from deleting trapping from the calculation. Note that the hydrogen production numbers are not significantly affected by deleting the mitigation by heat transfer.

Since DCH is generally thought of as being a very rapid event, it may seem surprising that heat transfer could have such a large effect. There are at least two reasons for this effect:

1. Without mitigation, very extreme temperatures (>2000 K) are calculated to develop in the subcompartment volumes, which have high surface/volume ratios. Heat transfer is very rapid under these conditions.

2. Much of the total energy release in the DCH events is due to combustion of DCH-produced hydrogen. However, most of this is produced in the oxygen-starved cavity and subcompartment volumes. Its combustion must await transport to regions of the containment with adequate oxygen, and the time required provides additional opportunity for mitigation by heat transfer.

The processes involved are illustrated in more detail in Figure 6.7-1, which presents pressure-time histories for Case I3c1407 (the standard case) and Case I3c1415 (no heat transfer). Also shown is the total hydrogen consumed as a function of time (dotted curves and right-hand axis). Debris dispersal and de-entrainment are largely completed within the first second in this experiment, and the two calculated curves are fairly close together at this time, indicating that mitigation during the debris dispersal time is only a moderate effect. Neither the experimental nor the calculated pressure curves have approached their maxima at this time, however.

Figure 6.7-1. SNL/IET-3 experimental and calculated pressure-time histories, and calculated hydrogen combustion histories, illustrating mitigation by heat transfer and delayed hydrogen combustion in oxygen-starved subcompartments.

By the time the experimental peak pressure is reached, at about 2.5 s, significant heat transfer has occurred and the pressure with heat transfer is about 0.1 MPa lower than the adiabatic case. Some hydrogen is left unconsumed at this time and it continues to burn in both calculations, but the energy input becomes too small to compensate for energy losses and this late combustion does not contribute to the peak ΔP in the case with heat transfer. Without heat transfer, however, the late combustion contributes just as effectively as the early combustion and the pressure continues to rise.

It is for this reason that the mitigation effect should be thought of as representing the combined effects of heat transfer and incomplete or delayed hydrogen combustion. If all the hydrogen could burn as soon as it is produced, the mitigation effects would no doubt be less; if it were not for the heat transfer effects, the delay in combustion would not matter. (There also may be some DCH-produced hydrogen that never does burn; hence the addition of "incomplete combustion" to the description.)

Unlike the situation with trapping, there is no experimental measurement against which one can directly check the calculated mitigation due to heat transfer, since no measurements of total heat transfer from atmosphere to structure during the event are available. Hence additional checking of the mitigation calculation seemed warranted. The first check involved performing some sensitivity studies on the heat transfer rates, and the second involved a simplified analytical calculation of the magnitude of the mitigation to be expected.

Sensitivity Studies. The results are summarized in Table 6.7-2 for some sensitivity studies involving heat transfer uncertainties for the IET-3 and IET-11 experiments. Case I3c1437 was run with all heat transfer structures deleted in the cavity, the chute, and the subcompartment cell closest to the cavity exit (Cell 5), and with structure surfaces reduced 50% in the next two subcompartment cells closest to the cavity exit (Cells 6 and 7; see Appendix A for a nodalization diagram). The resulting increase in ΔP, though not totally trivial, is less than 10%. This case may be best viewed as a simple sensitivity study directly varying the heat transfer rates, although its original motivation was to investigate the possible effect of reductions in heat sink efficiency if some of their surfaces become coated with hot debris. Even if the effect were larger, it probably would not be justifiable to explicitly take into account the reduced heat transfer efficiency resulting from hot debris on structure surfaces in the current standard prescription, because parametric features of the NAD model have been developed, in part, by comparisons with the experimental results. Any effect of reduced heat sink efficiency would already be reflected in the value of d_t selected. Thus attempting to take the effect into account explicitly, by reducing the structure surface areas, would risk double-counting the effect.

Table 6.7-2 Heat Transfer Mitigation Sensitivities for SNL/IET-3						
Case	Description	ΔP (MPa)	f_{dome}	H_2 Data (g-moles)		
				$N_{f,H2}$	$N_{H2,burn}$	$N_{H2,prod}$
	IET-3 Experimental Results	**0.246**	**0.088**	**37**	**190**	**227**
I3c1407	Standard Prescription	0.228	0.101	21	232	253
I3c1437	No struc. cavity, chute; structures reduced in subcompartments	0.244	0.100	11	248	260
I3c1438	Default radiation heat transfer	0.251	0.109	18	238	256
I3c1439	Default radiation in dome	0.232	0.101	21	232	253
I3c1443*	ε_g=-0.4, all cells	0.247	0.105	17	238	255
I3c1410	No NAD	0.110	0.099	18	84	103
I3c1440	No NAD; no struc. cavity, chute; struc. reduced in subcompartments	0.113	0.099	21	81	102
I3c1441	No NAD; default radiation hx	0.122	0.109	20	83	104
I3c1442	No NAD; default rad. hx in dome	0.111	0.099	18	84	103

In the standard prescription, the emissivity of the atmosphere, ε_g, is set equal to 0.8 in order to represent the effect of aerosol clouds that are expected to enhance atmospheric emissivities (see Section 3.3.2). A limiting estimate of the impact of this assumption was made by running Case I3c1438 with the default treatment of atmosphere-structure radiant heat transfer restored. Again, there is a small increase in ΔP, about 10%.

It might be more realistic to argue that a value of the emissivity as high as 0.8 should not be used in the dome, since aerosol clouds there may not be as dense. In Case I3c1439 the default emissivity treatment was restored in the dome only. Here the differences with respect to the standard prescription are trivial.

Although dense clouds of hot aerosols have been assumed to enhance emissivities in defining the standard prescription, concerns do exist that the emissivity could actually be reduced if the aerosol clouds are so dense that the optical mean free path is less than that of the thermal boundary layer, so that structures cannot "see" the hot gas/aerosol cloud beyond the boundary layer. In this event, the standard value could prove nonconservative. Little quantitative guidance as to the possible magnitude of this effect is currently available, however. Case I3c1443 in Table 6.7-2 was run with ε_g reduced from 0.8 to 0.4. The increase in calculated ΔP is less than 10%. The calculated value of ΔP is not very sensitive to the emissivity assumed because radiant energy transfer varies approximately as T_{gas}^4. Only a limited change in the temperature (and therefore the energy) of the gases flowing through the subcompartments is required to compensate for even a relatively large change in the emissivity. Hence the change in the emissivity does not result in a large change in the amount of energy reaching the dome, which is the primary factor controlling the extent of containment pressurization.

Another concern raised during the review of this document was that CONTAIN's well-mixed atmosphere assumption might overestimate the atmosphere-structure heat transfer in the subcompartments. It was suggested that only part of the subcompartment volume might be heated to very high temperatures if the gas flow through the subcompartments is sufficiently nonuniform, and that the amount of mitigation by atmosphere-structure heat transfer might therefore be considerably less than calculated by CONTAIN. Actually, the 14-cell deck does capture the nonuniformity effects to some degree; for example, in the IET-3 analysis, maximum subcompartment temperatures calculated ranged from ~2350 K close to the cavity exit to ~1540 K in subcompartment volume farthest from the cavity exit, and about 75% of the DCH-produced hydrogen entered the dome from the cavity side of the subcompartments. On the other hand, the 5-cell Zion deck represents the entire subcompartment as a single well-mixed cell. Comparison of the 14-cell results with the 5-cell results (see Section 6.1.3 and Table 6.1-3) shows no evidence that the extent of mitigation by heat transfer is very sensitive to the nonuniformity effect. Although CONTAIN cannot be expected to represent complex flow distributions in the subcompartments very accurately, there is sufficient nonuniformity in the 14-cell representation that significant differences would have been expected if the calculation were very sensitive to this effect. Hence it is concluded that nonuniformity is unlikely to result in large uncertainties in the calculated mitigation effect.

The IET-11 experiment provided a considerably more severe DCH event than IET-3, with higher atmosphere temperatures that would be expected to enhance the importance of atmosphere-structure radiant heat transfer. Some sensitivity cases for this experiment are also given in Table 6.7-2. The effect of using the default gas emissivity treatment was actually quite small in this case, probably because the atmospheric composition included considerable steam (unlike IET-3, in which there was little optically active gas present). Reducing ε_g from 0.8 to 0.4 increased the calculated ΔP by only ~11%; however, totally eliminating radiant transfer by setting ε_g to 10^{-10} increased ΔP by 32%. This case is considered quite unrealistic, even as a bound.

Before concluding this discussion of sensitivity calculations for heat transfer, we recall that it was noted in Section 4.2.3 that the arguments for believing NAD interactions and/or debris-water interactions are very important in the Zion IET experiments depend, in some degree, upon the assumption that CONTAIN does not greatly overestimate the mitigation due to atmosphere-structure heat transfer. It is therefore of interest to estimate the uncertainty in the heat transfer effects for the case with no NAD and no debris-water interactions (Case I3c1410). The sensitivity cases described above for the IET-3 experiment were therefore run with no NAD interactions modeled. An additional case was run with radiation turned off entirely by setting ε_g to 10^{-10}. These results are also given in Table 6.7-2. It appears that uncertainties in the atmosphere-structure heat transfer are not nearly large enough to explain the failure of the Case 3 results of Section 4 to account for the experimental measurements of ΔP, and postulating reduced heat transfer does nothing to improve agreement for the hydrogen production numbers. Even the case with radiation turned off entirely, which is very unrealistic even as a bound, does not come close to reproducing the experimental results.

Analytical Estimate of Mitigation. As an additional check on the modeling of mitigation due to heat transfer, an independent estimate was performed using an analytical "hand" calculation. One motivation for performing this additional check was to provide an additional test of the arguments (upon which much of the present work is based) that the large difference between the calculations without NAD and the experimental results in the Zion IET analyses necessarily implies that nonairborne debris processes and/or cavity water are making important contributions. Hence the check was performed on cases without NAD rather than the standard prescription (which would have been difficult to analyze with a hand calculation in any event).

IET-3 and IET-4 were selected for analysis because they include no pre-existing hydrogen whose partial combustion could complicate the treatment. In Table 6.7-1, Cases I3c1427 and I4c1415 are the same as Cases I3c1410 and I4c1410, respectively, except heat transfer to structures was deleted in the first two and 'srtemp' was set to 300 K in order to ensure that all the DCH-produced hydrogen would eventually burn.

Without heat transfer, the discrepancy between the calculated ΔP and the experimental value is much reduced. The discrepancies between the calculated and experimental values for hydrogen production and combustion remain, however. If the parametric features of the NAD model (or the debris-water interaction model) were adjusted to match the cases without heat transfer, the contributions from these processes needed to match ΔP values would be much smaller than is actually the case when heat transfer is included. Their contribution to the hydrogen production and combustion results would likewise be small and these results would continue to be substantially underpredicted.

It is apparent, then, that without the mitigation due to heat transfer, one could match either the ΔP values but substantially underpredict hydrogen, or match hydrogen and substantially overpredict ΔP. This result illustrates the point made in Section 4.2.3, that the validity of the present interpretation is supported by the observation that any input prescription giving satisfactory agreement with experiment for ΔP also yields reasonable agreement for hydrogen, when the atmosphere-structure heat transfer is included. For the cases without heat transfer, no amount of tuning of the parametric features of either the nonairborne debris model or the debris-water modeling would be able to bring the numbers into agreement for both ΔP and hydrogen.

The magnitude of the mitigation associated with heat transfer and incomplete/delayed hydrogen combustion was estimated using simplified analytical models in order to obtain an independent verification of the CONTAIN results. The heat transfer correlations used were those employed by CONTAIN, but the actual calculations were performed on a spreadsheet. The effect of hydrogen left unburned at the end of the accumulator blowdown was also estimated. Details are given in Appendix C.

The result obtained was that the simple analysis predicted that the mitigating effects would reduce ΔP by 0.11 MPa. The actual mitigation implied by the CONTAIN calculations summarized in Table 6.7-1 is 0.073 MPa for IET-3 and 0.094 MPa for IET-4. The agreement is considered to be good, in view of the approximations required in the simplified analysis.

6.8 Scale Effects.8 Scale Effects.8 Scale Effects

The question as to how to apply results obtained in small-scale DCH experiments to NPP events has long been recognized as a crucial issue for DCH analysis and it has received extensive study [Zub91]. The ability of a model such as CONTAIN to reproduce trends as a function of scale is vital to its utility. Significant uncertainty must always be allowed for when applying DCH models at NPP scale, since experiments inevitably must be performed at a small fraction of NPP scale and large extrapolations with respect to scale will always be needed in NPP analysis.

The scaled counterpart IET experiments performed at 0.0255 scale at ANL and 1/10-scale at SNL provide a very valuable resource for evaluating scale effects in the Zion geometry. Comparable studies for other containment geometries are not available and we consider only the Zion containment geometry here. We consider the ANL/IET-1RR, ANL/IET-3, and ANL/IET-6 experiments performed with a linear scale factor of 0.0255, together with their SNL counterpart experiments performed at 1/10-scale. Other ANL/IET experiments were not designed to be scaled counterparts of specific SNL experiments and will not be considered here.

Although the ANL/IET cases to be considered are close counterparts of the corresponding SNL experiments, they are not exact counterparts. The containment vessel used in the ANL experiments had a larger height/diameter ratio (~4.5) than did the Surtsey vessel (~2.9), the melt masses used in ANL/IET-1RR and ANL/IET-3 (but not ANL/IET-6) were overscaled 15% relative to their SNL counterparts, and the steam mass in the accumulator in ANL/IET-1RR and ANL/IET-6 was also overscaled about 15%, although the steam mass in ANL/IET-3 was within a few percent of being the scaled equivalent of SNL/IET-3. (The exact steam mass in the accumulator at the start of the experiment is difficult to control very accurately.)

These differences were taken into account in the CONTAIN calculations. The difference in height/diameter ratios for the containment vessel is reflected only through such parameters as the structure areas, cell height, and the trapping lengths. Otherwise, the geometric parameters used in the ANL/IET input decks were exact scaled counterparts of the SNL/IET deck calculated assuming a linear scale factor ratio of 0.255.

Scaling is a very large and complex subject [Zub91] and we make no attempt to address it completely here. We consider only the scale-dependence of certain features of the CONTAIN model as well as scaling of experimental phenomena which can affect the comparisons with experimental results, including scaling of inputs derived from the experiments such as fraction of the debris dispersed and the extent of debris-steam coherence. Some additional discussion of scaling for the ANL/IET and SNL/IET experiments is given in Reference Kme93.

