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NUREG/CR-4896

SAND87-0633

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Printed May 1987

Received by CSTI

AUG 04 1987

Containment Loads Due to Direct Containment Heating and Associated Hydrogen Behavior: Analysis and Calculations With the CONTAIN Code

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Albuquerque, New Mexico 87185 and Livermore, California 94550
for the United States Department of Energy
under Contract DE-AC04-76DP00789

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CONTAINMENT LOADS DUE TO DIRECT CONTAINMENT HEATING AND ASSOCIATED HYDROGEN BEHAVIOR; Analysis and Calculations with the CONTAIN Code

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May 1987

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Operated by
Sandia Corporation
for the
U.S. Department of Energy

Prepared for
Accident Evaluation Branch
Division of Reaction Systems Safety
Office of Nuclear Regulatory Research
U.S. Nuclear Regulatory Commission
Washington, DC 20555
Under Memorandum of Understanding DOE 40-550-75
NRC FIN NOs. A1412, A1258

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ABSTRACT

One of the most important unresolved issues governing risk in many nuclear power plants involves the phenomenon called direct containment heating (DCH), in which it is postulated that molten corium ejected under high pressure from the reactor vessel is dispersed into the containment atmosphere, thereby causing sufficient heating and pressurization to threaten containment integrity. Models for the calculation of potential DCH loads have been developed and incorporated into the CONTAIN code for severe accident analysis. Using CONTAIN, DCH scenarios in PWR plants having three different representative containment types have been analyzed: Surry (subatmospheric large dry containment), Sequoyah (ice condenser containment), and Bellefonte (atmospheric large dry containment). A large number of parameter variation and phenomenological uncertainty studies were performed. Response of DCH loads to these variations was found to be quite complex; often the results differ substantially from what has been previously assumed concerning DCH. Containment compartmentalization offers the potential of greatly mitigating DCH loads relative to what might be calculated using single-cell representations of containments, but the actual degree of mitigation to be expected is sensitive to many uncertainties. Dominant uncertainties include hydrogen combustion phenomena in the extreme environments produced by DCH scenarios, and factors which affect the rate of transport of DCH energy to the upper containment. The importance of hydrogen behavior is partly due to the fact that most of the metallic content of the dispersed corium is calculated to react rapidly with steam in the oxygen-starved lower containment; hence, the immediate energy release is reduced (relative to oxygen reactions) but large quantities of hydrogen are rapidly generated. In addition, DCH loads can be aggravated by rapid blowdown of the primary system, co-dispersal of moderate quantities of water with the debris, and quenching of de-entrained debris in water; these factors act by increasing steam flows which, in turn, accelerates energy transport. Assessment of the actual contribution of DCH scenarios to plant risk would require substantial additional work, but it may be noted that containment-threatening loads were calculated for a substantial portion of the scenarios treated for some of the plants considered.

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ACKNOWLEDGMENT

This work is the result of the timely identification of direct containment heating (DCH) as a key containment loading issue by members of the NRC's Severe Accident Analysis Branch. In order to support this effort, resources from two ongoing severe accident analysis programs were made available by re-prioritizing these programs. These programs were the Quantitative Uncertainty Evaluation for Containment Loads Analyses (QUECLA) program under the direction of Dr. Phillip M. Wood, and the Severe Accident Sequence Analysis (SASA) program under the direction of Dr. Thomas J. Walker. We are also indebted to a number of coworkers at Sandia who have contributed to our understanding of DCH through numerous discussions, related studies, and experiments. These coworkers include M. Pilch, W. W. Tarbell, D. A. Powers, and M. Sherman.

EXECUTIVE SUMMARY

Overview of Major Findings.

If molten corium is ejected from a reactor vessel under high pressure, a variety of complex physical and chemical processes known collectively as direct containment heating (DCH) may ensue which have the potential to threaten the integrity of even the most robust containment. Models for some of the dominant DCH-related phenomena have been developed and incorporated in the CONTAIN code for severe accident analyses. The code has been applied in an extensive series of calculations for DCH scenarios in representative Pressurized Water Reactor (PWR) containments. Although major uncertainties remain, results of these analyses provide a number of important conclusions concerning the phenomena governing DCH loads, some of which differ substantially from previous expectations with respect to DCH. Major conclusions drawn from this work include the following:

- Containment compartmentalization has the potential to greatly mitigate DCH loads, relative to the predictions of single-cell analyses; however, the degree and even the existence of this mitigation is sensitive to many scenario details and phenomenological uncertainties.
- Calculated pressures are sensitive to factors that govern the rate at which energy is transported from the lower to the upper containment.
 - Loads are sensitive to the rate at which superheated steam and gas can transport DCH thermal energy to the upper containment.
 - Transport of chemical energy in the form of hydrogen to the upper containment is very important if conditions permit the combustion of this hydrogen.
 - In none of the many cases analyzed was the degree of transport of core debris itself to the upper containment identified as being the dominant influence controlling the calculated containment pressures.
- Special features of hydrogen phenomenology associated with DCH can be extremely important contributors to the loads arising in DCH scenarios.
 - Metal-steam reactions in the oxygen-starved lower containment can generate large quantities of hydrogen within a very short time.
 - High temperatures and the catalytic effects of suspended oxide particles may promote hydrogen combustion even when atmospheric compositions do not meet the flammability criteria normally assumed in accident analysis codes.
 - In ice condenser plants, hydrogen phenomenology can result in severe loads being calculated, even in scenarios for which analyses neglecting hydrogen would predict that the ice condenser would effectively control the DCH threat.
- Due to the sensitivity to energy transport rates, DCH loads are sensitive to the rate of blowdown from the primary system, and may be

significantly augmented by interaction with water in the lower containment (in contrast with previous expectations that water co-dispersed with the debris necessarily mitigates DCH loads).

- The rate at which debris is de-entrained from the atmosphere by interaction with structures does not play as important a role as previously assumed, though this parameter remains significant.
- The mass of corium ejected from the vessel does not necessarily govern the resulting loads to the degree previously assumed; given inefficient energy transport, even high core participation fractions may generate only moderate loads.
- The present work does not assess the probability that DCH loads could actually cause failure in the plants studied. However, the results do indicate that containment capacity (i.e., volume and failure pressure) is likely to be an important factor governing the probability of DCH-induced failure in any given plant.

Background.

For many nuclear power plants, especially PWRs, hypothetical accident sequences in which core melt initiates with the primary system at high pressure are predicted to be important contributors to the total plant risk. In such sequences, the molten corium may melt through the vessel bottom while the system is still pressurized. It has been hypothesized that this corium can then be ejected under high pressure from the vessel and be dispersed into the containment atmosphere, thereby causing sufficient heating and pressurization of the atmosphere to threaten containment integrity. This phenomenon, called direct containment heating (DCH), is considered to be one of the most important unresolved safety issues in the area of severe accident analysis for many nuclear power plants. For example, the recent Severe Accident Risk Reduction Program (SARRP) at Sandia National Laboratories identified it as the dominant contributor to the uncertainty in the risk estimated for the Surry plant.

The DCH problem involves many physical and chemical processes which are extremely difficult to model. In the past, most DCH analyses have consisted of either stand-alone models for particular phenomena involved (such as debris-gas heat transfer and chemical reaction) or else relatively simple bounding calculations for evaluating the potential threat to containment of a specified energy release. These analyses suggested that dispersal of even moderate fractions (20 - 50%) of the total corium inventory, with efficient oxidation of the metallic content and efficient heat transfer to the gas, could present a severe threat to containment integrity, even for PWR large dry containments. Although it was recognized that many phenomena could mitigate the loads predicted by these highly conservative calculations, models for estimating the effects of these mitigating factors were inadequate or lacking.

The present report describes the Interim Direct Heating Model (IDHM) which has been developed and incorporated into CONTAIN, a state-of-the-art systems code for the analysis of containment response to severe accidents. This model treats phenomena governing containment loads due to DCH, but does not address potential radionuclide release associated with DCH. The CONTAIN model has been applied to the analysis of containment loading during DCH scenarios arising in connection with station blackout (TMLB') transients found to be potentially important to risk. Plants representing the three basic types of

U.S. PWR containments are considered: Surry (subatmospheric large dry containment), Sequoyah and Watts Bar (ice condenser), and Bellefonte (atmospheric large dry). A substantial number of parameter variations and alternative modeling assumptions have been investigated. Results provide a number of insights into DCH scenarios, some of them at odds with past conventional wisdom on this subject.

The CONTAIN Interim Direct Heating Model (IDHM).

The CONTAIN code models containments as a number of interconnected control volumes called "cells", with the atmosphere of each cell assumed to be well mixed. In the IDHM, those DCH phenomena which are reasonably well understood are treated with mechanistic models. Poorly understood phenomena are treated with simple parametric representations which nonetheless permit their potential effects to be propagated through subsequent stages of the calculation, even though the phenomena themselves are largely governed by user-specified parameters. This approach facilitates evaluation of uncertainties in the final results due to the less well understood phenomena. The models for DCH are coupled with the other models for containment thermal-hydraulic, aerosol, and radionuclide phenomena which have been implemented in the standard released versions of CONTAIN.

Debris-gas heat transfer and chemical reaction rates in the IDHM are treated using an approach similar to that reported previously by M. Pilch, but with extensions to include reaction with mixed air-steam atmospheres and reaction rate limits associated with condensed-phase as well as gas-phase mass transport. One important limitation of the IDHM is that airborne debris is represented by a single "field" of drops, with all drops in a given cell being characterized by a single drop size, composition, and temperature. This limitation seriously restricts the ability of the model to accurately predict the extent of chemical reaction when rapid cooling of the debris may cause partial quench before reaction is complete.

A key uncertainty in DCH analyses is the rate at which airborne debris is de-entrained from the gas streams due to interaction with structures and gravitational deposition. In the present work, these processes are referred to as debris "trapping". Useful mechanistic models for trapping are not available. In the IDHM, trapping is simulated by permitting debris to be removed from the atmosphere of each cell at a rate specified separately for each cell; these trapping rates are specified by the code user. Thus, the impact of any postulated rate of trapping may be investigated, even though no modeling is available to calculate what the actual trapping rate should be. Except for the effect of trapping, debris is assumed to transport with the flow of gases between cells, without slip.

DCH Scenarios in the Surry Plant.

A base case was defined in which it was assumed that 75% of the in-vessel inventory of corium would be injected into the reactor cavity region during a five second period; blowdown of steam and hydrogen from the vessel was assumed to require 30 seconds. When analyzed using a single-cell model of the containment, very severe loads (11 - 12 bars) were calculated, in qualitative agreement with earlier, simpler analyses. However, when a more realistic (though still quite simplified) 5-cell representation of the containment was used, peak loads for an equivalent scenario were reduced to about 7 bars.

There are several reasons why containment compartmentalization yielded this dramatic mitigation of the DCH loads calculated for the Surry base case. First, the lower containment was oxygen-starved and metal-steam reactions were calculated to rapidly consume the metallic content of the corium before it could be transported to oxygen-bearing portions of the containment; metal-steam reactions release substantially less energy than do the equivalent metal-oxygen reactions. Second, the lower containment becomes thermally saturated, in the sense that the limited masses of gas and steam available become heated to extreme temperatures, 1500-2500 K. Hence, most of the total thermal energy available remains in the debris, even when local debris-gas thermal equilibrium is achieved. Third, in the base case scenario, energy is transported to the upper containment more slowly than it is lost from the lower containment by gas-structure heat transfer (largely radiative) at the extreme temperatures developed.

In the past, debris de-entrainment by interaction with structures (represented here by "trapping") has been advanced as the most important of the potential mitigators of DCH, but trapping played only a secondary role in the present analyses. Totally eliminating trapping from the calculation increased peak pressures by only 0.7 bars because energy was still rapidly lost to lower-containment structures even though the debris itself remained airborne indefinitely, with trapping eliminated. On the other hand, only very rapid trapping could prevent chemical reaction and local (i.e., intra-cell) debris-gas heat transfer from being largely complete, because the latter processes were calculated to require only short times, ≤ 0.5 second. Hence, only very rapid trapping could have a dramatic effect upon the DCH loads.

A substantial number of sensitivity studies were carried out for Surry using the base case as a starting point. Minimal sensitivity was found for the extent of in-vessel zirconium oxidation and for chemical reaction rate uncertainties. Sensitivity to uncertainties in gas-structure heat transfer were not large. Even the sensitivity to the corium participation fraction (hitherto viewed as crucial) was only moderate. On the other hand, a high degree of sensitivity was found to the rate of primary system blowdown: postulating that blowdown would occur during only 10 seconds, instead of 30 seconds, increased the calculated loads by over two bars. These results may be understood in terms of the base case being considerably less sensitive to processes affecting total energy release in the lower containment than it is to processes affecting the rate of energy transport to the upper containment. The principal energy transport mechanism governing these results is the flow of superheated gases from the lower to the upper containment, not the transport of the debris itself.

It has been widely argued that interaction between debris and water in containment might substantially reduce DCH loads, due to co-dispersed water quenching the debris. In the present study, however, it was found that, with moderate amounts of co-dispersed water, the quenching effect could be overwhelmed by the effect of accelerated energy transport resulting from the steam generated, with the net effect being to increase DCH loads by up to 2 bars. The effect of co-dispersed water was, however, sensitive to the amount of water, and the time and location at which it was introduced; it was also quite sensitive to uncertainties in chemical reaction rates (unlike the base case calculation). An important related uncertainty concerns whether one assumes that the energy of debris trapped in the lower containment is effectively lost from the problem, as is plausible when debris is trapped by adhering to structures or falling on dry surfaces, versus whether the debris is quenched in water pools, thereby rapidly generating steam. In the latter case, peak

pressures were increased by 1.6 - 2 bars; again, improved energy transport to the upper containment was the principle factor. Since the existence of this effect requires trapping to occur, the neglect of trapping would actually be quite "nonconservative" in this scenario, in sharp contrast to the usual assumption that trapping will always act as a mitigating influence.

Some of the most important uncertainties involve hydrogen combustion phenomenology in the extreme environments produced by DCH. In the CONTAIN default burn model, it is assumed that steam mole fractions greater than 0.55 will prevent hydrogen combustion, and this condition (called "steam inerting") was always met in the upper containment for the Surry TMLB' scenarios considered. However, the default burn model is based upon experiments performed at temperatures near the steam saturation temperature. In contrast, the base case DCH scenario involved temperatures in the upper containment of up to 800 K; mixtures of steam, hydrogen, and debris entering the upper containment from below were calculated to be at still more extreme temperatures, 1500 to 2000 K. Under these conditions, the various flammability limits (including the steam inerting limit) of the default model likely have little meaning. It is at least possible that any mixture containing both oxygen and hydrogen will show near-hypergolic (i.e., spontaneously reacting) behavior at these temperatures, almost independently of steam concentrations.