6.8.1 Overview of Integral Result Scaling.8.1 Overview of Integral Result Scaling.8.1 Overview of Integral Result Scaling

In Table 6.8-1, experimental results and CONTAIN calculations (standard prescription and no-NAD cases) are given for the ANL and SNL scaled counterpart experiments. Both SNL/IET-1 and SNL/IET-1R are given as counterparts to ANL/IET-1RR since the two SNL experiments were intended to be replicates and thus both are considered to have equal claims to being a counterpart to ANL/IET-1RR, although it should be remembered that comparisons between CONTAIN and experiment for SNL/IET-1 sometimes do not fit the trends established by the other SNL/IET experiments. All ANL/IET hydrogen results have been multiplied by $(1/0.255)^3 = 60.3$ in order to facilitate comparison with the SNL/IET hydrogen results. Note that this treatment takes no account of the overscaling of the ANL melt masses and/or steam supplies that existed in some of the experiments.

Table 6.8-1: Results for Scaled Counterpart Experiments						
Case	Description	ΔP (MPa)	f_{dome}	Hydrogen Data (moles)		
				$N_{f,H2}$	$N_{H2,burn}$	$N_{H2,prod}$
	ANL/IET-1RR Experimental Results	**0.150**	**0.184**	**241**	**~0**	**241**
A1c1402	Standard input prescription	0.101	0.079	362	0.09	362
A1c1404	No NAD	0.068	0.078	153	0.06	153
	SNL/IET-1 Experimental Results	**0.098**	**0.116**	**230**	**3**	**233**
I1c1408	Standard input prescription	0.115	0.107	271	0.5	271
I1c1410	No NAD	0.076	0.117	130	0.8	131
	SNL/IET-1R Experimental Results	**0.110**	**0.105**	**238**	**11**	**248**
I1rc1407	Standard input prescription	0.101	0.096	248	0.6	247
I1rc1410	No NAD	0.063	0.095	101	0.5	99
	ANL/IET-3 Experimental Results	**0.190**	**0.060**	**69**	**211**	**280**
A3c1402	Standard input prescription	0.229	0.050	39	286	326
A3c1404	No NAD	0.124	0.053	26	119	144
A3c1407	d_t=0.00402 m [Eq. (3.2-6) with m=1]	0.227	0.051	42	260	302
A3c1409	d_t=0.01 m	0.168	0.052	24	165	189
A3c1410	d_t=0.00804 m, with cavity water	0.232	0.067	54	204	258

Inert Atmosphere Cases. Considering first the IET-1 group, it is apparent that the small-scale experiment yielded a $\triangle P$ almost 50% greater than the larger-scale experiments, yet scaled hydrogen production was essentially scale-independent. The CONTAIN standard prescription results go the other way; that is, the calculated $\triangle P$ in the small-scale experiment is about the same as in the larger-scale experiments while the calculated scaled hydrogen is larger. The reasons for these differences have not been fully established, but the easy explanation is that ANL/IET-1RR had a relatively large value of f_{dome} (0.184), which CONTAIN underpredicted by more than a factor of two. Debris transported to the dome may contribute effectively to $\triangle P$ by heating the atmosphere without contributing to hydrogen production, since the atmosphere is inert (N_2) in these experiments.

Reactive Atmosphere. The trends for the experiments with a reactive atmosphere are somewhat different. The standard prescription overpredicts $\triangle P$ somewhat for ANL/IET-3 and is about right in ANL/IET-6. There is some tendency to overpredict hydrogen production in the two ANL experiments, but the tendency is not as large as in the inert case. Taken together, the IET-3 and IET-6 cases exhibit less evidence than did IET-1 of any scale effects that the code cannot reproduce. Deviations for the ANL/IET cases are not larger than the variability of the experiments or larger than the variability in the degree to which the code calculations agreed with the larger-scale experiments.

Differences between individual experiments are not very well reproduced. The difference between $\triangle P$ for ANL/IET-3 and for ANL/IET-1RR is considerably less than the difference between the corresponding SNL counterpart tests, while the difference between ANL/IET-3 and ANL/IET-6 is greater. The code results follow the trends of the SNL/IET cases more closely than they do the trends of the ANL/IET experimental results themselves.

Some of these behaviors will be discussed further in terms of the scale dependencies of specific phenomena in the following subsections.

6.8.2 Scale Dependence of Dispersed Fraction and Debris-Steam Coherence.8.2 Scale Dependence of Dispersed Fraction and Debris-Steam Coherence.8.2 Scale Dependence of Dispersed Fraction and Debris-Steam Coherence

In the calculations, the fraction of the debris dispersed from the cavity, f_{disp}, is taken directly from the experimental reports. It is in effect an input to the code calculations.

An experimental value of the extent of coherence between the debris dispersal interval and the blowdown steam was defined based upon the amount of steam that had left the accumulator at the time the debris dispersed from the cavity in the CONTAIN calculation reached 95% of

Table 6.8-2 Scale-Dependence of Experimental Values of f_{disp} and f_{coh}					
ANL/IET Experiments			SNL/IET Counterpart		
Experiment	f_{disp}	f_{coh}	Experiment	f_{disp}	f_{coh}
ANL/IET-1RR	0.705	0.58	SNL/IET-1	0.859	0.34

its final value. The procedure is the same as that used in Sections 5 and Section 6.3.3. Although the accumulator pressures and debris dispersal histories used in calculating f_{coh} are taken from the CONTAIN calculation, it is important to recognize that the value of f_{coh} so obtained is basically an experimental quantity, not a model prediction. The reason is that this value of f_{coh} is governed by the blowdown rate, which is matched to the experimental blowdown curve; and by the airborne debris source, which is derived from the measured cavity pressurization history (Section 3.2.2).

This definition of f_{coh} is somewhat formal and it is not claimed that it necessarily gives the best possible estimate of the "correct" value for the experiments. Indeed, the imprecision of the coherence concept (Section 6.3.3) precludes any precise definition of the "correct" value. The definition does have several virtues for present purposes: it can be applied objectively, it is not expected to seriously distort trends when the results of different experiments are compared, and it can be applied equally well to other code calculations in order to obtain measures of coherence that can be compared with the experimental values cited in this assessment.

Values of f_{coh} obtained in this way are tabulated for the counterpart experiments in Table 6.8-2 along with the experimental values of f_{disp}. It is commonly assumed that, at sufficiently high driving pressures, debris dispersal will be virtually complete except for films that freeze on cavity and structure surfaces, and that this effect will reduce f_{disp} more at small scale than at large scale due to higher surface/volume ratios at small scale. The IET driving pressure (6-7 MPa) would be expected to qualify as "high" in view of the fact that f_{disp} in the WC experiments was on the order of 0.8-0.85, and these had lower driving pressures ($\leq$4.6 MPa).

There is, however, no evidence of decreasing f_{disp} with decreasing scale in the data; f_{disp} appears to be approximately scale independent. Consideration of f_{disp} for the other ANL/IET and SNL/IET experiments also supports this conclusion. (Although they are not scaled counterparts of one another, most of the other experiments do not differ in ways expected to substantially affect f_{disp}.)

In contrast, the values of f_{coh} do show evidence of a significant scale effect, possibly as much as a factor of two. If extrapolated to NPP scale, this result would imply improbably small values of f_{coh}. The reason for this scale dependence is not known. It is not even clear whether f_{coh} should be a monotonic function of scale, since different phenomena may be controlling at different scales.

Of the cavity entrainment correlations considered in Section 5 of this report, the modified Whalley-Hewitt correlation is expected to be almost scale-independent while the Levy correlation is expected to yield some decrease in f_{coh} with increasing scale; note that these expectations are based upon behavior with low-temperature simulants [Wil96] and thus neglect the feedback between interactions of the airborne debris and the forces driving dispersal. The low temperature simulant experiments themselves appeared to imply trends that were the reverse of those found here, in that dispersal appeared to decrease with increasing scale, which would imply f_{coh} should increase with scale. However, there were some ambiguities in this result; see Reference Wil96 for details.

Implications of these results for definition of debris sources for NPP calculations are considered in Section 7.3.3.

6.8.3 Airborne Debris Interactions.8.3 Airborne Debris Interactions.8.3 Airborne Debris Interactions

In the CONTAIN model, the efficiency of the airborne interactions is expected to increase with increasing facility scale until a limiting case is reached in which the airborne debris comes into local thermal and chemical equilibrium with the atmosphere, in which case additional increases in efficiency with increasing scale are not expected. The reason is that the characteristic times for debris transport and trapping approximately scale with the facility, while the characteristic time scales for debris-gas interactions are approximately independent of facility scale, providing particle size is independent of facility scale. (If particle size were to be proportional to facility scale, a decrease in efficiency with increasing scale would be predicted in the CONTAIN model.)

Since debris-gas equilibrium was not completely achieved even in the 1/10-scale calculations, the calculated interactions would be less efficient at the scale of the ANL/IET experiments. Sensitivity studies to directly evaluate this effect would have been somewhat tedious to set up and were not performed. (Due to the different values of f_{coh}, the actual analyses of the SNL and ANL experiments differ considerably from what one would obtain if the calculations were exact scaled replicas of one another.) However, earlier pretest analyses of SNL/IET-1 and ANL/IET-1 were performed with decks that were almost scaled replicas of one another, with very similar values of f_{coh}. When particle size distributions were the same as those assumed here, the larger-scale calculation gave ΔP values 30% and hydrogen production 36% higher than the small-scale calculation. Neither NAD nor water was included in these calculations.

In Table 6.8-1, comparison of the cases without NAD shows that the calculated ΔP and hydrogen production values were somewhat higher in the smaller-scale experiments. To a considerable degree, this result probably reflects the larger f_{coh} values at small scale overcoming the scale dependence of the airborne debris-gas interactions. However, other departures of the experiments from being exact counterparts would also contribute to this effect.

Experimentally, there is little direct evidence that debris-gas interactions are less efficient at the smaller scale, although conclusive evidence would be difficult to come by. One could interpret the larger ΔP in ANL/IET-1RR than in SNL counterparts as indicating that the debris-gas interactions were equally efficient, thereby permitting the larger value of f_{coh} to dominate the results. However, this explanation would lead one to expect that hydrogen production would also be greater in the small-scale experiment, which was not the case.

6.8.4 Nonairborne Debris Interactions.8.4 Nonairborne Debris Interactions.8.4 Nonairborne Debris Interactions

Scaling of the NAD model is of special concern, in view of the uncertainties associated with this model. The three ANL/IET experiments analyzed were similar with respect to parameters affecting the NAD model and the irregularity in the ΔP results summarized in Section 6.8.1 is unlikely to be due to the NAD model. Comparing the experimental results and the standard calculation results for ANL/IET-3 and SNL/IET-3, we note that it is for the experimental results, not the calculated results, that the ΔP values differ significantly. This is true despite the fact that the scaled hydrogen production was somewhat greater in ANL/IET-3 than in SNL/IET-3. This result is consistent with evidence summarized in Section 6.8.5 indicating that hydrogen combustion did not contribute as efficiently or as consistently to containment pressurization in the ANL/IET experiments as it did in the SNL/IET experiments. These considerations suggest that the hydrogen production results for ANL/IET should be given more weight than the ΔP results when considering scaling of the NAD model, and we tentatively accept this conclusion in the following discussion.

The value of d_t used in the ANL/IET analyses, 0.00335 m, was calculated from Eq. (3.2-7) with m = 0.8, which yields a weak negative dependence upon scale (efficiency varying as S^-

$^{0.2}$), based upon the analysis in Appendix B. If one attributes the tendency of the standard prescription to overpredict hydrogen production in the small-scale experiments to uncertainties in the scaling of the NAD model, the results imply that the dependence of d_t upon scale assumed here may be somewhat too strong. Note that this could mean that NAD interactions would be underpredicted at NPP scale.

Since uncertainties in scaling the NAD model are substantial, sensitivity studies are recommended in NPP analyses. As a starting point, using Eq. (3.2-7) with m = 1 instead of m = 0.8 might be more appropriate for defining a base case. This recipe would give a nonairborne interaction efficiency approximately independent of scale. Applied to the ANL/IET experiments, this prescription gives d_t = 0.00402 m. Case A3c1407 was run with this value. It is evident that agreement for hydrogen production would be improved somewhat, although the effect is too small to be at all conclusive.

Case A3c1409 in Table 6.8-1 was run without rescaling d_t at all; i.e., d_t = 0.01 m was assumed. Hydrogen production is considerably underpredicted in this case. This result is consistent with the arguments given in Appendix B that, for a best estimate, d_t should increase with increasing scale, and that a conservative case can be defined for NPP analysis by not scaling d_t; i.e., by running the calculation with the 1/10-scale value, d_t = 0.01 m. Scaling d_t in calculations including water is briefly considered in Section 6.8.5.

6.8.5 Scaling of Other Phenomena.8.5 Scaling of Other Phenomena.8.5 Scaling of Other Phenomena

Here we very briefly consider how a number of other DCH-related phenomena might be expected to vary as a function of scale in the CONTAIN model. There is no attempt to be complete and details will be omitted.

Transport Time Scales. Simple analysis indicates that characteristic time scales for gas flow will vary as the linear scale factor. Kmetyk [Kme93] has compared the ANL/IET and SNL/IET blowdown curves after scaling the time in proportion to the linear scale factor and found that this simple scaling law worked well. Since the blowdown rate governs gas flow rates generally during the DCH event, the same scaling law is expected to hold for gas flow through the subcompartment. When the time scale for hydrogen combustion is controlled by rates of flow to oxygen-bearing portions of the containment, the time scale for this energy release will also vary as the geometric scale, to lowest order.

In the CONTAIN model, debris transport rates are also proportional to gas flow rates assuming one specifies the slip factors to be the same, as was done in this work. Actual slip factors as a function of scale are not known.

Trapping. To lowest order, time scales for trapping and for transport through the subcompartments will both vary as the linear scale factor in the CONTAIN model; hence, f_{dome} would be expected to be approximately scale independent. In the actual calculations, the calculated values of f_{dome} were somewhat higher for the SNL/IET experiments than for the ANL/IET experiments. However, this is probably due to the lower coherence ratio for the SNL/IET experiments. In the 'rhodg = mix' option of the TOF/KU model, rapid dispersal increases the density of airborne debris and makes it less likely that the de-entrainment criterion will be satisfied. In SNL/IET-7, which had a larger value of f_{coh} (0.42), f_{dome} was calculated to be only 0.057, which is similar to the values calculated for ANL/IET.

Experimentally, the situation is ambiguous. The ANL/IET experiments exhibited greater variability in f_{dome} than did the SNL/IET experiments, especially if one discounts the SNL/IET-4 case in which it is known that structure damage contributed to increased values of f_{dome}. The experimental value of f_{dome} in ANL/IET-3 was small and in agreement with the calculations, while the experimental values for ANL/IET-1RR and ANL/IET-6 are two to three times the calculated value. The reasons for these differences are not known. Damage to subcompartment structures was not involved in any of the three ANL/IET experiments analyzed.

H_2 Combustion. Temperature and concentrations thresholds for self-sustained hydrogen combustion are expected to become somewhat less restrictive as scale increases. This trend has already been discussed in connection with the DFB and BSR models in Section 6.6. CONTAIN does not model these scale dependencies, although the user can attempt to take them into account through the values assigned to the various burn parameters.

Experimentally, the tendency of ΔP values in the noninert experiments to be lower and less consistent in the ANL/IET experiments than in the SNL/IET experiments has been commonly attributed to scale effects in the hydrogen combustion behavior. In addition, Kmetyk [Kme93] has noted that the larger height/diameter ratio of the ANL vessel could also have played a role, in that the narrower vessel could have slowed the rate of access of oxygen to the combustion zone in the smaller facility.

If scale effects are involved in the differences between the ANL and SNL hydrogen behaviors, the consistency of hydrogen behavior in the SNL experiments may mean that the effect is largely saturated at 1/10-scale. If this hypothesis is valid, it would imply that these effects would not lead to further large increases in efficiency at NPP scale.

Assuming conditions for self-sustained combustion are satisfied, the rate of energy release from combustion of DCH-produced hydrogen may be governed by the rates at which the hydrogen can find oxygen. This time scale, in turn, will often be proportional to the geometric scale factor, as noted above.

Mitigation by Atmosphere-Structure Heat Transfer. In lowest order, time scales for heat transfer are governed by surface-volume ratios, and thus increase linearly with scale as a first approximation. Since the overall time scale of a DCH event also increases approximately linearly with scale, the relative importance of mitigation due to heat transfer is not expected to be a strong function of scale. The CONTAIN models for heat transfer include some details that result in some deviation from the scaling law noted here, but these deviations are not expected to be very large.

Natural Convection. Since the buoyancy heads that drive natural convection increase with scale, convective velocities increase with scale. The increase is less than in proportion to the linear scale factor, and the time scale for convective mixing therefore increase with scale, but less than proportionately. Hence, the importance of natural convection may increase with scale, relative to other processes whose time scales increase proportionately with scale. The CONTAIN model should be capable of representing these effects as a first approximation, provided the problem is set up with flow path specifications adequate to represent the natural convection patterns. However, this only applies to convection through subcompartments and other largely enclosed volumes; the ability of CONTAIN to calculate convection and gas distributions within open volumes is questionable.

Debris-Water Interactions. As is the case for FCI effects generally, scaling of the debris-water interactions is not well understood. In the ANL/IET experiments, the cavity pressurization histories reveal no FCI "signatures" as were characteristic of the SNL/IET experiments. If this difference is real, and not a measurement artifact, it may imply a substantial scale effect for debris-water interactions.

Case A3c1410 in Table 6.8-1 was run using d_t = 0.008 m (i.e., twice the value used in Case A3c1407) and with the cavity water assumed to participate, in analogy with the approach used in Section 6.4 for the SNL/IET experiments. The results are fairly similar to A3c1407, and the degree of agreement with the experimental results is about the same, just as doubling d_t and adding the water yielded results similar to the standard prescription without water for the SNL/IET Zion experiments. Evidently this prescription for including both NAD and water interactions did not introduce severe scale distortions.

Case A3c1411 was run with water included and d_t = 0.02 m, which is the value used in the SNL/IET analyses that included cavity water, and it is seen that hydrogen production is substantially underpredicted. Again, the results are consistent with the hypothesis that d_t should be scaled in accord with the scaling law of Eq. (3.2.6) with $m \approx 1$ in order to obtain a best estimate, and that a conservative case can be defined for NPP analysis by not rescaling d_t from the values found appropriate for 1/10-scale analyses.

6.8.6 Perspective on DCH Scaling Uncertainties.8.6 Perspective on DCH Scaling Uncertainties.8.6 Perspective on DCH Scaling Uncertainties

Although the discussion given above shows that there are number of loose ends concerning scaling, one should not lose sight of the fact that, as a first approximation, comparison of the integral results for the ANL/IET and SNL/IET counterpart experiments does not reveal any dramatic scale effects. Likewise, the CONTAIN code results do not exhibit any major scale distortions with respect to experiment, especially in the cases with oxygen in the atmosphere. Some cancellation of opposing effects appears to be involved, and there may be less cancellation in going from 1/10-scale to full scale than there is between 1/40-scale and 1/10-scale. When applying the code at full scale, uncertainty associated with scaling clearly must be allowed for. Nonetheless, the results obtained to date are encouraging in that they do not indicate any gross scale distortions in the CONTAIN model, nor do they indicate that scaling uncertainties in NPP calculations will be so large that the results of the calculations would have little value.

Although one cannot draw rigorous inferences concerning scaling from experiments in different geometries, it is still worth remembering that the complete data base includes experiments with linear scale factors ranging from 0.0255 to 1/5.75, a factor of about 6.8. This factor is actually slightly larger than the increase in scale in going from the Surry IET experiments in CTTF to full NPP scale. Once again, the fact that the full data base reveals no very conspicuous scale distortions suggests that scale effects will not introduce gross error when the CONTAIN model is applied at full scale.

6.9 Selected IET Surry Analyses.9 Selected IET Surry Analyses.9 Selected IET Surry Analyses

6.9.1 Effect of Initial Containment Atmosphere.9.1 Effect of Initial Containment Atmosphere.9.1 Effect of Initial Containment Atmosphere

In the Zion-geometry SNL/IET experiments, by far the most important experimental variable studied was found to be the atmospheric composition, i.e., whether DCH-produced hydrogen could or could not burn. In those experiments in which hydrogen could burn, the range of ΔP values obtained was only 0.246-0.279 MPa, indicating that other experimental variables studied were much less important.

In the Surry-geometry IET experiments, the range in ΔP values was considerably larger, 0.283-0.430 MPa, even though most DCH-produced hydrogen burned in all three cases [Bla94]. Independent variables which differed for these experiments (see Table 2.1-4) included the initial steam inventory in the accumulator, the extent of a gap around the RPV, the presence or absence of simulated RPV insulation, and melt generator hole size. There were also significant differences in the extent of debris dispersal from the cavity (f_{disp}) and the degree of debris-steam coherence (f_{coh}). Although f_{disp} and f_{coh} are not independent variables in the experiments, these quantities are treated as if they were independent variables in the analyses, in the sense that they are determined through the input.

It is also apparent from Table 2.1-4 that there were significant differences in the containment atmosphere initial conditions for these three experiments. IET-9 had the lowest oxygen supply, the smallest number of total moles of atmosphere, and highest steam mole fraction; IET-11 was at the opposite end of the range for all three of these parameters, and IET-10 was intermediate. In order to investigate the possible implications of these differences in the atmosphere, several cases were run in which the input deck for a given experiment (e.g., IET-11) was modified by specifying the atmosphere initial conditions of another experiment (e.g., IET-9 or IET-11), without making any other changes.

The results are summarized in Table 6.9-1. In the first block of three lines, the experimental results are given and in the next block CONTAIN results are given using the standard prescription. The third block gives results calculated for the permuted-atmosphere cases.

Table 6.9-1 Effect of Initial Atmosphere Conditions in the Surry IET Experiments						
Case	Description	ΔP (MPa)	f_{dome}	Hydrogen Data (moles)		
				$N_{f,H2}$	$N_{H2,burn}$	$N_{H2,prod}$
	SNL/IET-9 Experimental Results	**0.283**	**0.21**	**413**	**847**	**968**
	SNL/IET-10 Experimental Results	**0.326**	**0.132**	**186**	**1352**	**1227**
	SNL/IET-11 Experimental Results	**0.430**	**0.307**	**137**	**1828**	**1517**
I9c812	IET-9 Standard input prescription	0.292	0.121	437[a]	1093	1270
I10c812	IET-10 Standard input prescription	0.345	0.089	30	1637	1370
I11c801	IET-11 Standard input prescription	0.437	0.262	9	1902	1462

A comparison of Case I11c813 with the IET-10 and IET-11 standard cases indicates that, in the CONTAIN calculation, about half the difference between the IET-10 and IET-11 ΔP values can be accounted for by the difference between the initial conditions in the containment atmosphere. Comparison of Case I11c814 with the standard cases for IET-11 and IET-9 suggests that about two-thirds of the difference in calculated ΔP values for these two experiments can be accounted for by the differences in the containment atmospheric conditions. Likewise, comparison of Case I10c825 with the standard cases for IET-9 and IET-10 indicates that much of the difference in the calculated results between these two experiments may be attributed to the difference in the containment atmospheres.

Finally, Cases I9c822 and I9c823 are the reverse of Case I11c813, i.e., the IET-9 experiment is simulated with the IET-11 initial atmosphere conditions. Case I9c822 recovers only about a third of the difference in ΔP values for these two experiments. However, in this case, the BSR threshold was not exceeded in the dome and most of the pre-existing hydrogen did not burn, while it did burn in the standard case analysis for all experiments. In Case I9c823, the BSR threshold in the dome was lowered from 840 K to 795 K in order to obtain hydrogen burn behavior comparable to what was obtained in the other cases. Again, the results support the conclusion that, given comparable assumptions concerning the pre-existing hydrogen behavior, about two-thirds of the differences between the IET-9 and IET-11 calculations may be attributed to the initial atmosphere conditions.

It may be noted from the results that permuting the atmospheres did not have a significant effect upon the amount of hydrogen produced. Interchanging the IET-10 and IET-11 atmospheres did not even affect the amount of hydrogen burned significantly. There were substantial differences in the amount of hydrogen left unburned in the cases run with the IET-9 atmosphere. In all cases with the IET-9 atmosphere, the unconsumed hydrogen was principally DCH-produced hydrogen; the pre-existing hydrogen burned. Evidently, mixing required to burn DCH-produced hydrogen in the oxygen-starved subcompartments did not occur before conditions dropped below the thresholds required to sustain combustion in these cases.

The point that unconsumed hydrogen was DCH-produced, not pre-existing, in the cases with the IET-9 atmosphere (including the standard IET-9 case itself) is of some interest in the interpretation of the experimental results. When measured hydrogen consumed is less than that produced, it has been customary to assume that what hydrogen did burn was DCH-produced hydrogen, and that the pre-existing hydrogen did not burn. However, this was not true in the CONTAIN analyses. Experimentally, of course, there is no way to determine which hydrogen burned. (It was possible to determine this in the calculation because a carbon monoxide mole fraction of 10^{-5} was specified, and the CONTAIN combustion models will always burn the CO and the pre-existing hydrogen in equal proportion. The fraction of the pre-existing hydrogen that is burned in the calculation is therefore the same as the fraction of the carbon monoxide that is burned). Note, however, that these results are subject to the nodalization uncertainties discussed in Section 6.6.3, and different results might have been obtained if the 12-cell deck had been used in this study.

In the calculation, the difference in steam concentrations probably did not play a significant role because the DFB model standard prescription includes a very high inerting threshold (90% in the dome, 95% elsewhere) and the BSR model includes no concentration thresholds. It is likely that oxygen supply played a dominant role in these results. Global oxygen starvation did not occur in any of the calculations, but the amount of oxygen per unit volume governs how much containment atmosphere must mix in with the DCH-produced hydrogen, and this will affect combustion rates. In addition, the total number of moles of atmosphere can play a role in that, with more moles, obtaining a given ΔP does not require as high a temperature, and with lower temperatures, the containment atmosphere does not lose energy to structures as rapidly. (As a compensating effect, the lower temperature also may be less likely to result in combustion of pre-existing hydrogen, as in Case I9c822.)

In this connection, it is interesting to note that the initial volumetric oxygen concentrations were about 2.55, 5.3, and 9.1 g-moles/m^3 in IET-9, IET-10, and IET-11, respectively. For comparison purposes, the volumetric oxygen concentration is about 5.5 g-moles/m^3 in subatmospheric large dry containments (including Surry) and about 8.4 g-moles/m^3 in an atmospheric containment. Thus, IET-9 was subprototypic in oxygen supply except, possibly, for scenarios in which substantial hydrogen combustion occurs prior to vessel breach. IET-10 oxygen supplies were prototypic of Surry, while IET-11 was more nearly prototypic of an atmospheric containment than a subatmospheric containment. It would seem that oxygen supply is something that needs to be taken into account when comparing DCH vulnerabilities of subatmospheric and atmospheric containments. Subatmospheric plants have sometimes been judged to be somewhat more vulnerable due to somewhat lower containment capacities, but these comparisons have not taken into account the oxygen supply effect.

6.9.2 Effect of RPV Insulation.9.2 Effect of RPV Insulation.9.2 Effect of RPV Insulation

In IET-11 only, the gap around the RPV and the RPV insulation (made of stainless steel sheet and foil) were modeled in the experiment. The insulation was almost totally removed by melting ablation. In the standard input prescription, the insulation was modeled in the CONTAIN calculation as iron and chromium sources that were added to the debris sources (see Section 3.2.2).

One consequence of the removal of the insulation is that it affects the estimates of f_{dome} calculated for both the experiment and the CONTAIN analysis. In all other experiments, the experimental value of f_{dome} was calculated directly from

$$f_{dome} = \frac{m_{d,dome}}{m_{d,sub} + m_{d,dome}} ,$$

12 (6.9-1)

where $m_{d,dome}$ and $m_{d,sub}$ are, respectively, the mass of debris located in the dome and in the subcompartments after the experiment. In IET-11, two experimental values of f_{dome} were reported [Bla94]. The first was calculated directly from Eq. (6.9-1) as in the other cases, while in the second, the mass of the insulation (29 kg) was subtracted from $m_{d,dome}$. In the present work, the first method of reporting has been used in all cases, for both the experimental results and the CONTAIN results.