By overriding the default burn criteria, it is possible to force CONTAIN to burn hydrogen unconditionally whenever the hydrogen enters any cell containing oxygen, which provides a rough simulation of hypergolic behavior. Peak pressures calculated using this unconditional burn option were two to almost three bars higher than those obtained with the default burn model. Hydrogen generated by metal-steam reactions during DCH played an important role; hydrogen generated by in-vessel metal oxidation (and assumed to be released to containment prior to vessel breach) was also important. There was some synergism between the effects of the unconditional burn assumption and effects such as rapid blowdown which accelerate transport to the upper containment: very severe loads, 10 to 12 bars, were calculated for a number of scenarios involving both features.

Potential threats to containment integrity associated with DCH thermal loads are of some interest, but they received only limited attention in this work. In the upper containment, temperatures achieved in the dome walls were moderate (≤ 450 K) and probably do not present a large threat. In the lower containment, much more extreme structure temperatures were achieved, but they persisted only for seconds and affected only the immediate surface. A much more detailed containment model would be needed in order to determine whether such extremes occurred in any location relevant to containment integrity.

DCH Analyses for Ice Condenser Containments.

A simple three-cell model was used in the study of DCH scenarios in ice condenser containments. Plant parameters were based upon the Sequoyah plant, but calculated loads are equally applicable to Watts Bar, which is very similar except that the estimated containment failure pressures in Watts Bar are higher. In the base case scenario, 75% of the in-vessel corium inventory was assumed to be injected, as in Surry. Hydrogen released prior to vessel breach was assumed to have been burned off, and therefore was not assumed to be present in containment at the start of the DCH calculation. The importance of this assumption was checked and its impact upon peak loads calculated was found to be relatively minor in the base case, though it could be important in some other scenarios.

Were it not for hydrogen phenomenology, ice condensers would appear to be very efficient in reducing DCH loads: with hydrogen generation artificially suppressed, maximum pressures calculated were only about three bars in the base case. Hydrogen produced by metal-steam reactions during DCH substantially increased the non-condensable gas fraction in the ice condenser, thereby improving energy transport through it; even with combustion artificially suppressed, including hydrogen increased peak pressures to over four bars. In ice condenser plants, steam inerting is not expected in the upper containment, and the flammability criteria for the CONTAIN default burn model were easily met in this scenario. With the default burn model active, peak pressures of about 7 bars were calculated in the base case.

Sensitivity to the amount of corium injected was investigated and was not found to be great, provided only that sufficient corium was injected to generate enough hydrogen to meet the default burn model's flammability criteria; this required about 25% of the corium inventory, depending upon the metallic content of the corium. Sensitivity to trapping rates was not large.

Some of the sensitivities studied for the Surry plant were considered for Sequoyah. The most important difference between the two plants involved the choice of burn model (i.e., default versus unconditional burn). In Sequoyah, the peak pressures were generally less sensitive to this choice and, furthermore, the default model gave the higher pressures in most (not all) cases considered. The reason is that the ice condenser prevents steam inerting of the upper containment and, hence, burns occurred in both models for most choices of the other parameters considered; since the default model allows hydrogen to accumulate before ignition occurs, it typically yields the more severe burn. Another difference between the two plants was that the ice condenser somewhat reduces sensitivity to effects which, in Surry, accelerated the rate of energy transport to the upper containment, e.g., rate of blowdown and co-dispersed water. Nonetheless, these issues appear to remain potentially significant.

Comparative Study of DCH Scenarios in Surry and Bellefonte.

At an early stage in the development and application of the IDHM, DCH scenarios were analyzed for both the Surry and the Bellefonte plants (the latter is an atmospheric large dry containment with a large volume and high failure pressure). Although no longer quite "state of the art", the results obtained are still of some interest for purposes of illustrating sensitivity to differences between plants having the same basic containment concepts (i.e., large dry containments). In general, sensitivities of the DCH loads to the parameters considered were found to be somewhat less for Bellefonte than for Surry, but were otherwise similar. The most striking feature of the comparison was the degree to which the large capacity of the Bellefonte containment can mitigate the threat to containment integrity in otherwise-equivalent DCH scenarios. (However, no true comparison as to actual DCH risks for the two plants can be made, since it is by no means apparent that "equivalent scenarios" are equally probable for the two plants.)

Conclusions.

The results obtained here show that the effects of containment compartmentalization do have the potential to substantially reduce thermal and chemical interactions between the debris and the containment atmosphere, and to thereby reduce containment loads. However, the degree and even the existence of this mitigation is quite sensitive to many scenario details and phenomenological uncertainties.

One of the most important and general of the phenomenological uncertainties concerns the combustion behavior of hydrogen in the highly abnormal DCH environments, which involve much higher temperatures than those which have characterized the initial conditions in the experimental studies of hydrogen combustion upon which the default flammability correlations in nuclear safety analysis codes such as CONTAIN are based. In addition, there is a high degree of sensitivity to effects which can accelerate the transport of energy (including chemical energy, e.g., hydrogen) from the lower containment to the upper containment. On the other hand, the base cases defined for these studies showed only limited sensitivity to variations in the total energy release in the lower containment. The rate at which debris-structure interactions result in de-entrainment of airborne debris (i.e., trapping) was found to be less important than has been widely assumed, though its effects are still quite significant and will inevitably become dominant if trapping rates are sufficiently large.

The various phenomena involved in DCH interact strongly in a highly non-linear way, and valid generalizations as to the magnitude or even direction of a given effect are often difficult to make. Effects found to matter little under some conditions may prove very important under others; except when explicitly stated otherwise, the descriptions of sensitivities given here apply only to the base cases used as starting points. Even generalizations as to whether neglecting a given effect is "conservative" or "nonconservative" are likely to be in error because many such effects aggravate DCH loads under some circumstances but reduce them under others. Examples include postulating unconditional hydrogen combustion in place of the default model, the effects of co-dispersed water, and even the effects of trapping. Often the impacts of various phenomena upon the calculated loads were found to be quite different from what has been widely assumed in the past.

Despite the large numbers of parameter variations and alternative modeling assumptions treated in this work, it is by no means complete. Many possible combinations of parameters have not been treated. Some important uncertainties have not been considered at all, e.g., uncertainties introduced by the highly simplified geometries used to represent containments whose actual geometric configurations are far more complex. Use of the results obtained here to judge the threat to containment integrity due to DCH in any specific plant or plants should be done with great caution if it is to be done at all: for one thing, no assessment has been made of the probability of the various plant/scenario/parameter combinations considered, other than an attempt to eliminate some obvious impossibilities. On the other hand, it is expected that the results of the present work will prove quite useful for improving understanding of the phenomena governing the DCH loads, and identifying those phenomena which most merit additional theoretical and experimental study.

1. INTRODUCTION

Since the publication of the Reactor Safety Study (RSS) in 1975 [NRC75], it has been apparent that, in many nuclear power plants (especially PWRs), scenarios in which core melt initiates with the reactor coolant system (RCS) at elevated pressures can be important contributors to the total risk associated with severe accidents. Among these scenarios are the small-break LOCAs (e.g., S₂D sequences, in RSS terminology) and the "station blackout" or TMLB' sequence. In the latter sequence, the absence of all offsite and onsite AC electric power implies that active containment engineered safety features (ESFs) will generally be unavailable, which in turn enhances both the conditional probability of containment failure and the potential source term associated with these sequences; hence the potential importance of TMLB' to risk.

Traditionally, it has been assumed that, in TMLB' and similar sequences in PWR plants, the core would melt down, slump to the vessel bottom, and cause vessel breach with the RCS under high pressure. Should this be the case, the melt could be ejected from the vessel under high pressure, in which case both theory and experimental data indicate that significant fractions of the molten corium may be dispersed as finely divided particulate [Pi85, Ta86b]. This particulate could rapidly transfer its heat to the containment atmosphere and cause substantial containment pressurization. Furthermore, the effect could be considerably augmented by chemical energy release due to the reaction of any unoxidized metals in the melt with oxygen and steam in the containment atmosphere. Collectively, these phenomena and their associated threat to containment integrity have come to be known as direct containment heating (DCH).

More recently, it has been suggested that the core melt environment might cause RCS failures which would result in partial or total depressurization prior to melt-through of the vessel lower head, and that this effect would mitigate or prevent DCH [NRC85]. Though this hypothesis represents an important insight which is receiving active study [NRC87a], it lies outside the scope of the current report and will not be considered further here.

The potential importance of DCH phenomena was recently highlighted by the Severe Accident Risk Reduction Program (SARRP) carried out at Sandia National Laboratories [Bn87a, NRC87b]. The results indicated that DCH was the dominant contributor to the uncertainty in the risk estimated for the Surry nuclear power station, and was also the dominant contributor to the mean risk estimated in the SARRP uncertainty study for Surry.

The DCH scenario includes many phenomena which are extremely difficult to model at the present level of understanding. Notable among these is the question of debris transport through complex containment geometries: the degree to which the debris will be entrained with, and carried along by, steam and gas issuing from the RCS versus being removed from the gas stream by contact with various structures and obstacles in the path. This issue has been accepted as being central to the DCH question [NRC87b] because the reactor cavity is relatively remote from the upper containment region which constitutes the main supply of atmospheric oxygen and atmospheric heat sink. In the conventional picture of DCH, development of a severe threat to containment integrity arises if and only if there is reasonably efficient transport of debris to the main thermal and chemical atmospheric reservoir.

Despite the formidable difficulties of modeling some aspects of DCH, it remains useful to analyze the problem with the best calculational tools available in order to assess the important uncertainties as well as interpret the results of the ongoing DCH experimental program as efficiently as possible as these results become available. Hence, an Interim Direct Heating Model (IDHM) has been developed for incorporation into the CONTAIN computer code for the analysis of containment response to severe accidents [Be85]. The goal of this interim model is to treat the highly uncertain phenomena parametrically in a context where the better-understood phenomena are simultaneously being treated mechanistically with the state-of-the-art models incorporated in the standard released versions of CONTAIN.

Outline of This Report. The next section is introduced with a brief description of some previous work that is closely related to the CONTAIN IDHM. The major features of the IDHM are then presented, along with a brief description of some standard CONTAIN models important to DCH scenarios as well as a description of the modeling of DCH itself. Sections 3 through 5 constitute the heart of this report in a practical sense; they present, respectively,

results for three major series of calculations of DCH scenarios in representative PWR nuclear power stations:

- Analyses performed for Surry, a PWR with a subatmospheric large dry containment, in support of the Quantitative Uncertainty Evaluation in Containment Loads Analyses (QUECLA) program (Section 3).
- Analyses of DCH in the Sequoyah ice condenser plant. Many of these calculations were performed in support of the preparation of the NRC staff position paper on DCH phenomena which is a part of the ongoing major NRC risk rebaselining effort, to be documented in [NRC87b] (Section 4).
- Calculations of DCH loads in the Surry and Bellefonte plants performed for the Severe Accident Sequence Analysis (SASA) program. Bellefonte is a PWR with an atmospheric large dry containment.

These calculations were performed over a period of several months, during which the CONTAIN code and the IDHM underwent substantial revision (including discovery and correction of some minor coding errors). During this period, our understanding of DCH phenomena also underwent substantial evolution. In addition, the calculations were performed in support of different programs which had different requirements. As a result, the studies are divided into several series with some mismatches between the modeling and/or input assumptions employed in the different series. The effects of these mismatches have been examined and are not large enough to significantly impact the important conclusions to be drawn from this work. For the sake of completeness and accuracy, these mismatches and their effects will be acknowledged in the appropriate passages of the text as the various results are presented. It is hoped that the reader will not be excessively inconvenienced by the occasional digressions required by these acknowledgements.

Section 6 of the report summarizes some of the most important results obtained in these studies, and offers some conclusions.

During the course of this work, a number of miscellaneous studies were performed in order to assess (in part) the importance of the various approximations and omissions in the present model. This work included some separate-effects evaluations of various phenomena which are not treated in the IDHM, or which may be treated inadequately. Some of this material is reviewed in the

Appendix to this report. While not strictly necessary to following the case studies described in Sections 3 through 5, the information given there may be of some help in guiding judgments as to when the present model is expected to be reasonably reliable versus when substantial uncertainty in the modeling requires more caution in interpreting the results. The Appendix is also helpful in guiding decisions as to where future modeling efforts might be most fruitful.

2. THE CONTAIN IDHM

2.1 Review of Previous Work.

DCH has been a subject of active study during the past three years. The present brief review will be limited to mentioning those contributions that were the most influential to the development and application of the CONTAIN IDHM.

During 1983 and early 1984, under NRC sponsorship, a group known as the Containment Loads Working Group (CLWG) held a series of meetings in order to evaluate the state of the art of predicting containment loads under severe accident conditions [NRC85]. Computational analyses were focused on a series of rather stylized "standard problems" designed to represent some of the important issues affecting U.S. containment designs, but not intended to represent best-estimate descriptions of specific accidents. Two of these standard problems, designated SP-1 and SP-2, were based upon PWR atmospheric and subatmospheric large dry containments, respectively. As a result of experimental data from the SPIT tests at Sandia [Ta84a], the subject of DCH was raised during the CLWG analysis of SP-1. Subsequent deliberations concerning its implications for SP-1 and SP-2 did much to heighten the awareness of this issue within the nuclear reactor safety community.

Calculations performed for the CLWG included a number of simple adiabatic calculations using the DHEAT code [NRC85, Be86a], in which postulated quantities of corium debris were allowed to thermally and chemically interact with the containment atmosphere. Heat transfer to surrounding structures, which would mitigate the response, was neglected in these calculations. Other calculations including some nonadiabatic effects were performed with the CONTAIN code. Since no models for DCH phenomena were incorporated in the code at that time, postulated time-dependent DCH energy releases were simply input to the code, and the response of the containment atmosphere was then calculated. These simple analyses did show that, given sufficiently pessimistic assumptions, the efficient participation of relatively moderate fractions of the total core inventory (20-50%) in DCH could generate serious threats to the integrity of PWR large dry containments [NRC85, Be86a]. These pessimistic assumptions included postulating complete reaction of the metallic content

with oxygen, thermal equilibration with the atmosphere, and a total pressure rise reflecting the full combined effects of steam spikes, vessel blowdown, and DCH itself. However, the lack of any coupled treatment of the various physical processes in a single integrated analysis severely limited insights as to the degree of conservatism (e.g., overprediction of peak pressure) that might be involved in these results and what the dominant phenomena might be.

A number of stand-alone models for specific aspects of the DCH problem have been developed. Among these, the rate-dependent model developed by Pilch [Pi86a] in support of the SPIT and HIPS experimental series [Ta84a] is noteworthy for its contribution to the present effort. This model treats the trajectory of a reacting drop as it falls through the atmosphere under gravity. Unlike the models described above, this calculation tracked the temperature and composition of the debris drop as a function of time, taking into account the heat and mass transfer rate limitations in the gas boundary layer surrounding the drop. Atmospheric temperature and pressure were simultaneously tracked, yielding a self-consistent calculation based upon a simple picture of a field of identical debris droplets falling through a single-volume containment. As in the DHEAT model, heat transfer to structures was neglected. Severe pressure rises were again calculated, even when moderate fractions of the total core were assumed to participate in DCH.