In order to investigate the contribution of the insulation, the problem was run with the sources representing insulation deleted. Some results are summarized in Table 6.9-2. In Case I11c804, the insulation was deleted and no other changes made; comparison with the standard case shows a significant reduction in ΔP, by about 0.08 MPa. However, much of this

Table 6.9-2 Effect of Insulation and Blowdown Sensitivity in IET-11						
Case	Description	△P (MPa)	f_{dome}	Hydrogen Data (moles)		
				$N_{f,H2}$	$N_{H2,burn}$	$N_{H2,prod}$
	SNL/IET-11 Experimental Results	**0.430**	**0.307**	**137**	**1828**	**1517**
I11c801	IET-11 Standard input prescription	0.437	0.262	9	1902	1462
I11c804	IET-11, no insulation modeled	0.354	0.199	374	1356	1280
I11c810	No insulation, dome 'srtemp'=795 K	0.425	0.198	10	1718	1279

difference is due to temperatures in the dome staying below the BSR threshold when the insulation is deleted. In Case I11c810, the insulation was again deleted but the BSR threshold was reduced to 795 K in order to obtain hydrogen burn behavior comparable to the standard case. The reduction in △P due to deleting the insulation is considerably less in this case. Hydrogen production and combustion numbers are still reduced by about 200 g-moles, relative to the standard case.

The open gap and the effect of the insulation combine to produce values of f_{dome} that are larger than in the other IET experiments, which produces somewhat more sensitivity to trapping than in the others. Case I11c807 was run assuming GFT trapping in the dome, which increased △P somewhat, about 0.014 MPa, relative to the standard case. It should be remembered that, when L_1 is large, the TOF/KU model often predicts trapping on first impact, which does run some risk of giving nonconservative results in the dome.

6.9.3 Sensitivity to Blowdown Rate.9.3 Sensitivity to Blowdown Rate.9.3 Sensitivity to Blowdown Rate

In the present work, blowdown rates were matched to the experimental blowdown curves using simplified decks that included only those parameters needed to define and control the blowdown. After most of the IET-11 analyses had been performed, it was subsequently discovered that information was incorrectly transferred from the simplified deck to the IET-11 deck, and that the blowdown was somewhat too rapid in the IET-11 decks. The magnitude of the error is shown in Figure 6.9-1 in which the experimental blowdown curve is compared with the calculated blowdown curve with the error and with the error corrected.

Case I11c816 in Table 6.9-2 is the standard input prescription case recalculated with the blowdown error corrected. Cases I11c1202 and I11c1205 were both run with the 12-cell deck and no BSR in the dome, with the blowdown error corrected in I11c1205. Correcting the blowdown error reduced ΔP by a small amount, 0.003-0.006 MPa.

Figure 6.9-1 shows that the error in the blowdown, though not large, is larger than the degree of mismatch between the experimental and calculated blowdown curves that is normally achieved in this work. Since correcting the error had only a small effect, it follows that the degree of agreement between the experimental and calculated blowdown curves normally achieved is adequate to avoid significant error.

32Figure 6.9-1. Calculated and experimental accumulator blowdown curves for SNL/IET-11, used to investigate sensitivity to errors in matching the experimental blowdown.

7 User Guidance User Guidance User Guidance

7.1 Scope of this Section.1 Scope of this Section.1 Scope of this Section

The purpose of this section is to offer some practical suggestions for performing DCH calculations in NPPs. The discussion is limited to issues specific to DCH. Some guidance for the use of CONTAIN in general is provided in Reference Mur89, and additional guidance of this type will be available in the forthcoming CONTAIN 1.2 Code Manual [Mur95].

The suggested approach starts with the standard prescription defined in Section 3 for experimental analysis where it is applicable, and the details given in Section 3 are not repeated here. The present section emphasizes changes representing lessons from the experimental analyses, suggestions for dealing with the differences between experimental analysis and NPP analysis, and sensitivity studies designed to explore potentially important uncertainties.

A PWR containment is assumed. PWR ice condenser containments are included except that issues related directly to the ice condenser itself are not considered. In parts of the discussion, there is an implicit assumption that the containment is compartmentalized, with at most limited transport paths from the cavity directly to the dome being available; there is little experience in analyzing containments for which this is not true and no experimental data exist except for quite nonprototypic conditions. Initial conditions (melt characteristics, vessel pressure at breach, vessel failure size, etc.) are assumed to be known by the analyst, but no assumptions about the initial conditions are made here.

Uncertainties and the Role of Sensitivity Studies. The discussion that follows acknowledges the possible existence of a considerable number of uncertainties. As we have emphasized elsewhere in this report, this does not mean that any one calculation is likely to be sensitive to a large number of uncertain phenomena. Usually, at most a small number of the uncertainties will be found to have an important impact upon the results. However, the nature of the controlling uncertainties can be different for different DCH scenarios. Since it is intended that the present work be as widely applicable as possible, the range of uncertainties identified as being "potentially important" is considerably wider than what we would expect the user will find to be important in any single DCH scenario.

The sensitivity studies suggested are designed to explore uncertainties, and thus do not include cases that are demonstrably outside the credible range. There is a different type of sensitivity study that can be performed with CONTAIN in which extreme or limiting assumptions are made in order to determine the contribution of some specific phenomenon to the results. Examples are provided by the studies of mitigation effects in Section 6.7 in which trapping and/or heat transfer surfaces were eliminated. While the insights obtained from such studies can be very useful, they are not considered here.

To date, there has been relatively little experience in applying the standard prescription developed in this work to NPP analysis. It is inevitable that some modifications will be needed as experience accumulates, and some surprises may well be in store. The suggestions that follow must therefore be considered preliminary. Many of these suggestions are based upon the general body of experience with CONTAIN DCH analysis that has been accumulated by the authors over the last several years, and a specific justification is not given for every suggestion. Users are always encouraged to perform additional sensitivity studies to investigate uncertainties judged to be significant for their particular problem. On the other hand, not every sensitivity study suggested here will be needed for every problem.

7.2 Nodalization.2 Nodalization.2 Nodalization

Results obtained in Sections 6.1.3 and 6.6.3 demonstrated that CONTAIN DCH calculations can show nontrivial sensitivity to how the containment is nodalized. It was also apparent that the nature of these sensitivities could be very different in different cases, i.e., Zion versus Surry. Here we attempt to offer some guidelines that may be helpful in getting started. However, no general prescription can be given as to how to nodalize a containment of arbitrary geometry.

Identification of the Subcompartment Volumes. For compartmentalized geometries, one of the most important features that the nodalization must represent is the separation of regions referred to in this report as the "subcompartments" from the main open volume of the containment that has been referred to as the "dome." The "subcompartments" are defined to include those volumes for which structures provide sufficient physical barriers that two-way gas mixing between the subcompartments and the dome is not an important effect so long as blowdown of the primary system provides a strong forced flow of gas through the subcompartments. Thus defined, the subcompartments comprise a region that can become oxygen starved early in the DCH event.

Typically the structures defining the subcompartments will also limit the extent of debris transport to the dome. The definition of the subcompartments used here emphasizes the limitation upon gas mixing because trapping may limit transport of the debris to volumes that are small compared with the volumes that become oxygen starved during the DCH event, and it is important to capture the mitigation associated with this oxygen starvation. If only trapping effects are considered, the "subcompartment" volume so defined could be too small, and part of the mitigating effect associated with delayed or incomplete combustion of hydrogen that was described in Section 6.7.3 might be lost. Often there will not be a very large uncertainty in this mitigation effect, and failure to take adequate credit for it can therefore result in an unnecessarily conservative calculation.

The geometry of the regions represented by the subcompartments may be too complex for the best results to be obtained if it is modeled as a single cell in CONTAIN. Much of the remainder of this section addresses some possible guidelines for nodalization of the subcompartment region. The question of whether to subdivide the dome is also discussed.

Well-defined compartments should generally be assigned individual computational cells. Here a "well-defined compartment" may be defined to be a volume largely enclosed by structure such that flow path areas into and out of the volume are small compared with the cross section of the volume, while internal structure within the volume is sufficiently limited that, for the most part, there would be unobstructed line-of-sight across the volume in most directions. In such a case, CONTAIN's well-mixed assumption will generally be applicable within the volume, suggesting that it not be subdivided, while conditions within such a compartment may differ substantially from those outside the compartment, suggesting it should not be combined with adjacent regions.

In some cases, even well-defined compartments may be combined if there is good reason to believe that little error can result. For example, there may exist several well-defined compartments in the same region of the containment and whose total volume is a small fraction of the containment. Lumping these volumes together may be an acceptable simplification, especially if they do not lie on a major flow path important to the problem (e.g., do not lie on one of the main flow paths from the cavity to the dome).

Large Open Volumes: The Dome. The dome volume is a special case of a "well-defined compartment," in that it would satisfy the preceding definition. It presents a special problem for two reasons. The first reason is the fact that the dome typically includes a large fraction of the total containment volume (and hence a large fraction of its total oxygen supply and pre-existing hydrogen). This large size gives the dome a special importance in DCH calculations.

The second reason is that experimental evidence shows that the well-mixed assumption often does not apply in the dome. In the Surry-geometry IET experiments, thermocouples demonstrated that a large amount of thermal stratification existed in the dome, with temperatures in the upper part being substantially higher than in the lower part [Bla94]. Gas samples, though less conclusive, also indicated that there was stratification with respect to composition, as one would expect, given the thermal stratification. Among its implications is the possibility that stratification could inhibit the combustion of pre-existing hydrogen to a large degree. The reason is that the hot upper region likely consists largely of burned-out gases from the DCH-produced hydrogen plume, and most of the containment oxygen and pre-existing hydrogen are likely present in the cooler, lower region.

In the Zion-geometry experiments [All94b], thermal stratification was observed in the SNL/IET-7 experiment, although not to the extent observed in the Surry experiments. Temperature measurements in the other Zion-geometry experiments did not imply thermal stratification [All94b], but the temperature instrumentation was less complete in these than in SNL/IET-7 and it is not certain the behavior was actually as different as the measurements suggest.

If stratification exists and the dome is treated as a single cell, the temperature calculated for the dome will be higher than the actual temperature in the lower region, which contains most of the pre-existing hydrogen, and an otherwise-reasonable BSR temperature threshold could overpredict the tendency of pre-existing hydrogen to burn on DCH time scales. Nonetheless, subdivision of the dome (or any other well-defined compartment) in an attempt to capture stratification effects in CONTAIN calculations is not recommended, except in appropriately designed sensitivity studies.

One reason is that gas and debris transport through the dome may be heavily affected by momentum-governed transport and mixing processes which the CONTAIN code cannot capture. Some early CONTAIN calculations for the Surry NPP [Wil88], in which the dome was subdivided, gave stratification effects the reverse of those subsequently observed experimentally; that is, hot debris and hydrogen entering the dome via the RPV gap made the lower part of the dome much hotter than the upper part, probably because the calculation could not reflect any tendency of the momentum of the material to carry through the lower part and into the upper dome. Since the lower part of the dome also became oxygen starved while the upper part still had sufficient oxygen for hydrogen combustion, this treatment was potentially nonconservative and it was subsequently abandoned. The dome was modeled as a single cell in all the Surry IET analyses.

Another possible departure from well-mixed conditions in the dome may result from what has been called the "cloud effect." If a well-defined jet of debris enters the dome, its interaction with the dome atmosphere may be limited to a cloud of gas in the immediate vicinity of the jet. The volume of this cloud could be considerably smaller than the total volume of the dome and the total debris-gas heat transfer and chemical reaction could then be smaller than what CONTAIN would calculate if the entire dome volume is modeled as a single well-mixed cell. Some early CONTAIN experimental analyses sought to represent this effect by suitably subdividing the dome [Tar88]. However, for NPP analysis, this subdivision risks introducing nonconservatism; e.g., by artificially restricting the access of DCH-produced hydrogen to oxygen. It is not recommended except for possible sensitivity calculations. Note also that the CONTAIN analyses of the open-geometry experiments in the present work overpredicted the experimental ΔP by relatively small amounts, $\leq 15\%$, suggesting that any conservatism resulting from neglecting the cloud effect may be small.

In the 14-cell Zion-geometry deck, the dome was subdivided into two cells, but the plane separating the cells was a vertical plane through the Surtsey vessel axis, not a horizontal plane, and did not reflect any attempt to represent stratification effects. The two halves of the dome were connected by two flow paths, rather than only one, in order to permit intercell recirculation. The purpose of this division was to represent the cavity side of the Surtsey dome separately from the side opposite the cavity exit, and thereby represent the fact that flows entering the dome on the cavity side are at a higher temperature and carry more hydrogen than do flows entering on the far side. This is a real effect, confirmed by experimental measurements (at least for temperature; hydrogen concentration measurements at this level of detail are not available), and the CONTAIN code gives at least a qualitative representation of the effect. Subdividing the dome for this purpose is probably reasonable, although it did not have a large effect upon the results for the conditions of the Zion IET experiments. Even this type of subdivision is potentially nonconservative if it is found that oxygen starvation in part of the dome restricts hydrogen combustion.

<u>Subcompartments with Large Amounts of Internal Structure</u>. The Zion subcompartment region satisfies the first of the above criteria for a "well-defined compartment" in that flow path areas into and out of it are small compared with the subcompartment cross-sectional area. However, it definitely does not satisfy the second criterion: it is a "busy" volume with an irregular shape and a large amount of internal structure that would block a line-of-sight path across the subcompartment region in most directions. Debris transport beyond the subcompartments typically requires several changes in the direction of the flight of debris particles.

In such instances, experience with the Zion nodalizations described in Section 6.1.3 leads to the recommendation that, ideally, the subcompartments should be subdivided such that the dimension of the individual cells is of the same order of magnitude as the unobstructed line-of-sight flight path of debris. The $6V_{cell}/S_{str}$ rule probably gives an adequate estimate of this "unobstructed flight path." This guideline may be relaxed for regions sufficiently far from the cavity exit that they are unlikely to play an important role in debris trapping and transport processes, unless there is some other reason for subdividing these regions. Comparison of the 14-cell deck results with the simple 5-cell deck, in which the entire subcompartment volume was represented with a single cell, suggests that the guideline given here can be too prescriptive and that simpler representations can be acceptable for some purposes; see Section

6.1.3. However, there were some irregularities in the behavior of the 5-cell deck and a more detailed representation is believed to be preferable if time and resources permit it.

Non-Isotropic Quasi-Open Volumes. This awkward term is used for a category of volume which can be equally awkward for the definition of nodalization guidelines. The subcompartment region in the Surry experiments provides an example. This region consisted principally of the basement and the annulus outside the crane wall. Both these volumes are relatively open in the sense that they do not include a large amount of internal structure, nor are there partitions which physically divide them into well-defined subvolumes. However, they are characterized by shapes such that their dimension in one direction is very different from the dimensions in the other two directions. The basement volume is disk-shaped, with a diameter (~5.6 m) considerably greater than its height (~1.2 m), and the width of the annulus (~0.54 m) is much less than its height or its azimuthal extent.

Owing to their shape, the well-mixed assumption can be poor for such volumes, yet there is no obvious prescription for subdividing them. In some instances, a consideration of the specific geometry at hand may suggest an approach. If nothing else, sensitivity studies using different nodalizations may provide insights as to the magnitude of the uncertainties involved. This approach was used for the Surry IET subcompartments, as discussed in Section 6.6.3.

Momentum-Governed Transport Paths. When openings are aligned with the expected debris trajectories, debris transport through these openings may be much greater than CONTAIN calculates due to momentum-controlled transport which the CONTAIN code cannot represent. An approximate simulation of this effect can be attempted by specifying a fictitious flow path bypassing the intermediate cell(s). This approach was used in the Surry IET analysis, in which a flow path was specified directly from the cavity cell to the seal table room (STR), thereby bypassing the RHR platform cell, even though no such direct connection actually exists. The area of this flow path was determined by estimating the fraction of the coffer dam exit (the opening from the cavity to the RHR platform) which is subtended by the seal table opening from the RHR platform to the seal table room. Note that this approach likely overestimates gas flow to the seal table room, since the momentum-controlled transport is probably less important for the gas than for the debris.

One can also investigate sensitivity to f_{dome} by specifying an extra flow path directly from the cavity to the dome. Some sensitivity studies of this type were performed in the IET-10 analyses, since f_{dome} was underestimated in the standard prescription, even with the RHR platform bypass described above. Results (see Appendix D) indicated sensitivity was low.

In the Zion analysis, no attempt to simulate the momentum-driven transport was made. The approach based upon subtended areas was less applicable because the transport probably included some low-angle glancing impacts of debris upon the crane wall and the seal table room walls. In addition, f_{dome} was not systematically underpredicted by the standard prescription in the SNL Zion IET experiments. In some early analyses of the SNL/IET-1 experiment, sensitivity studies that included a 10% bypass path from the cavity to the dome were performed. The calculated ΔP was increased from 0.081 MPa without the bypass to ~0.095 MPa with the bypass, while the fraction of the debris transported beyond the subcompartments was increased from 0.078 without the bypass to 0.17 with the bypass. (The latter numbers are not precisely comparable to f_{dome} as currently defined, but they do represent a substantial overprediction of f_{dome} when the bypass was included.)

It is clear that momentum-driven transport into the seal table room was an important factor in the Zion-geometry experiments because 20%-30% of the debris dispersed from the cavity was found in the STR after the experiment. CONTAIN underpredicted this transport by an order of magnitude because the STR entrance flow path area is very small compared with other available paths for gas flow, which is the only transport mechanism that CONTAIN models.

Natural Convection. In CONTAIN, countercurrent circulation through a single opening is not modeled. For adjacent cells at approximately the same elevation and separated by a vertical interface, countercurrent flow can be at least qualitatively simulated by dividing the flow path into an upper half and a lower half. This approach was used in the 14-cell Zion deck except when the openings connecting the two cells were small (i.e., small compared with the cell cross sections). It was not used in the other decks, except for the Surry 12-cell deck employed in the nodalization sensitivity studies.

When two cells are located approximately above one another, with a horizontal interface separating them, there is no analogous approach that permits simulation of countercurrent flow between them. (If one attempts to subdivide the opening and assign different elevations to the two flow paths, spurious circulation can result and this approach is not recommended.) Modeling the countercurrent flows would require subdividing at least one of the two cells. The usual caveats concerning subdividing open volumes will apply and it is up to the user to determine whether subdivision can introduce significant spurious effects for the specific analysis under consideration.

7.3 Debris Sources, Particle Sizes, and Particle Compositions.3 Debris Sources, Particle Sizes, and Particle Compositions.3 Debris Sources, Particle Sizes, and Particle Compositions

In the assessment of the RPV and cavity models described in Section 5, we concluded that use of these models can only be recommended for "friendly users" knowledgeable with respect to the phenomenologies involved and who are willing to take on the responsibility of ensuring for themselves that the results being obtained are reasonable. Hence the present section emphasizes the specification of user-defined debris sources. However, much of the discussion is equally relevant as a guide to assist users of the RPV and cavity models in deciding whether the results obtained are "reasonable."

The analyses described in the main body of this work relied upon experimental results in order to define the debris sources input to the problem, and this approach is not directly applicable when the code is being used to make predictions for scenarios not studied, including NPP events. In this section, we offer some guidance for defining debris sources for analysis of scenarios not studied experimentally, including the analysis of NPP DCH scenarios.

7.3.1 Debris Characteristics and Dispersed Fractions.3.1 Debris Characteristics and Dispersed Fractions.3.1 Debris Characteristics and Dispersed Fractions

Debris Characteristics. Initial values for the debris characteristics (mass, composition, temperature) must be defined by the user. As in the experimental analyses, we recommend that no credit be taken for possible retention of molten material in the RPV (see Section 3.2.2 for the rationale). Hence, all the initial molten mass should be placed in the cavity prior to the start of the RPV blowdown.

Fraction Dispersed from the Cavity. For driving pressures greater than a few megapascals, experimental data suggest that the fraction of the initial mass which is ejected from the cavity can be spanned by the range 0.6-0.85,[*] but a sensitivity calculation using a value close to 1.0 is suggested on order to allow for scaling uncertainties and any other effects that might increase f_{disp}. (Assuming f_{disp} = 1.0 is not necessarily the most conservative assumption; see Section 6.3.2.) For pressures of a few megapascals or below, smaller values of f_{disp} are likely but, for compartmentalized geometries, DCH loads are expected to be moderate under these conditions for reasons summarized in Section 2.2. For open-geometry containments, sensitivity to f_{disp} under these conditions could prove important.

7.3.2 Time Dependence of the RPV Blowdown.3.2 Time Dependence of the RPV Blowdown.3.2 Time Dependence of the RPV Blowdown

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[*]*Note that "f_{disp}" in this discussion actually corresponds to the experimental value of the product $f_{eject}f_{disp}$, since we recommend taking no credit for melt retention in the melt generator.

Blowdown steam sources are most conveniently provided by using one or more cells to model the RPV, as was done in the experimental analyses described here. The rate of blowdown of the RPV can have important effects upon DCH loads, with rapid blowdown tending to favor larger loads [Wil87, Wil88]. The rate of blowdown is largely governed by the vessel hole diameter, d_h. The CONTAIN RPV models include a model for hole ablation [Gri94], with the user required to specify an initial hole size. However, when the user specifies the debris sources through input, the user must also specify the RPV hole size, including any time dependence.

Experimental depressurization curves, such as those in Figure 3.2-1, show that the rate of depressurization does not reach its maximum until some time after the initial failure. Instantaneously opening the vessel failure orifice to its maximum value would not reproduce this behavior. DCH loads are not expected to be sensitive to minor details of the shape of the depressurization curve, provided the overall time scale for depressurization is approximately correct. However, it is recommended that the vessel failure orifice not be instantaneously opened to its final size; instead, the orifice area may be increased linearly from a value of zero to its maximum value over a time period, τ_h, controlled by the user.

A value of τ_h can be estimated by noting that, in the SNL/IET (Zion) experiments, the time interval between gas blowthrough and the maximum depressurization rate was about 0.3 to 0.7 s in most cases, as estimated from the experimental accumulator depressurization curves [All94b]. The rate of hole enlargement was not strictly linear, and a value of τ_h equal to about 0.4 s would provide a reasonable approximation when a linear time dependence is used. Simple scaling arguments suggest that τ_h should be proportional to the linear scale factor, S; inversely proportional to the square of the scaled hole size, d_h/S; and inversely proportional to the square root of the accumulator (or RPV) initial pressure, P_0. For the SNL/IET Zion experiments, $d_h/S \approx 0.4$ m, S = 0.1, and P_0 = 6.3 MPa on average. Hence, one may estimate τ_h from

$$\tau_h = (0.4)\left(\frac{S}{0.1}\right)\left(\frac{0.4}{d_h/S}\right)^2 \sqrt{\frac{6.3}{P_0}} ,$$

13 (7.3-1)

where τ_h is in seconds, d_h is the final hole size in meters, and P_0 is in megapascals. Approximate checks against blowdown curves given in the experimental reports for the ANL/IET experiments [Bin94] and the WC-3 experiment [All93] indicate that Eq. (7.3-1) gives a reasonable account of the variation with scale and with hole size, although the dependence upon d_h may be somewhat too strong. Since τ_h is being introduced simply to avoid an unrealistically rapid onset of depressurization, only large uncertainties in this parameter would be of concern and we do not believe that sensitivity studies for this parameter will usually be necessary.

7.3.3 Coherence Between Blowdown and Debris Dispersal.3.3 Coherence Between Blowdown and Debris Dispersal.3.3 Coherence Between Blowdown and Debris Dispersal

Although results given in Section 6.3.3 indicated that sensitivity of DCH to coherence is not large in some cases, we still consider coherence to be a potentially important DCH parameter. Hence we will discuss the problem of defining coherence for the debris sources in greater detail than is done for other source parameters.

The suggested approach starts with values of f_{coh} based upon experiment and uses a correlation to guide extrapolation to estimate coherence for conditions not studied experimentally. For the latter, we suggest, with some qualifications, a model presented by Pilch [Pil94a], who has parameterized coherence in terms of a dimensionless quantity called the coherence ratio, R_τ. This coherence ratio may be thought of as the ratio of the characteristic time required for debris entrainment, τ_e, to the characteristic time for blowdown, τ_b: $R_\tau = \tau_e/\tau_b$. Derivation of experimental values of R_τ does not require determination of experimental values of either τ_e or τ_b. Instead, the experimental values of R_τ are estimated from the initial accumulator pressure, P_0, and the accumulator pressure, P_e, at the end of the entrainment interval, much as f_{coh} has been estimated in the present work:

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

14 (7.3-2)

For use in Eq. (7.3-2), P_e may be defined as the accumulator pressure at the time the debris mass dispersed from the cavity reaches 95% of its final value, as was done in Sections 5 and 6 of this work. In terms of R_τ, the coherent fraction f_{coh} is given by

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

15 (7.3-3)

For the same experimental value of P_0/P_e, Eqs. (7.3-2) and (7.3-3) will yield the same value of f_{coh} as that used in Sections 5 and 6, i.e., as given by Eq. (3.2-1).

As represented in the Pilch model, the parameters of greatest interest are the vessel failure size (diameter d_h), the initial melt mass m_d^0, the initial mass of steam (m_g^0) within the RCS, and the volume of the RCS, V_{RCS}. The dependence upon these parameters in the Pilch model may be represented as

$$R_\tau = C_1 \left(\frac{m_d^0 V_c^{1/3}}{m_g^0 V_{RCS}} \right)^{1/2} d_h ,$$

16 (7.3-4)

where V_c is the cavity volume and C_1 is a coefficient to be determined by fitting to experimental values of R_τ calculated from Eq. (7.3-2). The model as presented in Reference Pil94a includes some additional dependencies upon the debris temperature and the gas temperature in the RCS. These dependencies are weak and we would view them as being insufficiently motivated either experimentally or theoretically to recommend their use here. We would also place the weak dependence upon V_c in Eq. (7.3-4) in the same category but have included it in the equation in order to maintain C_1 as a dimensionless constant.

The data base available for validating the dependencies implied by Eq. (7.3-4) is limited, there is considerable scatter in the coherence data, and there is considerable uncertainty in the estimates of coherence based upon the cavity pressurization histories. Qualitatively, however, the dependence upon the major parameters implied by Eq. (7.3-4) is physically reasonable and in agreement with the trends of the data where trends can be established. Hence we believe that use of Eq. (7.3-4) is preferable to simply using the experimental values of f_{coh} directly, without allowing for the differences in parameters such as d_h, m_g^0, etc.

Experimental Values of Coherence. Data on coherence potentially useful as a starting point are summarized in Table 7.3-1. The experimental values of f_{coh}, etc., are derived as described in Section 6.8.3 and may therefore be compared with values used in NPP CONTAIN calculations provided the latter are defined similarly. In the table, the experiments are divided into three groups: ANL/IET Zion, SNL/IET Zion, and SNL/IET Surry. The LFP and WC experiments are not included because the debris sources were obtained using the simpler method described in Section 3.2.2 and values of f_{coh} obtained from them might not be comparable with the values obtained from the IET experiments.

Table 7.3-1 Experimental Estimates of Coherence Parameters						
Experiment	P_0	P_e	f_{coh}	R_τ	--- C_1 ---	
					Values	Group Avg. ±Std. Dev.
ANL/IET-1RR	6.70	2.12	0.58	0.93	6.79	6.84 ±0.39
ANL/IET-3	5.70	2.10	0.53	0.80	6.39	
ANL/IET-6	6.60	2.42	0.53	0.81	7.35	
SNL/IET-1	6.82	3.96	0.34	0.42	3.63	2.71 ±0.82
SNL/IET-1R	6.05	3.78	0.30	0.36	3.06	

For each experiment, values are given for P_0, P_e, f_{coh}, R_τ, and C_1. The latter are obtained by inverting Eq. (7.3-4). The geometric parameters V_{RCS} and V_c are given at the bottom of the table and other parameters required to obtain C_1 are obtained from the tables of initial conditions given in Section 2.1. In the last column, the mean value and the standard deviation of C_1 are given for each of the three groups of experiments.

Uncertainty in Coherence. Experiments within each of the three groups are quite similar in terms of the parameters expected to affect coherence. The extent of variation of C_1 within a group gives a measure of the variation due to uncontrolled experimental variations (including truly stochastic effects such as FCIs). Comparison of the means for the three groups provides a measure of the degree to which Eq. (7.3-4) compensates for differences in the experimental parameters characterizing the three groups. Somewhat surprisingly, the difference between the mean C_1 values for the SNL/IET Surry and Zion-geometry experiments is no greater than the variation within the groups despite the many differences between these experiments, while the difference between the ANL/IET and SNL/IET values of C_1 is large, much greater than the variation within either group.