Corradini and his colleagues and students at the University of Wisconsin [Go86, Po86] have developed a model, DIRHEAT, which incorporates physics similar to that of the Pilch model. They have used the energy releases calculated by this model as input to a suite of containment analysis codes to perform calculations for some DCH scenarios. However, the DIRHEAT code was not coupled to the containment analysis codes.

The reaction models considered above include the assumption that reaction rates are limited only by gas-phase transport rates. L. Baker of Argonne National Laboratories has reported results [Ba86] obtained using a model for dispersed debris droplets which treats reaction rate limits associated with mass transport within the drop, as well as gas-side limits. However, the heating of the atmosphere by the debris was not modeled; since the atmosphere therefore remained cool in his calculations, cooling of the drop resulted in early shutoff of the chemical reactions in many of the cases that were considered.

Recent experimental studies have provided information on the debris transport question. Experiments using thermitic melts ejected under high pressure at Argonne and Sandia National Laboratories, as well as other experiments with less prototypic materials, have shown that most of the debris is likely to be ejected out of the immediate cavity region [Sp86, Ta84a]. However, debris transport through the intervening compartments between the cavity and the upper containment remains a very open question.

Very recently, in an experimental program utilizing the Surtsey facility at Sandia, the first of a series of tests was performed [Ta86a, Ta86c] in which thermitic melts are injected into a large (103 m^3) pressure vessel which may contain scaled containment structures, etc. In the Surtsey facility, the actual pressure rises (along with many other parameters) are being determined, something not possible in earlier, unconfined, experiments. Data obtained in this facility are being used for the development and validation of phenomenological models which can be incorporated into future versions of the CONTAIN direct containment heating model.

2.2 Description of CONTAIN and the Interim Direct Heating Model

There are two aspects of the new calculational capabilities under discussion: standard CONTAIN models which play important roles in DCH scenarios, and the new features of the IDHM itself. These will be briefly discussed below, with no attempt at completeness.

2.2.1 Relevant CONTAIN Models

CONTAIN is a system-level best-estimate containment analysis code specifically designed for analysis of severe accident containment phenomena. Details of the CONTAIN models can be found in the CONTAIN User's Manual [Be85] so only a brief description of the standard features which have been utilized in the direct heating calculations will be presented here. All of the CONTAIN models are keyword-enabled; if the appropriate keyword does not appear in the input deck, the model is not activated and it has no effect upon the calculation. The present descriptions will be limited to those models which were employed in the work to be described. The code has been undergoing rapid development during the period of the present work, so not all calculations were performed with exactly the same models. Where changes significant to the

results were introduced, the code version number to which they apply will be included for reference purposes. All calculations to be discussed were performed with version 1.04 or higher (version 1.05 or higher with respect to hydrogen burn phenomenology).

The code features which play significant roles in the present work include the following:

a. Intercell Flow. CONTAIN uses a control volume approach to gas transport, treating each specified volume or cell as a well-mixed repository for the gases. Flow between cells occurs via an orifice flow correlation when a flow path of a given cross-sectional area and friction coefficient is specified between the cells. Any number of computational cells is allowed and arbitrary interconnections between them are permitted, except that no two cells may be directly connected by parallel flow paths in the code versions employed here.

b. Two-phase Gas-Steam-Water Thermodynamics. A realistic equation of state for two-phase water and a variety of noncondensable gases is solved at every time step to give the pressure and temperature of each computational cell, based on the internal energy and masses of the constituent gases.

c. Heat Transfer to Structures. Each cell can have an arbitrary number of heat transfer structures (e.g., walls, internal components, etc.) inside the volume. Heat transfer occurs via convection, condensation (or evaporation), and radiation between the gas and the structure surfaces. Gas-structure radiation heat transfer utilizes a model based upon the Cess-Lian correlation for the emissivity of atmospheres containing steam [Ce76]. CONTAIN 1.06 and higher versions include more detailed modeling for the atmospheric emissivity based upon the work of Modak [Mo79]; it accounts for CO₂ and CO in the atmosphere and also provides an improved treatment of steam.

Heat sink geometries in CONTAIN may be slab, cylindrical, or spherical, and the heat sinks may be composed of layers of different materials. The one-dimensional heat conduction equation is solved to obtain the temperature profile in each structure.

d. Hydrogen Combustion. The default hydrogen burn model is taken from the default burn model used in the HECTR code [Di86], which was developed at Sandia for the analysis of containment problems involving hydrogen transport and combustion. In the default model, it is assumed that an ignition source is always present, and that a burn occurs whenever the mole fractions of hydrogen and oxygen exceed 0.08 and 0.05, respectively, provided further that the steam mole fraction does not exceed 0.55. (In CONTAIN 1.06, the default flammability limit for hydrogen was reduced to a mole fraction of 0.07.) Propagation from cell to cell is also assumed to take place depending on whether certain other concentration criteria are satisfied. All burns are treated as deflagrations occurring over a time period determined by the characteristic length of the cell and a flame speed which is calculated from correlations. In CONTAIN 1.05 and higher versions, the user may override any or all of the default correlations for hydrogen burn phenomenology, and this capability was used in a number of the DCH calculations as is described in Section 2.2.2.

e. Ice Condenser. The ice condenser model involves both thermal-hydraulic and aerosol decontamination modeling, but since fission products are not treated in the direct heating calculations to follow, the scrubbing model will not be described. The ice is modeled as a surface held at the ice temperature; the surface area changes as the ice melts. Condensation and radiation heat transfer is modeled between the atmosphere and the ice with a thin water film separating the two. Doors between the lower compartment and the ice bed and between the ice bed and the upper containment can be modeled as being either one-way or two-way; in the latter case, the effective flow area can be different depending on which direction the flow occurs. In all calculations to be presented for ice condenser plants (Section 4), it is assumed that the doors do not fully close upon flow reversal.

2.2.2 Direct Heating Models

This section provides a relatively brief overview of the major features of the IDHM, with many details concerning the approximations and assumptions required in developing and implementing the model omitted. Some selected features of the model and its limitations are discussed in more detail in the Appendix, with emphasis upon the uncertainties that may result from the model's limitations under various conditions.

The present version of the CONTAIN IDHM is limited to assessment of the containment loading phenomenologies associated with DCH. In addition to providing a potentially severe threat to containment integrity, DCH events can also release copious aerosols and significant quantities of radioisotopes to the containment atmosphere [Ta86a]. At present, the code could address the subsequent fate of these materials only if the user specified their quantity and other characteristics through code input. No mechanistic models for actually calculating the generation of aerosols and release of fission products during DCH are available, but it is hoped that models suitable for incorporation into CONTAIN will become available in the future. In the mean time, the present work addresses containment loading issues only. Aerosol and radionuclide phenomena associated with DCH will not be discussed further.

a. Dispersed Debris Field. The principal modification to the standard versions of CONTAIN is that a new field has been added to the code in order to represent the dispersed debris. The debris field is like the gas in that each cell is a well-mixed repository of the debris mass and its energy. However, the debris mass in each cell is assumed to be composed of a large number of spherical droplets having identical composition and temperature. A realistic debris equation of state is solved at each time step to give the debris temperature in each cell. There are five debris constituents allowed: Zr, ZrO_2 , Fe, FeO, and UO_2 . Chromium and nickel, which are present in significant quantities in reactor stainless steels, are neglected.

The debris flows with the gas in a dispersed droplet mode; that is to say, debris is transported without slip from one cell to the next with the gas in proportion to the mass of debris and gas present in the donor cell at each timestep. Such a model is sometimes called a homogeneous flow model. In the cavity area, this approach can be justified by the expectation that gas velocities are so high that droplets which impinge on surfaces are quickly resuspended in the gas stream and fragment down to about the maximum Weber-stable radius. In the model, however, the droplet diameter is specified in input and does not change throughout the calculation. Qualitatively, this picture of transport of a fluidized debris/gas mixture at gas velocities well in excess of the critical Kutateladze velocity is justified by theory, the HIPS experiments [Ta86b], and simulant fluid experiments conducted at Brookhaven [Gi87]. Quantitatively, there are many potentially-significant

aspects of debris behavior which are not treated. One of these, interactions between drops leading to drop agglomeration, is discussed in the Appendix.

b. "Trapping" of Airborne Debris. As gas velocities drop, it is to be expected that some de-entrainment will occur which is not followed by reentrainment. This process will be referred to as "trapping" in the present work; it is defined to include any process which removes debris from the atmosphere and transfers it to an environment such that it can no longer effectively exchange heat and/or mass with the atmosphere on the very short time scales characteristic of DCH. Trapping is partially analogous to the transition from dispersed droplet flow to annular flow in two-phase flow in pipes. However, so little is known about the flow patterns under these conditions in the complex geometries and large scales of reactor containments that it is not possible to apply conventional correlations for two-phase flow in the situation under consideration. Furthermore, there are additional complications associated with the interaction of hot debris with surfaces: freezing may lead to debris adhering to surfaces under conditions for which re-entrainment would otherwise be expected, while ablation and gas generation at some surfaces (paint, concrete, or even wet metal) may favor re-entrainment. Therefore, the process of trapping is treated parametrically: a user-specified fractional removal rate, λ_{tr} , is assigned to each cell. Debris is then assumed to be removed from the atmosphere and deposited in a debris layer at the bottom of the cell at a rate equal to $\lambda_{tr} m_d$, where m_d is the mass of debris airborne within the cell. The units of λ_{tr} are 1/s, and its inverse is the characteristic trapping time for debris suspended in the volume. For many of the calculations to be presented in this report, a simple formula is used (following Pilch [Pi86a]) which equates the trapping time to an effective drop fall time:

$$\lambda_{tr} = v_t / V^{1/3}, \quad (2.1)$$

where v_t is the terminal velocity under gravity for the droplet and V is the cell volume. The processes which actually control the trapping of debris are, of course, highly complex, and highly uncertain. The parametric treatment used here is only intended to provide a simple way of accounting for the effects of debris removal in the absence of detailed calculation of particle and gas flow patterns and detailed models for debris-structure interactions. The purpose of Eq. 2.1 is to introduce a reasonable scaling for each cell, and

to allow parameter variations which affect the different cells in approximately the same way.

The debris which is not de-entrained is transported, without slip, with the gas to downstream cells. The mass of the airborne debris is included in evaluating gas density when the flow equations are solved. The mass and energy of debris entering a cell is added to that cell's debris field, resulting in a new debris temperature and a new composition.

c. Heat Transfer from Debris. Heat transfer occurs between the debris and the gas by conduction (with convection) and by radiation. As in Pilch's model [Pi86a], a heat transfer coefficient for conduction/convection is calculated based on a Reynolds correlation for flow over a sphere [Bi60], with a droplet velocity, v_i , for cell i relative to the gas; the v_i are specified for each cell by the user and are constant for the calculation. The Nusselt number and associated heat transfer rates are given by:

$$Nu = 2.0 + 0.6 (Re^{1/2})(Pr^{1/3}) \quad (2.2a)$$

$$\dot{Q} = \frac{k Nu}{d} S_d (T_d - T_g) \quad (2.2b)$$

where Re is the Reynolds number (based upon particle diameter), Pr is the Prandtl number, $\dot{Q}$ is the rate of heat transfer from the debris to the gas, S_d is the total surface area of the airborne debris, k is the thermal conductivity of the gas, d is the diameter of the debris drops, and T_d and T_g are, respectively, the temperature of the debris and of the gas. The various gas properties required in Eq. 2.2 are evaluated at a film temperature, T_f , which is assumed to be equal to $(T_d + T_g)/2$. The properties are evaluated for a gas of the bulk composition; i.e., variation of properties due to variations in the gas composition through the boundary layer are neglected. Significant uncertainty can result when steam is the dominant reactant, because the generation of hydrogen can then lead to large variations in the gas properties (e.g., the thermal conductivity) within the boundary layer, as is discussed further in the Appendix.

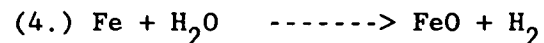
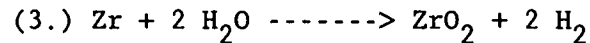
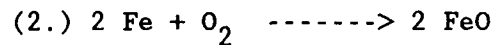
Significant uncertainty is associated with the application of Eq. 2.2 to heat transfer in DCH scenarios. As an aid to performing sensitivity studies, the heat transfer rate calculated using these relations may be multiplied by an arbitrary factor specified through the code input.

The use of a non-zero relative velocity of the droplets in Eq. 2.2a is not necessarily inconsistent with the zero-slip assumption employed in calculating the inter-cell transport of debris. The underlying assumption is that the debris field consists of a collection of particles moving in random directions superimposed on an overall drift equal to the gas velocity.

Debris-gas and debris-wall radiation transfer are treated independently and somewhat parametrically. The debris-gas transfer is a simple gray gas model, in that radiation from the debris is evaluated using the black-body radiation law and a multiplier is available to the user to reduce the heat flux from the pure black body value. Similarly, a second multiplier is provided to reduce the direct black body radiation transfer from debris to structure surfaces. The area for debris-structure radiative heat transfer is the minimum of the droplet field surface area and the structure area. Care must be taken in selecting the values of the two gray body multipliers not to remove an unphysical amount of heat from the droplet field (roughly speaking, the sum of the multipliers should be less than 1). In practice, side calculations are often used to select reasonable values for these multipliers. Radiation and convection heat transfer from the gas to the walls is part of the standard CONTAIN modeling, and is calculated in a much more mechanistic fashion than is debris-gas or debris-wall radiation. Improved models which self-consistently calculate all three heat transfer rates are now under development.

d. Co-dispersed Water. A water droplet field could be approximately modeled using either the CONTAIN containment spray model or the aerosol model, but a simpler approach is to assume that gas-droplet heat transfer is very efficient, and not rate limiting. Since CONTAIN has a true two-phase equation of state for water, it is possible to source in a mixture of non-condensable gas and extremely wet (i.e., low quality) steam; this is equivalent to a gas mixed with a water droplet field with extremely small droplet diameter. This approach will tend to exaggerate the effect of the presence of co-dispersed water.

e. Debris Oxidation Reactions. Chemical reactions can take place if the droplets contain oxidizable metal and the atmosphere contains steam and/or oxygen. The reactions considered are the following:



(H₂ is from Reactions 3 and 4)

Within each computational time step, the first four reactions are limited to (1.) the mass of metal in the droplet and/or (2.) the mass of oxygen or steam which can diffuse through the boundary layer to the droplet surface from the bulk gas during the time step. The metal oxidation reactions are treated in terms of a hierarchy favoring Zr over Fe and O₂ over H₂O when there is direct competition between these reactants. The Zr - Fe hierarchy is most plausible if it is assumed that Zr and Fe are initially intermixed in the same drops; in any case, the single-field debris model would have only very limited capabilities for representing drops having different compositions if it were assumed that the metals were initially segregated instead. The O₂ - H₂O hierarchy is applied only within the time step, which means that both the H₂O and the O₂ diffusing to the drop within a time step are allowed to react if there is sufficient metal even when oxygen is still available in the bulk cell atmosphere. Steam concentrations in typical DCH scenarios are much higher than oxygen concentrations, and this treatment therefore implies that most of the metal will be oxidized by steam rather than oxygen in such cases, even though there may be some oxygen in the cell. The heat from the metal oxidation reactions is added to the droplet field energy. All mass inventories (debris and gas fields) are appropriately updated in accordance with the extent of each reaction.

The fifth reaction listed above is treated separately from the normal hydrogen combustion event discussed in Section 2.2.1. The only hydrogen

involved in this reaction is the by-product of reactions 3 and 4, and the mass of oxygen consumed, if any, is taken from the bulk gas, rather than the quantity which can diffuse to the droplet surface. Likewise, the heat from this reaction is added to the bulk gas, not to the debris. This reaction represents the result of diffusion of the hydrogen byproduct back to the bulk gas. It is assumed that the near-drop environment is so hot that hydrogen-oxygen recombination occurs without need of a flame or spark source, as long as any oxygen is present in the bulk gas of the cell. (The code user may disable this recombination through code input, but this option was judged less realistic and it has been little used in the present work.) The effect of this reaction upon the local concentrations of oxygen and water vapor in the drop vicinity is neglected; hence, the reaction is assumed to have no effect upon the rates at which the first four reactions occur. In terms of total energy release, the combined effect of the steam-metal reaction plus the $H_2 - O_2$ recombination reaction is, of course, the same as if the metal were restricted to reacting with oxygen only. However, the resulting distribution of the energy between the debris versus the gas fields is different, and the total reaction rate is considerably greater for typical DCH conditions than would be the case if reaction were allowed to occur with the oxygen only.

A limitation of the present model is that chemical equilibria are ignored, and it is assumed that all reactions go to completion. The resulting errors are probably negligible except for the steam-iron reaction. Thermodynamically, the equilibrium steam/hydrogen ratio in the presence of iron is about 0.5, over a wide range of elevated temperatures; thus the reaction will not proceed at lower steam/hydrogen ratios. Even at higher steam/hydrogen ratios, this effect will reduce the rate of reaction because the steam/hydrogen ratio at the drop surface can not fall below this value, while the present model assumes zero reactant concentration at the surface. Hence, the present model overestimates the reactant concentration gradients which drive the transport of reactant through the gas phase to the drop surface. It should be noted also that the steam/hydrogen ratio of 0.5 applies only to equilibrium between the Fe/FeO couple; dilution of either the metallic or the oxide phase with other species could alter this ratio appreciably. Metals more reactive than iron (e.g., Zr and Cr) can react with steam even at much lower steam/hydrogen ratios, and the present treatment will not introduce significant error so long as such metals are present. Future versions of the model will treat chemical equilibria and will also treat chromium, which is present in significant

quantities in typical stainless steels. Additional discussion of some of these subjects is given in the Appendix.

Oxidation of UO_2 by oxygen is not treated in this model since it is not favored under many of the conditions of high temperature and limited oxygen availability of interest in DCH scenarios. In addition, it has limited significance energetically.

Mass transfer through the gas boundary layer to the droplet is calculated with a mass transfer coefficient based on a heat transfer/mass transfer analogy [Bi60]. The dimensionless Sherwood number, Sh , is calculated from a correlation analogous to that of the Nusselt correlation in Eq. 2.2a, except the Prandtl number is replaced by the Schmidt number. (Again, this is the same approach used earlier by Pilch [Pi86a].) Thus,

$$Sh = 2.0 + 0.6 (Re^{1/2})(Sc^{1/3}) \quad (2.3a)$$

$$\dot{M}_j = \frac{D_j}{d} \frac{Sh}{S'_d} C_j, \quad (2.3b)$$

where $\dot{M}_j$ is the reaction rate for the j th gaseous reactant and D_j and C_j are the diffusivity and concentration, respectively, of the j th reactant in the gas phase. As in Eq. 2.2, gas properties are evaluated at the film temperature, T_f , but correspond to the composition of the bulk gas. The area used for diffusion of oxygen and steam to the droplets, S'_d , is equal to S_d in Eq. 2.2b, multiplied by an estimated fraction of debris particles which still have some metal left, as is discussed further in the Appendix.

As in the case of the heat transfer calculation, the mass transfer rates calculated using Eq. 2.3 may be multiplied by an arbitrary user-specified factor. This factor may be specified separately for oxygen and for steam.

The rate of chemical reaction may also be limited on the drop side of the interface by the rate at which oxidant and/or metal species can diffuse within the drop. This rate can depend strongly upon the length of time the drop has been exposed to oxidant, i.e., drops with fresh surfaces may react much more rapidly. In the current treatment, it is not possible to model this process in detail since the code does not keep track of how long the various droplets

have been reacting with the gas. Therefore, a reaction rate is calculated which would give the correct time to react half the metal if it were released as a puff into the cell. The treatment is based upon diffusion within a sphere. The code user can specify a temperature-dependent diffusivity and, in addition, the user can specify a reaction threshold temperature, below which no chemical reaction can occur. The utility of these temperature-dependent features is limited by the lack of a detailed description of the thermal history of the debris droplets in the present single-field model. The subject of drop-side reaction rate limits is discussed in more detail in the Appendix.

f. Hydrogen Combustion. An important result of the calculations performed for typical DCH scenarios with the present model is that the metal in the debris is rather efficiently oxidized by the steam which accompanies it. Furthermore, the resulting steam-hydrogen gas mixture moves into upper containment volumes with an extremely high temperature, sometimes as high as 2000K. Moreover, there may be a significant quantity of very hot oxidized particulate material accompanying the gas. The question then arises as to what are the appropriate criteria for hydrogen combustion (e.g., ignition thresholds and completeness) under these conditions. As explained in Section 2.1, the default CONTAIN model for hydrogen combustion is based on the HECTR code, whose default burn correlations are based, in turn, on experiments performed at relatively low initial temperatures. The use of these correlations (e.g., steam inerting at steam mole fractions greater than 0.55) at such high temperatures is extremely questionable. The presence of hot oxide particulates which can act as ignition sources or catalysis surfaces makes the use of the conventional criteria even more dubious.

At sufficiently high temperatures, any mixture containing both hydrogen and oxygen is expected to behave as hypergolic (i.e., spontaneously reacting). Experimentally, such behavior has been observed for stoichiometric air-hydrogen-steam mixtures at temperatures as low as 790-820 K [Sh57] at relatively low steam concentrations (0-30%); at higher steam concentrations (30-80%), theoretically calculated values of 850-1300 K have been reported, with total atmospheric pressure and vessel size as well as steam concentration being important parameters [Ma66]. Autoignition temperatures of 930-1090 K have been reported for steam-hydrogen jets (0-60% steam) entering air [Ze56, Sh85]. No extensive review of this subject has been attempted as part of the present work, and there are many questions concerning the applicability of

these results for present purposes. Nonetheless, the concept of hypergolic behavior at sufficiently elevated temperatures seems almost certain to be valid. It is at least plausible that it should be considered for any mixture at or above temperatures of 900-1000 K, perhaps lower when steam concentrations are not too high and near-stoichiometric mixtures may exist at least locally. In the present work, the 900-1000 K temperature range will be used for the sake of illustrative discussion only. It is likely that firmer estimates of air-hydrogen-steam combustion behavior at elevated temperatures could be generated using detailed theoretical combustion models such as the CHEMKIN code [Ke80], but this task has not been attempted to date.

There are other scenarios in which the default burn model may not give a good representation of hydrogen combustion behavior. One such case arises in the analysis of ice condenser plants, in which the ice condenser prevents steam inerting of the upper containment even in station blackout scenarios. If the gas entering the upper containment is rich in hydrogen, it may ignite and continue to burn as a self-sustaining plume or jet flame, without the minimum flammable concentration of the default model ever having been approached in the bulk gas of the upper containment. Even in large dry containments, similar situations may arise in sequences other than station blackout, if ESFs (e.g., sprays or fan coolers) keep steam concentrations sufficiently low.

In the present work, an attempt to bound the hydrogen combustion effect has been made by employing an option in CONTAIN which permits the code user to override the default combustion criteria and prescribe the values of the various parameters governing hydrogen burns. This option was used to force burning of all hydrogen present in a cell whenever there is oxygen, regardless of the concentrations of hydrogen, oxygen, or steam. In the discussions that follow, this option is designated the "unconditional burn" option. Once the unconditional burn option is activated, any existing hydrogen in a cell burns off (given the necessary oxygen) during a specified burn time. Additional hydrogen entering the cell burns in an approximately continuous fashion as it enters. The latter combustion is only approximately continuous because the code's logic for time step control during burns imposes a dead time immediately after completion of a burn, during which no new burn can initiate. The duration of the dead time equals the duration of the burn that preceded it. The unconditional burn option was used to simulate both the hypergolic

combustion behavior and the plume combustion behavior noted above. Its use does not, of course, determine whether these behaviors will actually occur in a given scenario, but it does provide a reasonable representation of the consequences to be expected if they do occur.

2.2.3 Model Verification and Validation.

Code verification and validation efforts for the IDHM are not yet advanced, but a limited amount of work has been done. Comparisons with some of the stand-alone models [Be86a, Pi86a, Ba86] discussed in Section 2.1 have been performed. When closely equivalent problems have been defined, reasonable agreement has been obtained. In some cases, difference in modeling and/or problem definition have prevented close comparisons, but the reasons for these differences are believed to be known, i.e., they do not represent model malfunctions.

Of greater practical interest may be the comparison of CONTAIN predictions with the results of the first Surtsey test, designated DCH-1 [Ta86a]. The CONTAIN calculation is compared with the preliminary experimental data in Fig. 2.1. The calculation was "blind" in that all input parameters were frozen prior to the experiment, with the sole exception of the mass of debris actually ejected from the experimental cavity into the Surtsey vessel, which was taken from the posttest data. The agreement obtained speaks for itself. This result should not be over-interpreted; review of the detailed DCH-1 results suggests that this experiment likely was dominated by those phenomena for which the code does attempt a reasonably mechanistic treatment, with phenomena for which the code includes only a parametric representation (e.g., trapping) being less important than is likely to be the case in some other problems. Certainly realistic DCH scenarios are far more complex, and it would be naive to suppose that CONTAIN might predict them with comparable precision. Nonetheless, the importance of this result should not be downgraded: it is highly reassuring that the code does appear to do a good job on the phenomena which it treats mechanistically, and this result lends considerable support to its use in DCH containment analyses provided that its limitations are allowed for in interpreting the results.

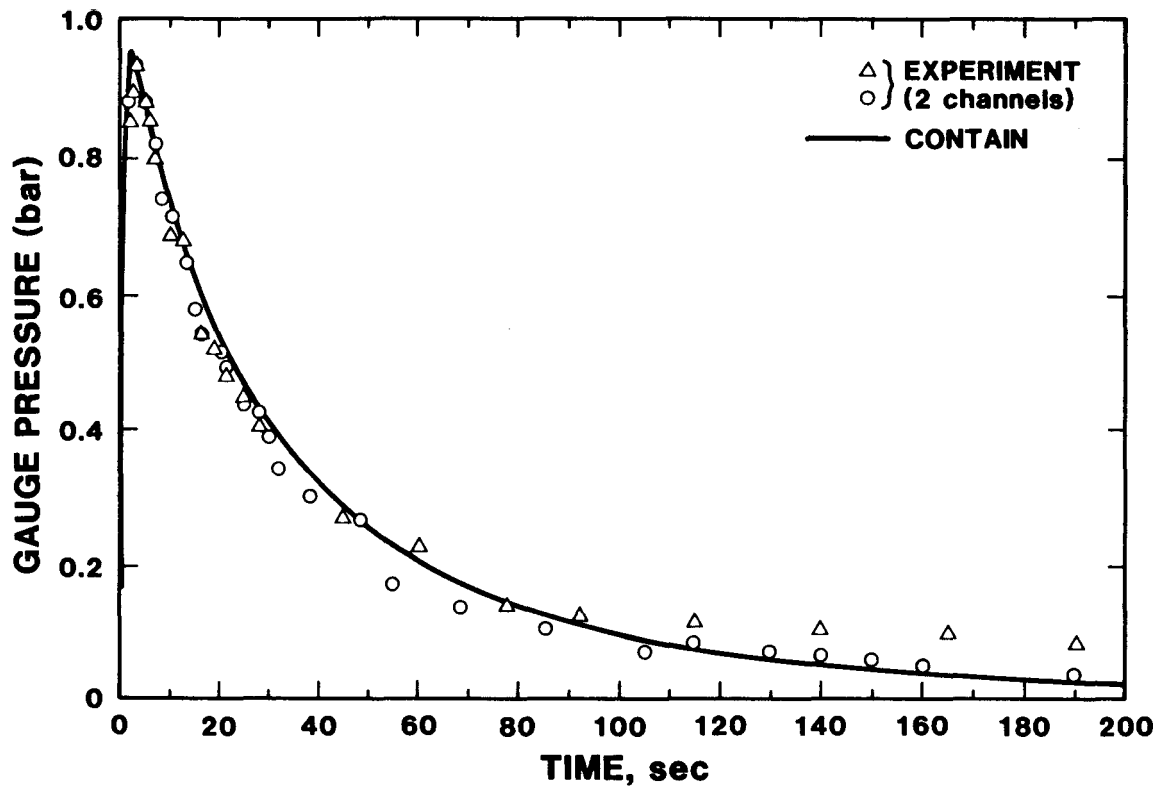


Fig. 2.1 Comparison of experimental results and CONTAIN predictions for the first Surtsey direct containment heating test, DCH-1.

3. ANALYSIS OF DCH IN THE SURRY TMLB' SEQUENCE

3.1 Introduction.

In this section, we present results obtained applying the CONTAIN IDHM model to DCH scenarios arising during the station blackout (TMLB') sequence in the Surry plant. This sequence was selected primarily for its potential importance to risk [Bn87a]. During the period over which these calculations were performed, there were some code modifications which should be kept in mind when comparing the various results:

a. Atmospheric radiation upgrade. As part of the upgrade from CONTAIN 1.04 (and 1.05) to CONTAIN 1.06, the Cess-Lian model [Ce76] for steam emissivity was replaced by a model based upon the work of Modak [Mo79] as the default calculation, although the Cess-Lian model remains available as an option. Steam emissivity is potentially important because DCH scenarios often involve extreme atmospheric temperatures which leads to thermal radiation being a very important mechanism for gas-structure heat transfer. Many of the calculations reported here employed CONTAIN 1.04, but sensitivity to this change has been explored. (The upgrade to CONTAIN 1.06 actually included some minor changes in the DCH model itself as well as important changes to many other parts of CONTAIN, but the refinement of the radiation model is the most important in the present context.)

b. Fixes to Minor Coding or Modeling Errors. The most important of these include fixes to a coding error which disabled the hydrogen recombination option discussed in Section 2.2.2 and a modeling error related to an inconsistency between the definition of the reaction energies and the definition of the CONTAIN reference energies for gaseous species. The impact of these corrections is believed to be small compared with the major effects of interest in this work, as is discussed further in Section 3.2.3.