The principal difference between the ANL and SNL Zion IET experiments is geometric scale. Neither Eq. (7.3-4) nor the complete correlation given in Reference Pil94a acknowledge any dependence of R_τ upon geometric scale, which is a major shortcoming of this method of estimating coherence if the ANL-SNL differences do represent a scale effect. Whatever the source of the differences between the ANL/IET and SNL/IET coherence results, these differences do suggest that substantial uncertainties should be allowed for when using Eq. (7.3-4) to estimate coherence. The fact that only a limited domain of parameter space has been studied experimentally reinforces this belief. Fortunately, the analyses described in Section 6.3.3 indicate that even large uncertainties in f_{coh} can be tolerated in some cases, but sensitivity to f_{coh} may depend upon other parameters of the DCH scenario and this sensitivity should be checked for the problem of interest. For example, it can be argued that sensitivity to coherence is likely to be greater when local debris-gas equilibrium is achieved, a condition that may be more likely to be met in CONTAIN calculations at NPP scale than at experimental scale. Neither calculations nor experimental data illustrating a higher sensitivity to coherence are currently available, however.

<u>Recommendations for Coherence</u>. We recommend use of Eq. (7.3-4) with a value of C_1 equal to about 4. This value is chosen to be intermediate between the ANL results and the SNL results, but with the latter given more weight on the grounds that the larger-scale experiments may be more prototypic. When Eq. (7.3-4) predicts small values of f_{coh}, we recommend that sensitivity calculations be performed assuming a larger value, $f_{coh} \geq 0.5$, in order to determine whether the results of interest are dependent upon f_{coh} being small.

<u>Time dependence of the Debris Sources</u>. Given the rate of blowdown and the value of f_{coh}, results given in Section 6.3.3 indicate that the calculation will be insensitive to the details of the time dependence of the debris source. Hence a simple trapezoidal time dependence is recommended. A procedure that should give reasonable results is the following:

- Run a calculation for the blowdown only, using Eq. (7.3-1) to define τ_h.

- Using the calculated RPV depressurization curve, find the time, t_e, at which the RPV depressurizes to the value of P_e such that Eq. (3.2-1) gives the desired value of f_{coh}.

" Define $t_{b,0}$ to be the time at which blowdown begins, and start the airborne debris source at time $t_{b,0} + 0.25\tau_h$ and terminate the source at t_e. Divide the interval between the source start time and the end time into three equal segments and use these to define a trapezoidal time dependence for the airborne debris source, normalized to integrate to the intended value of f_{disp}.

The suggested start time, $t_{b,0} + 0.25\tau_h$, is based upon the experimental observation that debris dispersal begins well before the rate of accumulator depressurization reaches its maximum. The prescription given here will not yield a value of f_{coh} corresponding exactly to the 95% dispersal criterion used to define the experimental values, but it should be reasonably close. Obtaining an exact match would require more iteration because dispersal from the cavity is delayed by the finite airborne residence time in the cavity. In view of the limited sensitivity of DCH loads to f_{coh} and the substantial uncertainty in the value of f_{coh} estimated from Eq. (7.3-4), this iteration is not likely to be worth the effort. As in the experimental analyses (Section 3.2.2), the debris should first be introduced into the cavity cell trapped debris field, and then transferred to the airborne fields; the time-dependence defined above applies to the transfer of debris to the airborne fields.

7.3.4 Debris Particle Size Distributions and Compositions.3.4 Debris Particle Size Distributions and Compositions.3.4 Debris Particle Size Distributions and Compositions

The present study revealed no evidence that the standard prescription particle size distribution needs to be redefined and it is still recommended as a starting point. The dominant effect of particle size is usually through the strong dependence of debris-gas heat transfer and chemical reaction rates upon particle size. In general, results will not be sensitive to reductions in particle size if debris and gas in any given computational cell already come into a close approximation of thermal and chemical equilibrium when the standard prescription is used. In the CONTAIN model, equilibrium is more likely to be approached at NPP scale than at experimental scale. Checking for sensitivity to particle size by running the problem with the mass median diameter reduced by a factor of two is suggested unless other evidence (results of similar studies, demonstration that equilibrium is achieved) indicate that it is not necessary. In performing this sensitivity study, there is usually no need to reduce further the size of the smallest debris field in the standard prescription, since it is already small enough to undergo very rapid interactions with the atmosphere and further reductions are likely to require very small timesteps in the calculation in order to maintain stability.

Another possible sensitivity to particle size is that the calculated transport of debris beyond the subcompartments (i.e., f_{dome}) may be increased when the particle size is reduced. Although this trend is reasonable in a qualitative sense, there is much more uncertainty in CONTAIN's simulation of this effect than there is in its modeling of the dependence of debris-gas thermal and chemical interactions upon particle size.

Even if there is little sensitivity to reductions in particle size below the standard prescription values, calculated loads will be affected (decreased) by increases in the particle size if it is made large enough. If desired, sensitivity studies with increased particle size can be performed to explore, for example, the implications of the hypothesis that the particle size increases with facility scale.

Particle Compositions. The standard prescription of uniformly well-mixed debris appears to be satisfactory. There is currently no evidence that uncertainties resulting from this treatment are sufficient to require sensitivity studies with respect to debris composition as a general rule.

7.3.5 RPV Insulation.3.5 RPV Insulation.3.5 RPV Insulation

For NPP in which the RPV is covered with stainless steel foil insulation, as in the Surry NPP, the standard prescription includes adding the iron and chromium content of the insulation to the debris sources as was done in the SNL/IET-11 experimental analysis (Section 3.2.2). The area of the gap should be figured without allowing for any blockage by the insulation, since the experimental results for SNL/IET-11 indicated that the insulation is ablated away. As in the experimental analysis, half the insulation is added to the debris in the cavity and half is added to the debris entering the dome, and the time dependence of the sources representing the insulation is that of the airborne debris source. The initial temperature of the insulation may be taken to be the temperature of the RPV exterior.

Although the effect of the insulation in the SNL/IET-11 analysis was small, it could be larger in NPP analyses because the longer flight paths at full scale may permit a higher degree of oxidation of that portion which is carried to the dome. In addition, the insulation can make a greater contribution to hydrogen production if the metallic content of the debris itself is low. In the SNL/IET-11 experiment, metal-steam reactions tended to be steam-limited and hence adding more metal to the debris could not increase hydrogen production substantially. However, with a highly oxidic melt, hydrogen production would not be steam-starved and the insulation might therefore contribute more effectively.

The standard prescription may tend toward conservatism, as not all the insulation may be melted and mixed with the debris as assumed. Excessive conservatism seems especially likely if the amount of molten debris is relatively small. A treatment including only part of the insulation may then be more appropriate.

7.4 Debris Transport and Trapping.4 Debris Transport and Trapping.4 Debris Transport and Trapping

The standard prescription for NPP analysis specifies zero trapping in the cavity and chute, for the same reason zero trapping was specified in the experimental analysis (Section 3.2.4). In analyzing compartmentalized containments, the most important question concerning the trapping and transport models is usually whether uncertainty in f_{dome} is significantly affecting the results. When the calculated value of f_{dome} is relatively small, as it is in all the experiments performed for compartmentalized geometries, a substantial relative uncertainty (e.g., a factor of two) in this value can be tolerated and the only question of much importance is whether the uncertainties are sufficiently large that the prediction that f_{dome} is "small" is questionable. There are two situations which might possibly give rise to large f_{dome} values in compartmentalized containment geometries:

1. Paths for efficient momentum-controlled transport to the dome may exist.

2. Driving forces for transport of debris may be considerably greater than in the experimental data base, e.g., due to the combination of a high vessel pressure and a large vessel hole size.

The CONTAIN code makes no attempt to model processes involved in the first situation; this question can be addressed only by detailed consideration of the geometry at hand. The code does attempt to model processes involved in the second situation and the standard prescription has been defined in a way which we believe will make the results tend toward conservatism under these conditions. It is certainly not bounding, however, and even the claim that the results tend toward conservatism is difficult to defend in view of the absence of any experimental data for the more extreme scenarios for which large values of f_{dome} might be calculated. Note also that there was some tendency to underpredict f_{dome} in the Surry-geometry IET experiments.

Sensitivity studies are recommended whenever it appears that the calculated results may be sensitive to the uncertainties in trapping and transport. If the code calculates a large value of f_{dome} and the resulting loads are excessive, it is worth determining whether the calculation is sensitive to some of the potentially conservative modeling assumptions, i.e., the specification of 'rhodg = mix' and 'vnost = gft' in the TOF/KU trapping model and the assumption of no slip in the subcompartment. If relaxing these assumptions makes a substantial difference, the question of their validity for the specific case at hand may be considered further. However, any relaxation of the more conservative treatment clearly does require a defense, as results presented in Sections 4.3 and 6.1 show that less conservative treatments can underpredict f_{dome} in some instances, possibly by substantial factors.

A potentially nonconservative feature of the standard prescription is the use of TOF/KU trapping in the dome, because this model may predict more de-entrainment on first impact than is realistic. Sensitivity to this question can be checked by setting the critical threshold value of the Kutateladze number for the first impact [$Ku_{T,1}$ in Eq. (3.2-3)] to some very small value in the dome.

If the extent of cavity pressurization is of interest, available information (see Section 6.1.3) indicates that calculations with $s_d = 5$ specified for the cavity and chute volumes underpredict cavity pressurization, and more realistic results for cavity pressurization may be obtained with $s_d = 1$. Since the no-slip assumption ($s_d = 1$) is believed to be unrealistic in other respects, compensating errors may be involved and caution is warranted.

7.5 DCH Heat Transfer.5 DCH Heat Transfer.5 DCH Heat Transfer

7.5.1 Debris-Gas and Debris-Structure Heat Transfer.5.1 Debris-Gas and Debris-Structure Heat Transfer.5.1 Debris-Gas and Debris-Structure Heat Transfer

Given a realistic particle size distribution, we believe that the standard prescription provides a reasonable treatment of debris-atmosphere heat transfer, which is not one of the more uncertain processes involved in DCH analysis. Results of DCH calculations are generally not very sensitive to these uncertainties. Furthermore, uncertainty in the heat transfer rates for a given particle size will have effects similar to uncertainties in the particle size, and the latter uncertainties are probably more important. Hence, any reasonable allowance for uncertainties in the particle size will probably allow for uncertainties in heat transfer rates adequately. At this time, we do not believe it is usually necessary to conduct sensitivity studies on the debris-gas heat transfer models in NPP calculations.

In the standard prescription, direct debris-structure heat transfer due to thermal radiation is neglected. Due to the high atmospheric opacities expected to exist during DCH events, we believe this treatment is a good approximation, and it is conservative insofar as it is in error. Again, there is probably no need to conduct sensitivity studies on direct debris-structure radiant heat transfer in NPP calculations.

7.5.2 Atmosphere-Structure Heat Transfer.5.2 Atmosphere-Structure Heat Transfer.5.2 Atmosphere-Structure Heat Transfer

In Section 6.7, it was shown that atmosphere-structure heat transfer was a very important mitigation process in DCH analyses. Nonetheless, sensitivity studies did not reveal any major sensitivities to reasonable allowances for uncertainties in the heat transfer models themselves, and earlier experience with NPP analyses generally supports the belief that uncertainties that do exist in these models are not major contributors to uncertainty in the analysis of DCH events in NPP.

One complication in adapting the standard prescription for experimental analysis to NPP analysis is the use of the user-defined atmospheric emissivity set equal to 0.8 in the code input, in order to simulate the effects of aerosol clouds. The difficulty is that, when this option is used, the emissivity is held fixed throughout the calculation, and it is not appropriate during the period prior to vessel breach in an NPP analysis. CONTAIN's normal emissivity models, based upon a fairly sophisticated treatment of the optically active constituents of the atmosphere [Was91], should be used during this period. We suggest two possible ways to deal with the problem:

1. Run the problem with the normal emissivity model in use until the time of the DCH event, stop the calculation, and restart with the user-specified emissivity of 0.8.

2. Run the problem with the normal emissivity model in use throughout.

The first option is best in principle but is somewhat inconvenient. The inconvenience is lessened by the fact that the same analysis of the initial period up to vessel breach can be used as the starting point for a wide variety of DCH-related sensitivity studies, provided only that the rules governing use of CONTAIN's restart option are not violated [Mur89, Mur95].

The rationale for the second option is that it is "correct" up to the time of vessel breach and any error in the analysis of the DCH event itself is expected to be conservative. The degree of conservatism is believed to be small in many cases because, in NPP analyses, the default model for atmosphere-structure radiation normally calculates fairly high emissivities due to the relatively long optical path lengths at NPP scale and the high steam concentrations usually present in the containment atmosphere. Allowing for the enhanced emissivity due to aerosol clouds may not be very important. In the experimental analyses, it was considered more important to allow for the aerosol cloud effect because no optically active gases were present in the containment atmosphere in many of the experiments and, even when they were present, the shorter optical path lengths would result in lower emissivities.

A plausible-seeming approach that <u>cannot</u> be recommended without further study is to simply start the calculation at the time of vessel breach, estimating the initial containment conditions by other means and specifying these conditions through input. CONTAIN modeling of steam condensation upon structures includes an allowance for a water film developing on structures [Was91, Mur95] and which can re-evaporate when conditions are appropriate. In NPP analyses, films usually will be present on structure surfaces at the time of vessel breach, and they will evaporate rapidly once the DCH event begins. Under certain circumstances, this film evaporation can be a surprisingly important source of additional coherent steam, augmenting what would otherwise be available for debris-atmosphere heat transfer and hydrogen generation. In some earlier calculations for the Surry NPP, deleting the film was found to reduce the calculated loads by about 0.17 MPa [Wil88].

The conditions assumed in these earlier calculations likely exaggerated the role of water films for several reasons. Melt masses were larger than what is now considered plausible and the coherence relatively low, which made the calculations sensitive to the increased steam supply. The default film thickness was 0.5 mm, which is considerably greater than that given by the more mechanistic "filmflow" model now available as a modeling option; the newer model typically yields thicknesses of the order of 0.1 mm. The film effect was manifested primarily in the subcompartments and more recent modeling gives greater emphasis to debris-steam interactions in the cavity.

Unfortunately, relevant NPP sensitivity studies with more modern input and modeling are not currently available. Hence it is best to run the calculation from the time of reactor shutdown in order to obtain a realistic distribution of water films, unless sensitivity calculations establish that the effects of the water films are unimportant.

7.6 DCH Chemistry.6 DCH Chemistry.6 DCH Chemistry

As in the case of debris-gas heat transfer, use of the standard prescription with the CONTAIN DCH chemistry models is expected to give reasonable results. With one exception, the uncertainties in the reaction rates should be covered by any reasonable allowance for the uncertainty in particle size. The exception is that the reaction threshold should be left at the CONTAIN default value (273.15 K) for scenarios involving large amounts of co-dispersed cavity water or co-ejected RPV water to avoid a spurious quenching effect; additional details are given in Section 7.8. Use of this value for all calculations probably will cause no difficulty because trapping will normally prevent unrealistic low-temperature reactions from occurring in any case.

Once again the reader is reminded that the standard prescription for the drop-side reaction rate limit is no drop-side limit (infinite drop diffusivity), which is not presently the CONTAIN default. The default is a drop-side diffusivity of 10^{-8} m^2/s, which is nonconservative generally and will almost totally eliminate chemical reaction with the nonairborne field as the latter is normally used; see Appendix D for some analyses of the SNL/IET-1R and SNL/IET-3 experiments in which $D_d = 10^{-8}$ m^2/s was specified. No drop-side limit will become the default in CONTAIN 1.21 and later releases.

7.7 Nonairborne Debris.7 Nonairborne Debris.7 Nonairborne Debris

The standard prescription models nonairborne debris interactions in the cavity and the subcompartments, but not in the dome. The nonairborne debris interactions are not well understood and there are potentially important modeling uncertainties involved in the rationale provided here for scaling the model to NPP analyses. For a central estimate, use of the scaling law based upon Eq. (B.2-5) in Appendix B with m = 1 is now recommended rather than m = 0.8 as in Eq. (3.2-7). This gives

$$d_t(S) = d_t(S_e)\left(\frac{S}{S_e}\right)^{\frac{2(2-m)}{3}} = d_t(S_e)\left(\frac{S}{S_e}\right)^{\frac{2}{3}} \text{ for } m = 1,$$

17 (7.7-1)

where $d_t(S)$ is the appropriate value for a problem of scale S, $d_t(S_e)$ the value found to be appropriate for a scaled experiment with scale factor S_e. With $S_e = 0.1$, the recommendations are $d_t(S_e) = 0.01$ m for calculations without water and $d_t(0.1) = 0.02$ m for calculations with debris-water interactions, and S = 1 for NPP analysis. Use of m = 1 rather than m = 0.8 is now preferred because it yields an efficiency of nonairborne interactions which is, in lowest order, independent of geometric scale, which is considered to be reasonable as a first approximation. Use of m = 0.8 results in efficiencies that decline somewhat with increasing scale and thus runs more risk of being nonconservative at NPP scale. Note also that use of m = 0.8 overpredicted hydrogen production for the small-scale ANL/IET Zion experiments, although it is not certain that the nonairborne model is the reason for that result.

The next step should be to determine whether the nonairborne interactions are contributing substantially and estimating an uncertainty range for their effects. The uncertainty range for the potential nonairborne contribution can be estimated by running the problem with no nonairborne interactions and rerunning with $d_t = 0.01$ m; due to the scaling behavior discussed in Appendix B, it is believed that this value of d_t is quite conservative for applications at NPP scale. Results obtained for ANL/IET-3 without scaling d_t (Section 6.9.4) also support the belief that conservative results will be obtained at NPP scale if d_t is not scaled up at all from the value used for experiments.

If the range spanned by these cases is not large, or if even the most conservative result is acceptable, there may be no need to do more. Whether this is the case depends largely upon the initial conditions. The experiments analyzed here had a high metal content in the melt, and the dominant effect of the nonairborne interactions was due to enhanced hydrogen production and combustion. Uncertainties associated with this model are expected to be smaller if the amount of metal in the melt is small. Note also that the importance of the nonairborne model appears to depend upon the plant geometry. The user should therefore run the suggested sensitivity calculations for the specific problem of interest and not rely excessively upon the qualitative generalizations offered here.

The user should also recall that the standard prescription only shuts off the nonairborne model when the blowdown is nearly complete. Results given in Section 6.5 indicated that this prescription overestimates the contribution from interaction with the late stages of the blowdown relative to the early stages.

7.8 Debris Interactions with Water.8 Debris Interactions with Water.8 Debris Interactions with Water

As in the case of the nonairborne model, there are potentially important modeling uncertainties affecting the analysis of DCH scenarios that include debris interactions with water. Again, the suggested first step is to define an uncertainty range for the problem. This may be done by running the problem with no water and then varying the amount of water until one finds the approximate amount which gives the maximum effect. As described in Section 3.2.8., the water is introduced into the problem as a source of low-enthalpy steam, with the time dependence being that of the debris source. Note that when the amount of water is relatively small, the maximum effect is likely to result when all the water is included. However, the SNL/IET-8B analysis (Section 6.4.5) showed that the CONTAIN treatment can be nonconservative when the amounts of water are large, and the sensitivity studies involving smaller amounts should be performed in these cases.

When several sensitivity calculations varying the amount of water are needed, it is reasonable to perform them only for the case with the value of the nonairborne debris parameter d_t set equal to the base case value defined in Section 6.7. Once the amount of water giving the maximum effect has been identified, the sensitivity calculations for d_t recommended in Section 6.7 can be performed for this case. Although not bounding in any rigorous sense, this procedure is believed to provide a reasonable measure of the possible uncertainty range.

It is important to remember that debris reaction threshold temperatures used in the standard prescription for the experimental analyses (1200 K) could yield quite nonconservative results in NPP analyses involving water. The reason is that the CONTAIN model can combine fresh, hot debris that still contains reacting metal with cool, aged debris that no longer includes any metal in the same debris field. The result can be an artificial quench of chemical reaction. It can be shown that the severity of this effect increases as the ratio of the time scale for chemical reaction and heat transfer to the airborne residence time of the debris decreases. Thus, the spurious quench effect could be the most severe for the smallest particles that actually should react the most efficiently, and is expected to be more severe for NPP scale than for experimental analyses because the airborne residence times increase with increasing scale while the reaction and heat transfer times do not.

In analyses with substantial amounts of water, it is also important to eliminate the DFB temperature thresholds. These temperature thresholds were originally defined for analyses involving little or no water, and the SNL/IET-8B analyses in Section 6.4.5 demonstrate that very nonconservative results may be obtained if these temperature thresholds are left in place.

The fact that spurious quenching of chemical reactions can arise in the CONTAIN model does not mean that very real quenching effects cannot occur in reality when large amounts of water are involved. In principle, these might be investigated with CONTAIN using the multigeneration feature [Was95] to avoid mixing fresh debris with cold aged debris. Reaction temperature dependence could be controlled by using either the cutoff temperature or the drop-side reaction rate limit model with an appropriate temperature-dependent diffusivity specified, although the impact of the latter on the nonairborne debris model would require consideration. A major problem for this approach is whether it could be adequately validated by comparison with experimental results. The DCH data base involving substantial amounts of water is quite limited, and it is not clear to what extent other FCI experimental results would be applicable. On a practical level, a large number of debris generations might be needed to avoid the spurious quench effect, which could result in excessively long computer run times. In any event, this approach was not applied in the present work, and it will not be discussed further here.

If even the conservative case defined by the prescription summarized above (i.e., maximum water effect with nonairborne debris $d_t = 0.02$ m) implies acceptable loads, there may be no need to do more than what has already been outlined here. If the conservative case yields loads considered to be excessive, sensitivity studies can provide useful insights by determining how much relaxation in the pessimism of this conservative case is needed in order to reduce calculated loads to less threatening levels. With present levels of understanding, a general defense of these less pessimistic cases as being adequately conservative is difficult to define, and proceeding further may require an approach tailored more to the specific case at hand. The need for caution is highlighted by the analyses of SNL/IET-8B, in which the calculation with all the water assumed to participate underpredicted ΔP and also underpredicted the efficiency with which energy was extracted from the debris on DCH time scales. On the other hand, the experimental ΔP was considerably less than the maximum value obtained in the sensitivity studies on participating water fraction. It is apparent that a genuine quenching effect can exist in DCH events involving large amounts of water, even though the CONTAIN model can overpredict the effect.

The probability of an event approaching the worst cases considered here may be small; unfortunately, it may be difficult to actually establish a less severe result as still being reasonably conservative. Adopting a probabilistic approach would be one way of acknowledging that the conservative cases may not be absolutely ruled out without allowing them to completely dominate the overall assessment of DCH threats.

7.9 Gas Combustion.9 Gas Combustion.9 Gas Combustion

Analysis Prior to Vessel Breach. The user should consider what assumptions concerning hydrogen behavior prior to vessel breach are desired, and set the hydrogen burn parameters accordingly. Time-dependent burn parameters cannot be specified in CONTAIN, and the standard prescription burn parameters could easily allow hydrogen entering the containment prior to vessel breach to burn off as it is introduced. The deflagration model can also burn off hydrogen prior to vessel breach, if its concentration requirements are satisfied. There could then be little pre-existing hydrogen in the containment at the time of the DCH event, which could be quite nonconservative if this is not what was intended by the user.

The simplest way to prevent burning off the pre-existing hydrogen is through use of the CONTAIN input variable 'tactive', which suppresses all DFB and deflagration activity prior to the time 'tactive'. If 'tactive' is set to the time of vessel breach, hydrogen introduced prior to vessel breach normally will not be burned in the calculation. This procedure corresponds to the assumption that there will be no ignition sources prior to vessel breach. If it is desired to model the hydrogen behavior prior to vessel breach under the assumption that ignition sources are available, and that the hydrogen should burn if the conditions are suitable, it will probably be necessary to perform a restart at the time of vessel breach, since the DCH standard prescription parameters for the combustion models are not suitable for non-DCH conditions.

Deflagrations. In the experimental analyses, conditions for deflagrations during the DCH analyses were never approached in the dome, and the minor deflagrations sometimes calculated to occur in the small subcompartment cells had little effect. In NPP analyses, the wider range of conditions that can arise may permit deflagrations to have a larger impact upon the calculation.

The CONTAIN deflagration model uses correlations for hydrogen burn combustion rates, completeness, and concentration limits which are based upon experiments at relatively low temperatures, typically ~400 K or less. These correlations are not temperature-dependent and tend to be nonconservative under DCH conditions because flame speeds and combustion completeness increase as the initial temperature increases. Furthermore, the deflagration model calculates a characteristic burn time based upon a flame propagating from a single ignition source. In a DCH event, there may be vast numbers of ignition sources, which could greatly accelerate the combustion rate. For DCH conditions, it may be reasonable to manually override the correlation for flame speed with a value based upon the velocities of hot debris particles flying through the containment. These velocities are typically of the order of tens of meters per second.

If a deflagration is allowed to initiate in a cell, no BSR can initiate in that cell until the deflagration is complete and an additional "dead time" (equal to the deflagration burn time) imposed by the code has elapsed. If conditions suitable for a BSR would have otherwise developed, this "pre-emption" by the deflagration model may yield nonconservative results. However, if the flame speed has been set to high values, > 10 m/s, in order to simulate the effects of multiple ignition sources, the burn times and therefore the dead times will be short and the potential for a nonconservative suppression of the BSR model is less. If this approach is adopted, a start-stop-start behavior could result for the hydrogen burns and this may produce an unrealistic shape for the pressure-time histories. Since the peak pressure is controlled primarily by the total energy input and the length of time over which the energy is released, the sensitivity of the peak pressure to the irregular energy input is probably quite limited. There is currently no experience available using this approach, however.

It is recommended, therefore, that the user either suppress deflagrations altogether and use the DFB and BSR models to control hydrogen behavior, or else impose a high flame speed on the model as suggested above.

Diffusion-Flame Burn (DFB). For DCH analysis, it may not be fruitful to place too much emphasis on identifying the "correct" values of the various threshold parameters controlling the DFB model. Combustion behavior of the incoming gas jet under DCH conditions is actually a function of jet composition and temperature, receiving cell composition and temperatures, jet orifice size, jet flow velocities, and probably depends upon debris parameters (amounts, temperatures, compositions, particle sizes). The CONTAIN model is not sufficiently mechanistic to capture these dependencies, and the trends in the observed DCH combustion behavior support this belief (see Section 6.6.1). Hence the real "standard prescription" is to set DFB parameters to ensure that most DCH-produced hydrogen does burn upon reaching an oxygen-bearing atmosphere. Since it usually did burn in the experiments and one expects large scale to favor this trend, the assumption that it will burn is considered to be the most likely outcome and it is also the conservative prescription; hence it should be adopted as the standard.

Examination of the experimental hydrogen combustion systematics shows that combustion of DCH-produced hydrogen exhibited a quasi-threshold behavior, in that either much more than 50% burned, with a substantial contribution to ΔP, or much less than 50% burned, with at most a minor contribution to ΔP. Given that the hydrogen burned, it was found that ΔP was quite insensitive to the DFB parameters unless they were made sufficiently restrictive that DFB was effectively suppressed.

Results presented in Section 6.6 indicate that the DFB parameter set used for the experimental analyses (Table 3.2-1) generally does a good job for typical containment conditions unless large amounts of water are involved. In this event, SNL/IET-8B results (Section 6.4.5) show that the temperature thresholds can suppress combustion when it actually should occur. Hence the temperature thresholds should be eliminated. Without the temperature thresholds, the justification for a high value of the diluent/combustible ratio in the subcompartments is less and hence this ratio ('shratio') may be left equal to the CONTAIN default value of 9.0. These changes are now suggested for all DCH calculations.

In the standard prescription, the concentration limits specified for the receiving cell are sufficiently permissive as to almost constitute no limitation at all. One reason for these settings is that, with less conservative values, the composition of the receiving cell might initially permit combustion, but that steam and oxygen concentrations would rise and fall, respectively, as the event proceeds, possibly terminating combustion if less conservative values were used. In reality, temperatures would rise rapidly in the receiving cell, which would tend to compensate for the changes in atmospheric composition, but the temperature dependence of the flammability limits is not modeled in CONTAIN. Experimentally, combustion has been observed to occur during DCH events when the default flammability limits (55% steam and 5% oxygen) are not satisfied. In the SNL/IET-9 experiment, for example, even the initial steam concentration was about 67% and the final steam and oxygen compositions were estimated to be ~80% and ~2%, respectively, yet most of the DCH-produced hydrogen burned [Bla94].