3.2 Sensitivity Studies of the TMLB' Sequence in Surry.

3.2.1 Definition of the Base Case.

In defining the base case for the present work, it was necessary to make a large number of assumptions concerning many of the relevant parameters. Some of the values chosen can be defended based upon other analyses, while some of the other choices required are somewhat arbitrary. It is believed that all of the values chosen lie within the respective uncertainty ranges of the parameters involved, but no claim is made that they represent best estimate values. Time and resources have not permitted sensitivity studies varying all of the potentially important parameters used to define the base case. Parameters held fixed throughout the present study will be summarized first, followed by parameters whose impact was investigated to at least a limited degree in sensitivity studies.

Parameters Not Varied. The in-vessel inventory of molten corium was assumed to be at a temperature of 2550 K and to include 80,000 kg of UO₂, 16500 kg total Zr, and 16500 kg steel. These quantities were taken from the specification of the CLWG problem SP-2 [NRC85]. At the time of vessel breach, about 320 kg of hydrogen was assumed to be present within containment, with an additional 110 kg being introduced as part of the blowdown following vessel breach. This quantity of hydrogen corresponds to that produced by in-vessel oxidation of 50% of the zirconium, plus about 70 kg produced by the in-vessel oxidation of steel. These values for in-vessel zirconium oxidation and hydrogen inventories are consistent with the results of typical calculations using the MARCH code [Wo80, Wo84], but there are substantial uncertainties in either direction concerning these quantities. Corium injection into the containment was assumed to occur over a period of five seconds, based upon recent modeling of the process of melt ejection from the pressure vessel [Pi85]. In estimating the surface area of the reacting drops (i.e., S'_d in Eq. 2.3b), it was assumed that metals and oxides were initially in separate drops (oxide drop surfaces not credited), but that Zr and steel (modeled as Fe) were intermixed. As in the Pilch model [Pi86a], Re in Eqs. 2.2 and 2.3 was evaluated assuming the gas-particle velocity to be equal to the particle terminal fall velocity, v_t , which was typically 5 - 7 m/s for a 0.5 mm debris drop.

The emissivity of the debris was taken to be 0.8, consistent with typical values for oxidic materials and heavily oxidized metal surfaces. All of the radiation from the debris was assumed to go to the gas rather than to structures, as side calculations have indicated that aerosol clouds associated with DCH [Ta86a] are expected to make the atmosphere quite opaque.

Parameters Varied in Sensitivity Studies. In the base case, it was assumed that 75% of the total in-vessel corium mass would be injected into the containment and would participate in DCH, while the remaining corium inventory was assumed not to participate in any fashion. Half of the zirconium was assumed to be oxidized in-vessel, rather than 30% as in CLWG SP-2. The drop diameter was 0.5 mm, in agreement with Surtsey and other experimental values of debris mass median diameters except that the experiments showed a wide range of drop sizes [Ta86a], which the present model can not accommodate. For each cell, the base case trapping rate, λ_{tr} , was taken to be $v_t/V^{1/3}$, where V is the cell volume, except that λ_{tr} was arbitrarily taken to be 0.2 in the cavity cell. The latter value was chosen because it implies little retention of debris in the cavity region, in agreement with several experiments [Ta84b, Ta86b]. Hydrogen produced by metal-steam reactions during DCH was assumed to recombine with any oxygen present in the same cell, and hydrogen was otherwise modeled with the CONTAIN default hydrogen burn options.

In modeling the drop-side reaction rate limits, a drop diffusivity of $10^{-8} \text{ m}^2/\text{s}$ and a reaction threshold temperature of 1200 K were assumed. The rationale for these choices is discussed in the Appendix.

Upon vessel breach, blowdown of steam and hydrogen was assumed to begin at the same time as the injection of corium debris into the containment. In the base case, blowdown was assumed to occur over a 30 second time period. During the first 15 seconds, the blowdown was assumed to include 8800 kg of dead-ended primary system water plus 12500 kg of highly super-heated steam. The superheat of the latter was more than sufficient to complete the vaporization of the water, yielding a net input of about 21000 kg of superheated steam during this period. This was followed by another 10000 kg of near-saturated steam during the next 15 seconds, which completed the blowdown. This blowdown history was based upon calculations with the MARCH code [Wo80] performed for the QUEST program [Li85]. The calculation utilized here is a relatively old one, however, and there was some ambiguity in extracting detailed primary

system sources from the MARCH calculation; thus, these sources may deviate substantially from what a more recent best-estimate calculation might give. Since the sensitivity studies to be presented here identify the blowdown sources concurrent with debris injection to be of high importance, these sources should be reassessed in future work.

Containment Failure Pressure. It is not the purpose of this study to assess whether DCH will or will not cause failure of the containments in any of the plants studied. Nonetheless, it is difficult to evaluate the significance of the results to be presented without some reference to estimates of the failure pressure, which has been rather extensively analyzed in the case of Surry. The SARRP risk reassessment study employed a central estimate of the failure pressure for Surry equal to about 9.2 bars [Bn87b]. However, it was acknowledged that there is considerable uncertainty in this estimate. SARRP also carried out a Monte Carlo uncertainty study on the Surry risk using Latin hypercube sampling (LHS) techniques, with the containment failure pressure being one of the parameters sampled. In the LHS study, containment failure pressure values in the range 6.9 to 10.9 bars received about 95% of the total sampling weight [Bn87a]. Sample weights in that study were based upon the opinions of an expert review group, and the review group made it clear that these weights should not be equated to confidence limits. Nonetheless, a large amount of detailed containment analysis information provided considerable technical basis for the experts' judgments on this question. Hence, for present purposes, it seems reasonable to treat any pressure below about 7 bars as representing a rather minimal threat, while pressures above nine bars must be considered a serious threat.

3.2.2 Single-Cell Calculations.

As will be shown in Section 3.2.3, single-cell representations of the containment can not lead to realistic DCH calculations. Nonetheless, the results of such calculations, and their comparison with other calculated results, can illustrate some potentially important phenomenologies. In Fig. 3.1, pressure-time histories are given for single-cell calculations for four alternative assumptions affecting the release of chemical energy. In the figure, times are measured from the time of reactor shut-down; vessel breach is at 9375 seconds. Curve (b) gives the results for the base case. It represents a very severe threat, over two bars above the SARRP "central"

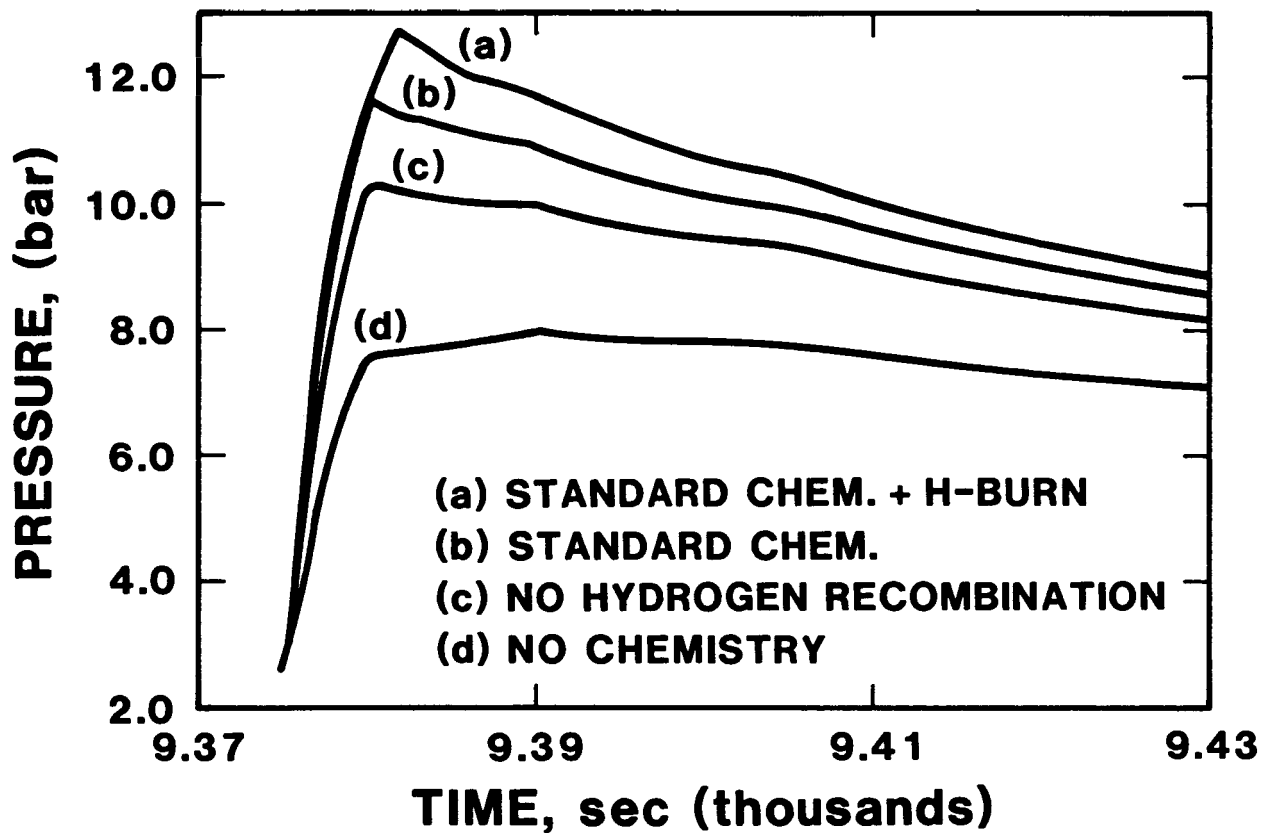


Fig. 3.1 CONTAIN calculations of DCH pressures in Surry for various chemistry assumptions, using a single-cell representation of the containment.

estimate of the Surry failure pressure (9.2 bars). Switching off the hydrogen recombination (curve (c)) drops the peak pressure by over a bar, because a substantial fraction of the total metal oxidation is due to reaction with steam even though oxygen is present, and full realization of the potential chemical energy release requires recombination of the hydrogen produced. Eliminating all chemical reactions (curve (d)) reduces peak pressures to under eight bars. On the other hand, overriding the default CONTAIN hydrogen burn parameters to permit all hydrogen (including the pre-existing hydrogen) to burn raises the pressure to almost 13 bars (curve (a)). These results indicate the large degree to which the potential DCH threat is dependent upon the release of chemical energy and its efficient transfer to the containment atmosphere.

In Fig. 3.1, it may be noted that the peak pressure in all cases arises at about the time that debris injection ceases except in the case without chemistry, in which the pressure continues to rise due to the continued injection of blowdown steam (less than 25% of the total blowdown occurs during the five-second debris injection period in this problem). For the other cases, the higher temperatures achieved result in more rapid heat transfer from the atmosphere to the heat sinks, and this effect dominates the effect of the continuing blowdown.

It is instructive to compare the results of the single-cell calculation with the results of adiabatic calculations performed using the DHEAT2 code, an improved version of the DHEAT adiabatic code used in the CLWG work [Be86a] discussed in Section 2.1. These results are compared in Table 3.1. Two sets of DHEAT2 results are included: those calculated with all steam and hydrogen from the vessel blowdown assumed to be present in the atmosphere and those with only 25% of the blowdown steam and hydrogen; the latter approximately corresponds to that portion of the blowdown occurring before the end of debris injection in the CONTAIN calculation. As expected from the preceding discussion of the CONTAIN results, the DHEAT2 results calculated with all the blowdown steam and hydrogen present imply pressures considerably higher than the CONTAIN results. On the other hand, the DHEAT2 results calculated with only 25% of the total blowdown in the atmospheric inventory are not much more severe than the CONTAIN results. This suggests that, in the single-cell

Table 3.1
Surry Single-Cell Calculations
Maximum Pressures (bars)

Case	CONTAIN	DHEAT2	
		100% Blowdown	25% Blowdown
a) All H ₂ Burns	12.7	15.0	13.2
b) Standard Chemistry	11.6	13.7	12.1
c) No H ₂ Recombination	10.2	(Option not available)	
d) No Chemistry	7.9	8.8	7.7

representation, mitigation due to heat transfer during debris injection is not very effective, nor is there a large amount of mitigation associated with CONTAIN's more realistic modeling for reaction rates and debris-gas heat transfer and the nominal trapping rate given by Eq. 2.1.

In the DCH calculations performed for the CLWG [NRC85, Be86a] which were discussed in Section 2.1, the blowdown steam was included in the total inventory of atmospheric gas. Furthermore, it was generally assumed there that the thermal energy of any corium not participating in DCH would simultaneously go into the generation of steam due to water quench, yielding still higher pressures. Hence, it was not surprising that this earlier work yielded a rather pessimistic picture concerning the potential threat of DCH to containment integrity. Since the only non-adiabatic calculations performed at that time employed single-cell representations of the containment, it was also not apparent that non-adiabatic effects could, by themselves, provide a large degree of mitigation. While it was recognized that these treatments probably were excessively conservative, no quantitative means of allowing for these conservatisms were available at that time.

3.2.3 Multi-Cell Sensitivity Studies.

In order to obtain more realistic results, a 5-cell model of the Surry plant was used, with containment nodalization and flow paths as indicated in Fig. 3.2. Both the debris and the blowdown steam and hydrogen are injected into the small cavity cell (Cell 1), and the principal flow path to the upper containment (Cell 3) is through the basement cell, Cell 2. The latter is the location of the steam sources from the primary system prior to vessel breach and is therefore oxygen-poor even before vessel breach.

The nodalization indicated in Fig. 3.2 still provides only a highly simplified representation of the actual containment geometry, which is extremely complex. Sensitivity to nodalization has not been investigated in the work to be reported here, except for comparisons with the one-cell calculations. It is clearly a potentially important source of uncertainty, however, and it should be investigated in the future.

The solid curve in Fig. 3.3 gives the results of applying the base case assumptions to the 5-cell Surry model. The other curves explore the

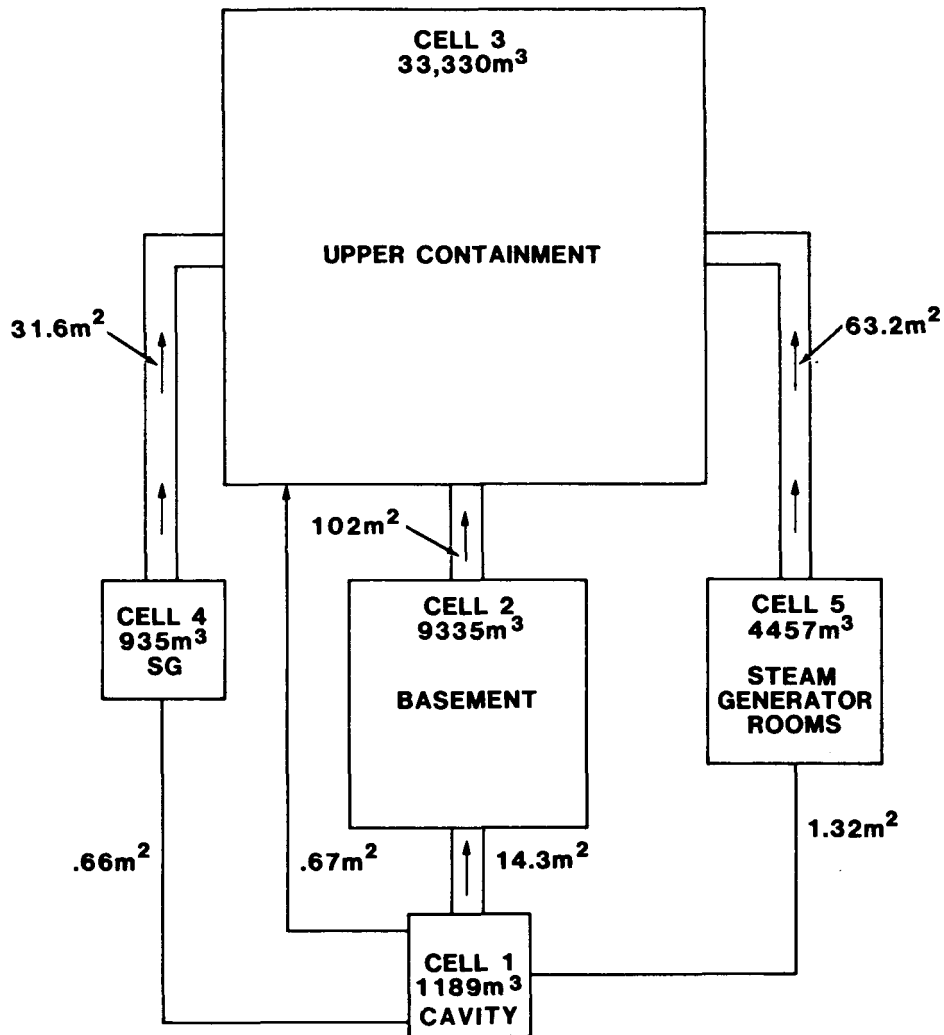


Fig. 3.2 Five-cell nodalization of the Surry containment used in the CONTAIN DCH calculations.

sensitivity to trapping, with λ_{tr} being varied from zero to ten times the base case values. Introducing containment compartmentalization reduces the peak pressures by over 4 bars in the base case (cf. curve (b) in Fig. 3.1), with the threat to containment integrity now appearing to be marginal at worst. Obviously, it is important to understand the reasons for this reduction, in order to determine the degree to which this dramatic mitigation effect is sensitive to unproven assumptions made in the calculation.

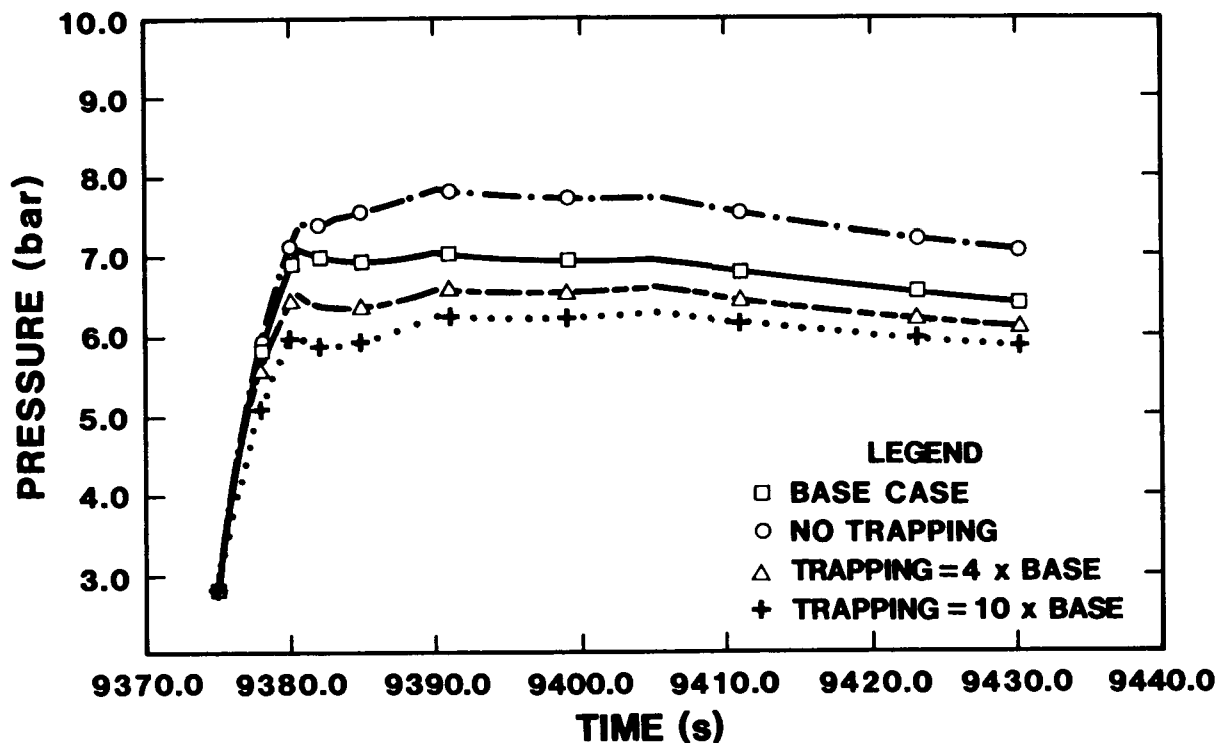


Fig. 3.3 CONTAIN 5-cell calculations of the pressure-time histories for four different values of the trapping rate. Times are referenced to reactor shutdown; vessel breach is at 9375 seconds.

Some insight may be obtained by reviewing some of the characteristic time scales and other governing parameters derived from the base case as summarized in Table 3.2. The trapping time scale, τ_{tr} ($= 1/\lambda_{tr}$) is seen to be comparable to, or somewhat less than, the mean debris residence time as determined by gas flow, τ_{fl} ; note especially the values for Cell 2. Hence, even the rather low base case trapping rates are adequate to substantially reduce the amounts of debris reaching Cell 3. On the other hand, the time scales for chemical reaction, τ_{rx} , are much shorter, and the time scales for debris-gas heat exchange are shorter still. Hence, large increases in trapping rates would be required in order to greatly reduce either the amount of chemical reaction or the amount of debris-gas energy transfer, and the calculated results are not very sensitive to moderate increases in trapping over the base case.

Table 3.2

Surry Base Case Chemistry and Debris Transport Characteristics

Cell	Residence Times (sec.)			Debris T(K)	Atmosphere Mole Fractions		
	τ_{tr}	τ_{fl}	τ_{rx}		O ₂	H ₂	H ₂ O
1	5.0	0.51	0.28	2540	0.0	0.57	0.43
2	3.1	1.8-9.0	0.28	2010	0.0	0.41	0.57
3	5.8	-	(∞)	840	0.050	0.055	0.70
4	1.7	(>10)	0.29	1840	0.10	0.11	0.30
5	3.2	(>10)	0.30	1310	0.14	0.041	0.27

Temperature histories for the base case are presented in Fig. 3.4. The extreme gas temperatures in Cells 1 and 2 (about 2500 and 2000 K, respectively), together with the relatively high surface/volume ratio of these smaller cells, lead to correspondingly rapid heat losses. Once debris

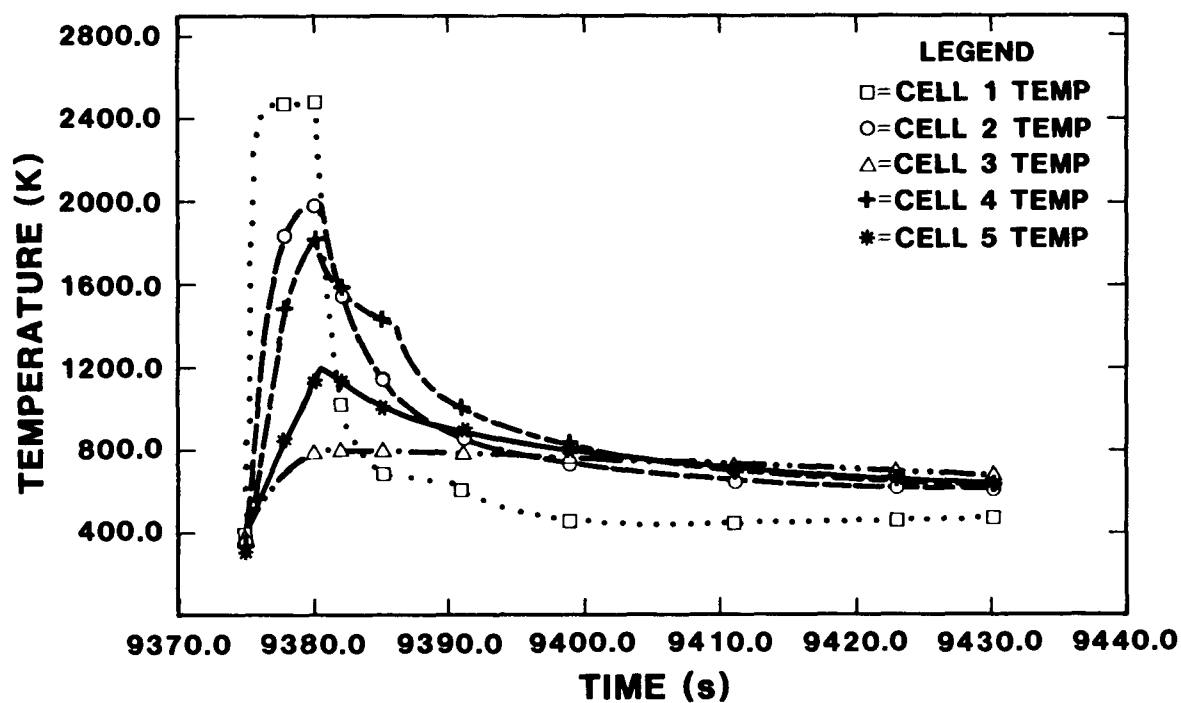


Fig. 3.4 Atmospheric temperatures calculated for the Surry base case DCH scenario.

injection stops, this effect prevents further transport of mass and energy to the upper containment, despite the continuing blowdown from the primary system. Hence there are no further pressure rises in the base case, and only moderate rises in the unrealistic no-trapping case. At the very high temperatures which occur during debris injection, much of the total thermal energy in these cells resides in the debris: 80-85% of the "atmospheric mass" in Cell 2 during this time actually consists of debris. Since the thermal energy can cause pressurization only insofar as it is transferred to gas, pressure rises are substantially reduced (relative to the one-cell case) by the lack of an adequate atmospheric heat sink in the superheated lower cells and the inability to transport this energy to the upper containment before much of it is lost to the lower-cell structures. Trapping increases this effect, but it is not the dominant influence.

The last three columns of Table 3.2 give the atmospheric compositions of the various cells at a time near the end of the debris injection period. The atmosphere in Cells 1 and 2 is roughly half hydrogen, because of rapid metal-steam reactions. The high diffusivity and high thermal conductivity associated with these hydrogen-rich atmospheres contributes to the very rapid reaction rates and heat transfer rates noted above. Since oxygen is almost immediately depleted in these cells, reaction is with steam only; due to the rapid reaction rates, relatively little metal reaches the cells which do contain oxygen. Since the Zr-steam reaction releases only about 56% as much energy as the Zr-oxygen reaction, and the energy release of the iron-steam reaction is very limited, the dominance of steam as the oxidant provides still another mitigating effect, relative to the single-cell calculation.

Oxygen is present in Cells 3, 4, and 5, but the hydrogen concentrations are too low and/or steam concentrations too high to meet the CONTAIN default burn criteria except in Cell 4. A burn does initiate in this cell during debris injection. However, this cell is too small for the burn to contribute significantly to the overall containment pressure.

Table 3.3 summarizes important data from a sensitivity study on the 5-cell Surry nodalization, including maximum pressures in the upper containment, maximum gas temperatures in Cells 2 and 3, and hydrogen production and distribution data. Case 1 in the table is the base case discussed above, while Cases 2-4 are the cases which explore the sensitivity to trapping rate.

Table 3.3
Summary of CONTAIN 5-Cell DCH Sensitivity Study
Cases with the notation "UCHB" were run using the
unconditional hydrogen burn option

Run		P _{max}	T _{max}	(K)	H ₂ After Injection, kg		
No.	Variations From Base Case	(bars)	Cell 2	Cell 3	Cells 1 + 2	Cell 3	Net Produced
1	Base Case	7.2	1990	800	450	440	590
2*	No Trapping	7.9	2020	860	490	450	630
3*	$\lambda_{tr} = 4\lambda_{tr}(\text{base})$	6.7	1890	750	390	420	500
4*	$\lambda_{tr} = 10\lambda_{tr}(\text{base})$	6.4	1750	700	310	390	380
5	No H ₂ Recombination	7.1	1990	800	460	460	610
6	E-Error Fix	7.0	1900	785	-	-	-
7	Unconditional H ₂ -Burn	9.3	1980	1160	520	-	-
8	UCHB, No Trapping	9.8	2010	1180	550	-	-
9	UCHB, $\lambda_{tr} = 4\lambda_{tr}(\text{base})$	8.8	1890	1110	450	-	-
10	UCHB, $\lambda_{tr} = 10\lambda_{tr}(\text{base})$	8.4	1740	1060	360	-	-
11	UCHB, E-Error Fix	9.1	1900	1130	520	-	-
12	UCHB (10-Sec. Duration)	9.3	1980	1170	490	-	-
13	UCHB at 9380 Sec.	9.6	1980	1220	480	-	-
14*	1-mm Particles	6.9	1910	780	350	390	400
15	UCHB, 1-mm Particles	9.0	1920	1120	390	-	-
16	10-Second Blowdown	9.5	1780	960	360	560	570
17	UCHB, 10-Sec. Blowdown	12.3	1790	1380	430	-	-
18	2x10 ⁴ Kg Cavity Water	8.8	1430	850	320	560	510
19	Cavity Water, UCHB	11.6	1440	1270	370	-	-
20*	Chem. rx. thresh = 400 K	7.2	1990	810	460	460	610
21*	No Trapping and D _d = ∞	7.9	1960	860	480	480	650
22*	Baker Diffusivity	7.0	1970	790	390	410	490
23	30% In-Vessel Zr Ox.	7.4	2080	830	520	460	680
24	30% Zr Ox., UCHB	9.5	2080	1180	590	-	-
25	Case 24, Adjusted H ₂ Inventory	9.1	2080	1100	550	-	-

Table 3.3 ... continued
Summary of CONTAIN 5-Cell DCH Sensitivity Study

Run No.	Variations From Base Case	$P_{\max}$	$T_{\max}$	(K)	H_2 After Injection, kg		
		(bars)	Cell 2	Cell 3	Cells 1 + 2	Cell 3	Net Produced
26	50% Core Injection	6.5	1760	730	310	390	380
27	25% Core Injection	5.9	1420	630	170	340	180
28	50% Injection, UCHB	8.5	1760	1060	360	-	-
29	25% Injection, UCHB	7.6	1430	960	200	-	-
30	C106, Cess-Lian Emiss.	7.0	1920	790	450	450	590
31	C106, Modak Emiss.	6.8	1840	770	460	440	590
32	C106, Cess-Lian, UCHB	9.1	1920	1140	520	-	-
33	C106, Modak, UCHB	8.9	1830	1110	520	-	-

* Small approximate corrections applied for H_2 -recombination error.