The SNL/IET-5 experiment does show that this parameter set can predict efficient combustion of DCH-produced hydrogen under conditions for which it actually will not occur. The initial containment atmosphere temperature in this experiment was low (302 K) and rose to only 400-450 K in the dome during the event; hence heating would not have had a large effect upon the flammability limits. NPP scenarios this heavily inerted may be unlikely to arise in practice, however. No changes are recommended for these parameters except for sensitivity calculations, e.g., if it is thought that the assumption that DCH-produced hydrogen may not burn due to high steam concentrations and/or low oxygen concentrations. It will then be up to the user to defend the assumption that the DCH-produced hydrogen will not burn for the scenario of interest.

Bulk Spontaneous Reaction (BSR). For the experimental analysis, the standard prescription for the BSR model temperature threshold was based upon an analysis summarized in Section 3.3.1 which yields thresholds that decline somewhat with increasing scale and, at NPP scale, would be close to the BSR default temperature (773 K). There is no evidence that the added complexity of the analysis referred to in Section 3.3.1 is justified and it is recommended that the BSR default temperature be used as the standard prescription for NPP calculations. The reaction rate assumed in the standard prescription, $5/V_{cell}^{1/3}$ s^{-1}, is also recommended based upon results given in Section 6.6.2. This value is no doubt quite uncertain and sensitivity studies are certainly justifiable in any analysis for which BSR is found to be important. At present, however, the principal issue appears to be whether the calculation should allow BSR in the dome to occur at all, and performing sensitivity studies on the BSR reaction rate may be of secondary interest until this question is better resolved.

Thus defined, the standard prescription predicts that there would be little contribution of pre-existing hydrogen to containment pressurization in the Zion-geometry IET experiments, which is in agreement with experimental results. The standard prescription also predicts that pre-existing hydrogen would contribute in the Surry-geometry IET experiments performed in the CTTF, but that the contribution is too small relative to other uncertainties to permit a clean test. This result reflects in part the limited amount of pre-existing hydrogen, equivalent to 14-24% Zr oxidation, in the experiments; pre-existing hydrogen could play a larger role in some NPP analyses in which a greater degree of Zr oxidation may be predicted to occur. Higher hydrogen concentrations would increase the potential importance of pre-existing hydrogen behavior and could also increase the likelihood of pre-existing hydrogen combustion. Note that the BSR thresholds depend upon temperature only, and it would be up to the user to reduce the thresholds to take into account any increased likelihood of combustion as the flammability of the atmosphere is increased.

It is our judgement that the BSR standard prescription (with the CONTAIN default for the initiation temperature) is unlikely to be overly optimistic to any great degree, and that it could be either reasonably best-estimate or overly conservative. It is recommended, therefore, that calculations be performed using the standard prescription with the recognition that the results may tend to be conservative. If calculated loads are acceptable, performing additional sensitivity analyses may be optional. The uncertainty associated with the pre-existing hydrogen behavior may be estimated by running the problem with a very high threshold temperature (e.g., 2000 K) specified for the dome. If the resulting uncertainty range is insufficient to alter the major conclusions to be drawn from the analysis, further study may not be needed.

Unfortunately, it is difficult to offer a general plan for proceeding further if the uncertainty associated with the pre-existing hydrogen behavior and the BSR model is found to be important. The problem is not that the approximate threshold for a rapid reaction under DCH conditions is tremendously uncertain; this uncertainty is not excessive and it could probably be reduced without a large amount of additional effort. However, the main source of uncertainty is now believed to be the possibility that stratification in the dome (clearly evident in the Surry IET experiments) may invalidate CONTAIN's well-mixed assumption. This effect cannot be reasonably represented by adjusting the threshold temperature because the latter is a chemistry parameter and cannot be expected to provide a satisfactory surrogate representation for what is basically a gas mixing uncertainty. While one can attempt to represent the effects of stratification by subdividing the dome volume, the ability of control-volume, lumped-parameter codes such as CONTAIN to capture gas mixing and stratification effects in open volumes is not established. At best, one could only hope to defend the results in the context of a specific analysis and a general prescription as to how to proceed cannot be given.

BSR could be favored if large amounts of hot debris enter the dome. Although the BSR model allows for triggering based upon airborne debris quantities and temperature, this feature of the model was not used in the present work, because of the lack of data available to support its use. Neglecting the effects of the debris on hydrogen combustion is potentially nonconservative, however. When large amounts of airborne debris reach the dome and BSR does not initiate, a sensitivity calculation with a lower threshold temperature that does allow combustion is suggested. In the CONTAIN default settings for the BSR model, hot debris can initiate reaction if its temperature exceeds 773 K and the concentrations exceed 1 kg/m^2. It would be unusual to have this much hot debris airborne in the dome and, if it were present, initiation of hydrogen reaction seems likely; hence leaving these parameters at the default values seems reasonable for DCH analysis

Monitoring Hydrogen Behavior. In any CONTAIN DCH calculation, it is recommended that hydrogen production and combustion be monitored in order to aid judgments as to whether the behavior calculated is reasonable. The amounts of hydrogen burned that are reported in the CONTAIN output (including the binary plot files) include hydrogen burned by all three of the standard combustion models but does not include the hydrogen recombination (Section 3.2.6) or direct metal-oxygen reactions calculated by the DCH model. A total combustion estimate that does include these processes also can be obtained simply by evaluating the decline in total oxygen inventory in the containment. Determining whether, and when, BSR initiates in the dome usually can be done by comparing the calculated temperature-time history for the dome with the specified value of the threshold gas temperature, since the debris concentrations are unlikely to exceed the 1 kg/m^3 threshold noted above.

7.10 Recapitulation.10 Recapitulation.10 Recapitulation

The standard prescription defined in Sections 3.2 and 3.3 was developed for experimental analysis and does not address some details needed for NPP analysis; additional modifications are recommended based upon the results of this study. Known modifications required or recommended for NPP analysis have been discussed in this User Guidance section and, for the sake of convenience, we recapitulate them here with little discussion. Some sensitivity studies suggested for scoping analyses are included. We then conclude the User Guidance discussion with some general observations on DCH analysis and uncertainties.

In what follows, we assume that the principal goal of the calculations is to determine whether threatening loads can arise, and that the possibility of unrealistic behavior late in the calculation (e.g., too much late hydrogen combustion) is not of concern if it occurs too late to affect the calculated loads. The sensitivity studies suggested here are based upon the assumption that the user will wish to estimate an uncertainty range for the results, especially in the conservative direction; if this is not the case, the suggestions given may be inappropriate. The user is again reminded that there has not yet been extensive experience in applying these procedures to NPP analysis and what follows must therefore be considered tentative.

- Debris Sources, Particle Sizes, and Particle Compositions. Simple time dependencies (e.g., trapezoidal) for the airborne debris sources appear to be acceptable, with f_{disp} in the range 0.7-0.95 and f_{coh} based upon experimental correlations for the coherence ratio, R_τ, summarized in Section 7.3; sensitivity studies with $f_{coh} \geq 0.5$ are also recommended. There is no known need for deviations from the standard prescription for particle size distribution and composition, but a sensitivity calculation with the mass median diameter reduced to 0.5 mm is recommended. RPV insulation, if present, may be added to the debris sources as in the SNL/IET-11 analysis.

- Debris Transport and Trapping. No need for deviations from the standard prescription has been identified. Sensitivity studies on the TOF/KU model are recommended (Section 7.4) if f_{dome} is greater than 0.1-0.2; sensitivity to subcompartment bypass should be studied if important momentum-driven transport paths appear to exist.

- DCH Heat Transfer. No clear need for deviations from the standard prescription, or even for sensitivity studies, has been identified for debris-gas and debris-structure heat transfer. For atmosphere-structure radiative heat transfer, the standard prescription for experimental analysis included use of a user-specified emissivity of 0.8, and this procedure is recommended for NPP analysis even though the user-specified emissivity value is inappropriate for the time preceding vessel breach.

- DCH Chemistry. Setting the reaction temperature threshold to a low value (e.g., the 273.15 K default) eliminates any known need for sensitivity studies unless unrealistic reactions of cold debris cause problems (usually trapping will prevent this).

- Nonairborne Debris (NAD). Use of Eq. (7.7-1) with $m = 1$ for scaling the NAD d_t is now preferred to using $m = 0.8$ as was done in the experimental analyses. For full-scale NPP calculations without co-dispersed water, the standard value of d_t then becomes 0.0464 m. It is recommended that an uncertainty range should be defined for the effects of NAD by running with no NAD and with $d_t = 0.01$ m.

- Water (including water and NAD). The approach suggested is to define the water source to be in parallel with the airborne debris source. Analysis of SNL/IET-8B implies the CONTAIN model can be nonconservative when amounts of water involved are large and all the water is assumed to participate. Hence sensitivity calculations varying the fraction of the water that participates are recommended in order to estimate an uncertainty range. The suggested values for the NAD d_t in analyses including water are equal to twice the values assumed for dry scenarios; i.e., 0.093 m for the standard case and 0.02 m for the conservative case.

- Gas Combustion. For the DFB model, we believe that the modified standard prescription developed for use in the SNL/IET-8B analysis (i.e., diluent/combustible ratio equal to 9.0 and no temperature thresholds) is actually applicable to all DCH scenarios and is recommended for general use. For the BSR model, the recommendations are to use the CONTAIN default values for the thresholds controlling initiation (gas and debris temperatures and debris concentrations) and the standard prescription values of the reaction rate. A sensitivity calculation evaluating the sensitivity to whether BSR initiates in the dome is also recommended. If the deflagration model is used, flame speeds should be set to high values ($>$ 10 m/s) to represent the effects of multiple ignition sources and to reduce the possible impact of the deflagration model preempting the BSR model.

- Based upon the results of the calculations suggested above, the nature of the DCH scenario, and the purpose of the analysis, it may be desirable for the user to consider additional sensitivity studies. Just which calculations, if any, should be performed depends upon too many contingencies to permit specific recommendations in this recapitulation.

The intent in defining these prescriptions has been to provide choices that will be "best estimate" for many DCH scenarios and that will tend to err on the side of conservatism in cases for which these choices are not best-estimate. However, the choices made are not bounding and in a few cases important upward uncertainties may exist. Sensitivity calculations are therefore recommended to assess these uncertainties. For the Zion-geometry IET experiments, the most important examples are the uncertainties involving debris-water interactions and nonairborne debris. In addition, the user may wish to perform sensitivity calculations using less conservative assumptions if it is believed that the less conservative assumptions can be justified for the particular problem of interest.

Dependence upon DCH Initial and Boundary Conditions. Although a considerable number of uncertainties in DCH phenomena have been identified in this report, analysis of any given DCH scenario is ordinarily expected to be sensitive to at most a small number of the uncertain phenomena. The identity of the important uncertainties can, however, depend upon the initial and boundary conditions of the problem.

For open containment geometries, it is expected that sensitivity to coherence and nonairborne debris may be substantially less than for compartmentalized geometries. The potential of water to augment DCH loads in open geometries will be less than for compartmentalized geometries if any such potential exists at all; the quenching effect of large amounts of water can still be important. On the other hand, sensitivity to the debris fraction dispersed from the cavity, to trapping rates in the dome, and to the particle size may be greater for open geometries. For compartmentalized geometries, a large vessel failure size and/or a high RPV pressure tend to enhance DCH because rapid blowdown accelerates transport of energy and hydrogen to the dome, reducing the effects of atmosphere-structure heat transfer; large vessel failure sizes are also believed to increase coherence.

If the metal content of the debris is low, the uncertainties associated with nonairborne debris interactions may be less than that implied by the present results, even for compartmentalized geometries. To a lesser extent, the same may be true of uncertainties related to debris-water interactions. Sensitivity to nonairborne debris tends to be minimal when the total blowdown steam supply is low and/or when the coherence ratio is large. On the other hand, sensitivity to debris-water interactions tends to be largest when interactions of debris with coherent steam are limited by the amount of steam available. Under these conditions, the increased steam supply from vaporized water has the potential to significantly enhance DCH loads.

8 Conclusions Conclusions Conclusions

The CONTAIN code's DCH models have been reviewed and a standard input prescription for their use has been defined. The code has been exercised against a large subset of the available DCH data base. Generally good agreement with the experimental results for containment pressurization (ΔP) and hydrogen generation has been obtained. Extensive sensitivity studies have been performed which permit assessment of many of the strengths and weaknesses of specific model features. These include models for debris transport and trapping, DCH heat transfer and chemistry, atmosphere-structure heat transfer, interactions between nonairborne debris and blowdown steam, potential effects of debris-water interactions, and hydrogen combustion under DCH conditions. Containment compartmentalization was found to be a major mitigation effect in the calculations, in agreement with experimental results. An important contributor to the calculated mitigation is the combined effects of atmosphere-structure heat transfer and delayed or incomplete combustion of hydrogen in oxygen-starved subcompartment volumes.

In many cases, obtaining satisfactory agreement between calculated and experimental results is not possible in calculations that consider only the interactions of airborne debris with blowdown steam and the containment atmosphere. It is also necessary to model interactions between the CONTAIN nonairborne debris field and steam, and/or to model possible effects of debris-water interactions. These processes are not well understood and the CONTAIN models for them are parametric in key respects. This fact adds to the uncertainty which must be allowed for in analyses of scenarios different from those studied experimentally, including NPP analyses.

A partial assessment is also provided for recently implemented models for ejection of melt from the RPV and entrainment and dispersal from the cavity. Results were encouraging in that good agreement was demonstrated for containment pressurization and hydrogen generation in the SNL/IET-3 experiment when these models were used. However, sufficient limitations to the current models were identified that their use is presently recommended only on a "friendly user" basis. Otherwise, the standard prescription employs user-defined sources based upon experimental results for the extent of debris dispersal from the cavity and for the degree of coherence between the debris source and the blowdown steam from the RPV. Though investigation of sensitivity to dispersed fraction and coherence for the specific problem of interest is advisable, results presented in the present work indicate that sensitivity to these parameters may be less than was previously thought.

The results of the assessment are employed to develop guidance for use of the CONTAIN DCH model in NPP analyses. This guidance includes some modifications to the standard prescription to take into account lessons learned from the study and also to take into account features of the prescription which were designed for experimental analysis and which are not optimum for NPP accident calculations. It also includes suggestions for sensitivity studies for the estimation of uncertainties. It is expected that, for any given scenario, the results will be sensitive to at most a limited number of the various uncertain phenomena that have been considered here, but that the identity of the dominant uncertainties will depend upon the specific scenario of interest. Since there has as yet been limited opportunity to apply the approaches developed in this assessment to NPP analyses, some of the suggestions offered must be considered tentative.

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