Effect of Hydrogen Recombination. Case 5 gives results for the base case with hydrogen produced by metal-steam reactions no longer assumed to combine with any oxygen present in the cell. In contrast with the single-cell treatment, the hydrogen recombination assumption now makes little difference (< 0.1 bar in the peak pressure) because the great majority of the hydrogen generation now occurs in cells which contain no oxygen. (As noted previously, a code error initially disabled the hydrogen recombination option, and many of the calculations performed in this work had been run by the time this error was discovered. Rather than rerun the considerable number of calculations involved, a small correction (<2%) equal to the difference between Case 1 and Case 5 results was applied to those cases which were similarly affected; these cases are marked with an asterisk in Table 3.3.)

Effect of the Error in the Energy Accounting. After most of these calculations had been performed, it was discovered that there was an inconsistency

in the treatment of reaction energies in the DCH model. The net effect was to introduce extra energy approximately equal to the latent heat of that steam which is consumed by chemical reaction. Case 6 in Table 3.3 illustrates the magnitude of its impact; it was run with the error fixed but with modeling otherwise essentially the same as in the base case. The effect is to reduce the peak pressure by about 0.22 bar, an amount which is not entirely negligible but which is small compared with the more important of the effects to be discussed here. In this case, applying a correction was judged to risk introducing as much error as it might remove. Hence, it should be remembered that this error is present in all the cases in Table 3.3 except those for which either the entry "E-error fix" or "C106" appears ("C106" refers to CONTAIN 1.06, in which the error was fixed). It is believed that the error will not significantly impact the trends as other parameters of interest are varied, but it does mean that the actual pressures given could be up to a few tenths of a bar too high.

Effects of Hydrogen Combustion. The last column of Table 3.3 indicates that, in the base case, almost 600 kg of hydrogen have been produced during and just after the 5-second debris injection period. This rate of hydrogen production is unusual in reactor safety analyses, and would tend to defeat such hydrogen mitigation schemes as igniters and catalytic recombiners. At the end of debris injection, substantial portions of this hydrogen still reside in Cells 1 and 2, where there is no oxygen, but equal portions reside in Cell 3, which does contain oxygen even though it is steam inert by the normal criteria (Table 3.2, last three columns). As can be seen from the cases with the variations in the trapping rate (Cases 2-4 in Table 3.3), large changes in trapping had only moderate impact upon hydrogen production, as expected from the preceding discussion of reaction rates.

During debris injection, Cell 3 temperatures rise to about 800 K and there is a flow of 3000 - 8000 kg/s of steam, hydrogen, and debris entering at temperatures of up to 2000 K from Cell 2. These harsh conditions justify serious skepticism as to whether the hydrogen and oxygen in Cell 3 will actually be prevented from reacting by the 70% steam concentrations, as assumed by the default burn criteria. It is at least plausible that conditions permitting hypergolic hydrogen combustion will develop as the entering hydrogen mixes with the oxygen-containing atmosphere of the upper containment. In order to explore the implications of this possibility, calculations were

run for the base case and the variations with altered trapping rates using the unconditional burn option discussed in Section 2.2.2. Burn parameters were prescribed to permit burns to initiate starting 2 seconds after vessel breach, at any time and location where both hydrogen and oxygen were present, independently of their concentrations or the concentration of steam. Burn duration was prescribed to be 5 seconds in the upper containment and in Cell 5, and 3 seconds in the other cells. With this treatment, hydrogen combustion in any cell was limited only by the complete consumption of one of the two reactants.

Results of the calculations with the unconditional burn option are summarized in Table 3.3 (Cases 7 - 10) and are compared with the corresponding cases assuming default burn parameters in Fig. 3.5, except that the figure does not include the no-trapping cases. Peak pressures are increased by two bars or more, and lie well within the uncertainty range for failure pressure. The effect of the hydrogen combustion is substantially larger than the effects of the factor-of-ten variation in trapping rates.

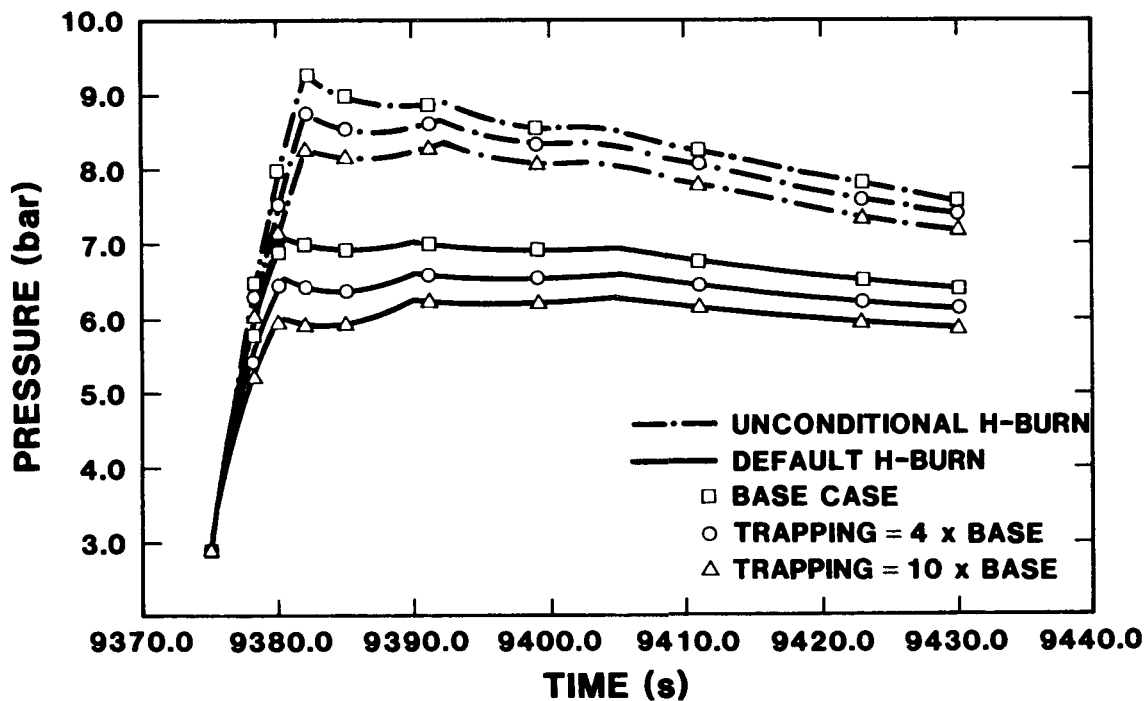


Fig. 3.5 Calculated pressure-time histories for different trapping rates and alternative assumptions concerning hydrogen combustion.

As a check, the base case with unconditional hydrogen burn was rerun after the energy accounting error had been fixed, with results given as Case 11 in Table 3.3. It is evident that the error has little impact on the main conclusions to be drawn from the various results presented.

There can be some sensitivity to the timing parameters of the unconditional hydrogen burns. Case 12 gives results obtained when the prescribed burn time in Cell 3 was changed from 5 seconds to 10 seconds, while Case 13 gives results obtained when the prescribed time for burn initiation was changed from 2 seconds after the initiation of debris injection to 5 seconds after initiation (i.e., at the time injection terminates). The first change had a trivial impact, but the second was of some significance, with maximum pressures being increased by about 0.3 bar. Presumably the reason is that the delay in burn initiation permits more hydrogen to enter the cells which do contain oxygen.

Since the potential effects of the hydrogen burns are so significant, many of the other parameter variations to be discussed below were run with both the default burn and the unconditional burn options.

Effects of Drop Size. Calculations were performed assuming 1-mm debris drops, which reduces reaction rates by a factor of almost four in this model. The input trapping rate was also approximately doubled, to represent the increase in v_t . Despite the large shift in the relative time scales of reaction and trapping, results were not greatly changed, as can be seen in Fig. 3.6 and Table 3.3 (Cases 14 and 15). The effect of the particle size is swamped by the uncertainty in hydrogen phenomenology.

Effects of Blowdown Steam and Cavity Water. It was earlier suggested that the large mitigating effects found in the 5-cell treatment relative to the single-cell calculations could be attributed to a number of interrelated factors which include the following:

1. Limited atmospheric mass in the lower compartments, which meant that much of the debris thermal energy remained in the debris and was thus unavailable for containment pressurization.
2. Extreme temperatures in the lower compartments, leading to very rapid losses of energy to the structures.

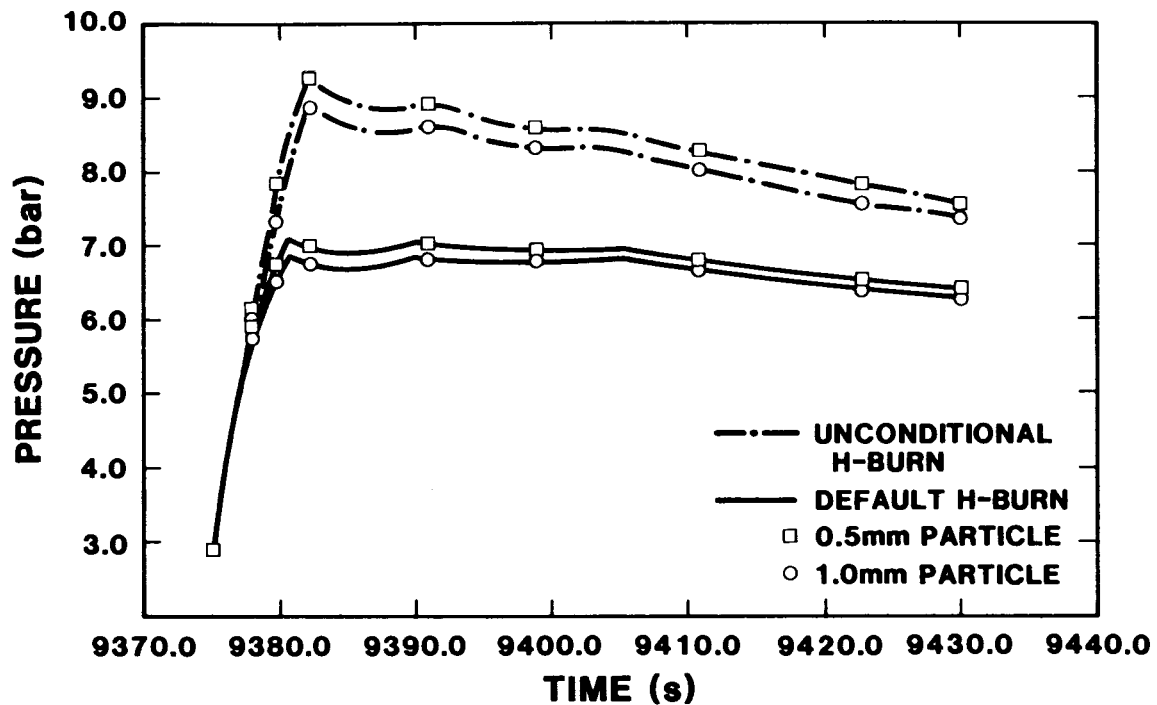


Fig. 3.6 Calculated pressures for different debris particle sizes and alternative assumptions concerning hydrogen combustion.

3. Limited rates of transport to the upper containment, which contains both the main atmospheric heat sink and the main reservoir of oxygen.
4. Reduction of the chemical energy release, due to consumption of metals by steam reactions in the oxygen-starved lower compartments.

The first three of the above mitigating effects would be reduced if more steam were to be introduced simultaneously with the debris, since there would be a greater atmospheric mass to which the debris could transfer its energy, reduced temperatures would lead to reduced heat loss, and flow rates to the upper containment would be greater. These considerations suggest that the maximum loads developed could be sensitive to the details of the vessel blowdown history, which is quite uncertain.

Calculations were performed assuming a vessel blowdown rate three times as high as in the base case (i.e., complete within 10 seconds). Comparisons with the base case (Fig. 3.7 and Case 16, Table 3.3) show there is indeed a major increase, over two bars, in the peak pressure. Furthermore, there is a synergism between more rapid blowdown and possible hydrogen burns: the improved energy transport increases the Cell 3 temperature, which presumably makes combustion more likely, and the improved transport also increases the Cell 3 hydrogen inventory. Imposing the unconditional burns upon the rapid blowdown scenario (Case 17 and Fig. 3.7) therefore yields an especially severe result, with pressures of about 12 bars; the mitigating effects associated with containment compartmentalization are largely eliminated in this instance, as the extreme pressures seen in curve (a) of Fig. 3.1 are approached.

It is important to understand that increased transport of debris to the upper containment does not play a dominant role in the augmented loads associated with the accelerated blowdown scenario. To investigate this question, a calculation (not listed in Table 3.3) was performed which was

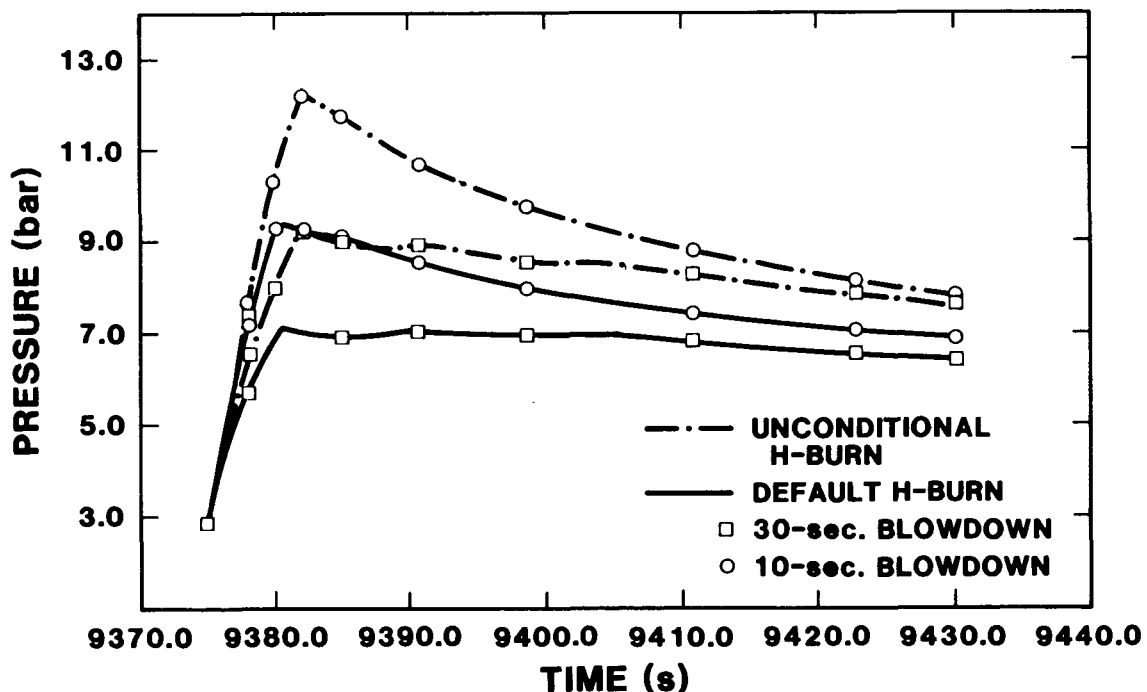


Fig. 3.7 Pressures calculated for different primary system blowdown rates and for alternative assumptions concerning hydrogen combustion.

identical to Case 16 except that the trapping rate in Cell 2 was increased by a factor of four. This change resulted in the amount of debris transported to Cell 3 being the same as in the base case, i.e., the effect of the accelerated steam flow upon debris transport was just compensated for by the effect of the accelerated trapping in Cell 2. The result was to reduce the calculated pressures by only 0.28 bar relative to Case 16, which is still two bars higher than the base case even though the amount of debris reaching the upper containment is the same as in the base case. Furthermore, this 0.28 bar reduction represents an upper bound for the possible importance of increased debris transport in Case 16, since the accelerated trapping in Cell 2 also reduces chemical and thermal interactions in that cell, which contributes to the total reduction in pressure obtained.

These results show that less than 15% of the total effect of the more rapid blowdown is due to improved transport of debris. The dominant effects are due to increased steam masses for debris-gas heat transfer in the lower containment, and increased flow of the resulting superheated steam and gas to the upper containment (plus hydrogen transport, in the unconditional burn scenario). Throughout this report, there will be repeated emphasis on "energy transport," not "debris transport." The principal vehicles for this energy transport are superheated gas and steam and, if it can burn, hydrogen. No cases have been identified in which the rate of debris transport to the upper containment appears to be the dominant factor governing the calculated pressures. (Among other things, this conclusion means that results are not sensitive to any tendency of the IDHM to overestimate intercell debris transport due to the model's neglect of particle-gas slip.)

Clearly, best-estimate assessments of DCH threats will require best-estimate evaluations of the blowdown occurring at and immediately after the time of debris injection. The blowdown is governed primarily by the end point of the in-vessel phase of the accident, the analysis of which is outside the scope of the present work. It is hoped that blowdown calculations based upon state-of-the-art analyses of the in-vessel phase will be available for DCH calculations in the future [Be86b].

The preceding results suggest that conventional thinking concerning the effects of cavity water which could be co-dispersed with the debris may require some modification. Hitherto, co-dispersed water has been almost

universally regarded as a potential mitigating factor due to its quenching effect, with debate limited to the question of whether water and debris will be sufficiently co-located to permit the required heat transfer. However, the steam so generated could act similarly to the increased steam supply in the rapid blowdown, though the need to supply the latent heat of vaporization would reduce the available energy. To examine this tradeoff, the base case was run with 2×10^4 kg of cavity water assumed to be dispersed along with the debris, with no heat transfer limitations other than heat transfer rates from the debris. The postulated co-dispersal of the cavity water increased resulting pressures from 7.2 bars to 8.75 bars in the case without unconditional hydrogen burns (Case 18 in Table 3.3), and from 9.3 bars to 11.6 bars with the burns (Case 19). Evidently, vaporized cavity water can produce much the same effect as the more rapid blowdown, with only a moderate reduction in the effect due to the need to supply the latent heat.

The potential effects of water in the containment have been the subject of considerable discussion in connection with DCH scenarios. A separate sensitivity study of this subject was therefore carried out, with results discussed in Section 3.3. As will be shown there, the effects of co-dispersed water are quite sensitive to the timing and location of water injection, the drop-side reaction rate limits, and the amount of water involved.

Sensitivity to Drop-Side Reaction Rate Limits. In Cases 20-22 of Table 3.3, some sensitivities involving the drop-side reaction rate limitations are examined. In Case 20, the reaction threshold was effectively eliminated by setting it equal to 400 K, while in Case 21, the drop-side reaction rate limit was eliminated by setting the diffusivity equal to infinity in the calculation with zero trapping (compare with Case 2). Even though the latter change increased reaction rates by a factor of about three, the overall impact of both these changes was slight because reaction was already nearly complete. Case 22 gives results obtained by imposing the drop diffusivity suggested by Baker [Ba86], which in CONTAIN can be represented using a diffusivity given by

$$D_d = 1.274 \times 10^{-4} e^{-22647/T_d}, \quad (3.1)$$

where D_d is the diffusivity of the debris particle (in m^2/s) and T_d is the temperature of the debris. This expression yields reaction rates that are strongly temperature-dependent and that are lower than the base case value for

any temperatures below about 2400 K; Eq. 3.1 is based largely upon extrapolations of solid-state oxidation studies and its use may underestimate reaction rates for molten drops. (See the Appendix for additional discussion of melt diffusivities and related questions concerning drop-side reaction rates.) Again, only minor changes in the peak pressure arise, and even the hydrogen generation was not greatly affected.

The reason that the base case calculation is little affected by substantial variations in the drop-side reaction rate limitation is that temperatures in Cells 1 and 2, where most of the reaction occurs, are so high. It is likely that any reasonable model for reaction rates would give a high degree of reaction for these conditions. It is possible that sensitivity to reaction rates would be greater for trapping rates higher than those assumed in the base case, but this possibility has not been investigated.

It is, however, clear that sensitivity to drop-side reaction rates can be important in scenarios in which atmospheric temperatures are lower, as is the case for the scenarios with cavity water and, to a lesser extent, scenarios involving the more rapid blowdown. Examples involving cavity water will be discussed further in Section 3.3, with conclusions that differ strikingly from those which might be drawn considering the response of the base case alone.

In-Vessel Zirconium Oxidation. Calculations were run assuming that only 30% of the zirconium would be oxidized in-vessel, as in CLWG SP-2. Case 23 in Table 3.3 gives results obtained assuming default hydrogen burn parameters. Comparison with the base case shows that the increased energy release associated with the additional zirconium has only a minor effect. The reason is that the lower compartments are almost "thermally saturated" in the sense that most of the thermal heat capacity in these cells is in the debris and, hence, most of the extra energy remains in the debris and thus does not cause additional pressurization. For the same reason, this additional energy release does not make transport of either energy or hydrogen to the upper containment substantially more efficient.

Cases 24 and 25 give results for the 30% in-vessel zirconium oxidation case with unconditional hydrogen burns. Case 24 was run assuming the same containment hydrogen inventories prior to vessel breach as in the base case, and comparison with Case 7 shows that, again, there is only a slight increase

in peak pressure due to the higher zirconium content of the melt. In Case 25, which may be more realistic, the inventories of hydrogen in all cells of the containment, and in the blowdown, were reduced in proportion to the reduced hydrogen production implied by assuming 30% in-vessel Zr oxidation instead of 50% as in the base case. In this calculation, the peak pressure is actually slightly less than in Case 7.

Sensitivity to Mass of Injected Corium. The sensitivity of the calculated results to the core fraction injected into the containment is investigated in Cases 26 - 29, which give results with and without unconditional hydrogen burns and for injection fractions of 50% and 25%. Without the unconditional hydrogen burn, there is only a moderate sensitivity to the injection fraction, considerably less than implied by earlier single-cell calculations [NRC85]. Again, saturation of the atmospheric heat capacity in the lower compartments is a major factor; that is, once the amount of injected debris exceeds a moderate fraction of the core inventory, most of the energy associated with further increases in the injection fraction remains in the debris. With unconditional hydrogen burns, sensitivity to injection fraction is somewhat greater because reducing the injection fraction also reduces the hydrogen production. It remains true, however, that quite substantial reductions in the injection fraction are required in order to make a qualitative change in the severity of the potential threat.

By comparing the cell temperatures calculated for Cases 26 and 27 with the base case values, it is seen that reducing the injection fraction leads to somewhat less extreme Cell 3 thermal environments, both in terms of the temperature in Cell 3 itself and in terms of the material entering Cell 3 from Cell 2. This reduction in temperatures could mean that the actual hydrogen behavior would trend away from the unconditional burn behavior and toward the default burn behavior as the injection fraction is reduced, which would increase the sensitivity of the actual peak pressures to the injection fraction. This effect, which could be important, is beyond the capability of the current treatment to model, except in a purely parametric sense.

Sensitivity to Gas-Structure Heat Transfer. Sensitivity to uncertainty in the radiant heat transfer between the atmosphere and the structures has been examined by comparing results obtained using the Cess-Lian [Ce76] and the Modak [Mo79] models. These calculations were run on CONTAIN 1.06 (designated

"C106" in Table 3.3), both with default burn parameters (Cases 30 and 31) and with the unconditional burn parameters (Cases 32 and 33). It is apparent that the effects are not large, despite the fact that the Modak model yields significantly higher steam emissivities at the temperatures involved. By comparing the Cess-Lian results using CONTAIN 1.06 with the results obtained using CONTAIN 1.04 with the energy inconsistency error fixed (Cases 6 and 11), it can be seen that other modeling changes involved in the CONTAIN 1.06 upgrade had little impact upon this particular problem.

The CONTAIN correlations for convective energy transport from the gas to the structures that were used here are the default correlations based upon natural convection. It is likely that they underestimate heat transfer rates in the current scenario for several reasons: they do not adequately treat the enhanced thermal conductivities associated with hydrogen-rich atmospheres, and high flow velocities existing in at least part of the containment have been neglected. In addition, there is no accounting for the fact that the superheated atmosphere of the lower compartments includes a dense dispersion of debris which actually includes most of the mass of the "atmosphere", which could increase heat transfer rates. Sensitivity to these effects has not been investigated, but it is apparent from the other results presented here that a substantial increase in heat transfer rates in the lower containment would be required in order to have a dramatic impact upon the outcome. In general, the results are considerably less sensitive to energy transfer to/from the lower containment than they are to factors altering the amount of energy transferred to, or released in, the upper containment. This lack of sensitivity is due to the thermal saturation effects arising in the lower containment that were discussed above in connection with the injected core fraction and the zirconium content of the debris.

3.3 Sensitivity Studies Involving Co-Dispersed Water.

3.3.1 Problem Definition.

As noted in the preceding section, the possible impact of water co-dispersed with the debris has been the subject of considerable discussion in connection with DCH. It has usually been invoked as a potential mitigating effect; however, the results given above showed that, under some conditions, the reverse can be true. In the particular scenario considered there, the

steam generated by the partial water quench improved transport of energy (including chemical energy in the form of hydrogen) to the upper containment. This improved transport reduced the mitigation otherwise associated with containment compartmentalization to a degree that overwhelmed the intrinsically mitigating effect of the debris quenching. However, it will be seen here that the impact of co-dispersed water is itself sensitive to a number of parameters, and any conclusions concerning this impact must be heavily qualified by proper consideration of these sensitivities.

For this portion of the study, a developmental version of CONTAIN 1.06 which includes the IDHM updates was employed. The Modak model for steam emissivities was also employed. Hence, pressures calculated are expected to be up to 0.5 bars lower than would be given by analogous calculations using the code version employed in calculating most of the results summarized in Table 3.3. For the co-dispersed water study, a base case was defined which differed from the base case used in Section 3.2 only in that it was assumed that 20000 kg of near-saturated water was injected into the Cell 1 atmosphere simultaneously with the debris, i.e., injected continuously during the same five-second period over which the debris was injected. (The quantity of water postulated was chosen to provide a useful starting point for the sensitivity studies; it does not correspond to any particular estimate of the quantity that might actually be involved.) Except for the code changes, this is the case treated in Case 18 of Table 3.3.

This water injection scenario maximizes the opportunity for debris-water interaction, since the time and location of water injection coincides with debris injection. In addition, the water was introduced as a low-quality steam, with a low enthalpy corresponding to that of the liquid, which means that instantaneous thermal equilibration between the liquid and the atmospheric gas is assumed in the calculation. Hence, any effects upon gas-water heat transfer due to the finite size of the liquid water drops was not included. It has been argued [Po86] that the drop size of co-dispersed water will be substantially smaller than that of the debris, in which case neglect of the finite size of the water drops should not introduce significant error in the rate of debris-water heat transfer, i.e., the debris-gas heat transfer should be the rate-controlling process. Likewise, "trapping" of dispersed water is neglected. Should the effects neglected prove important, the mass of water injected in the present study may still be thought of as the mass of

water which actually does participate effectively in energy exchange with the debris (i.e., which does vaporize), with this mass being smaller than the water mass actually present. Any additional water which may be present but which does not vaporize is not expected to have an important impact upon the problem.

The sensitivity of the results to the amount of water involved will be explored first in the next subsection, with several other important sensitivities being examined in Section 3.3.3. An important related uncertainty, the possible quench of trapped debris in water pools, will be considered in Section 3.3.4. Until the results of Sections 3.3.3 and 3.3.4 have been considered, no conclusions should be drawn from the results for the dependence upon water mass alone.

3.3.2 Sensitivity to Mass of Participating Water.

Maximum Pressures. Perhaps the most obvious sensitivity to investigate is the response as a function of the mass of water participating. Peak pressures generated are plotted as a function of water mass in Fig. 3.8, for both the default hydrogen burn parameters and the unconditional burn scenarios. In both cases, the pressure obtained initially rises rather rapidly as a function of injected water mass and reaches a maximum for about 20000 kg. For the default burn case (in which no significant burns occur), the maximum is quite broad, with substantial declines only for quite large masses (≥ 50000 kg). The unconditional burn case shows similar behavior except for a fairly small but sharp drop between 20000 and 25000 kg of water injected. The reason for this drop will be explained below. For a wide range of co-dispersed water masses, the unconditional burn scenario yields quite severe results.

Temperatures. Although Fig. 3.8 shows that the effect of co-dispersed water is potentially significant, it also provides a reminder that the impact of hydrogen combustion phenomenology may be even more important. By itself, therefore, Fig. 3.8 is potentially misleading because the co-dispersed water also heavily affects the thermal parameters which largely govern the credibility of the hypergolic combustion assumption which the unconditional burn option is intended to simulate. To illustrate this point, temperatures in Cells 1, 2, and 3 are plotted as a function of water mass for the default burn scenario in Fig. 3.9. Both atmospheric gas and bulk debris temperatures are

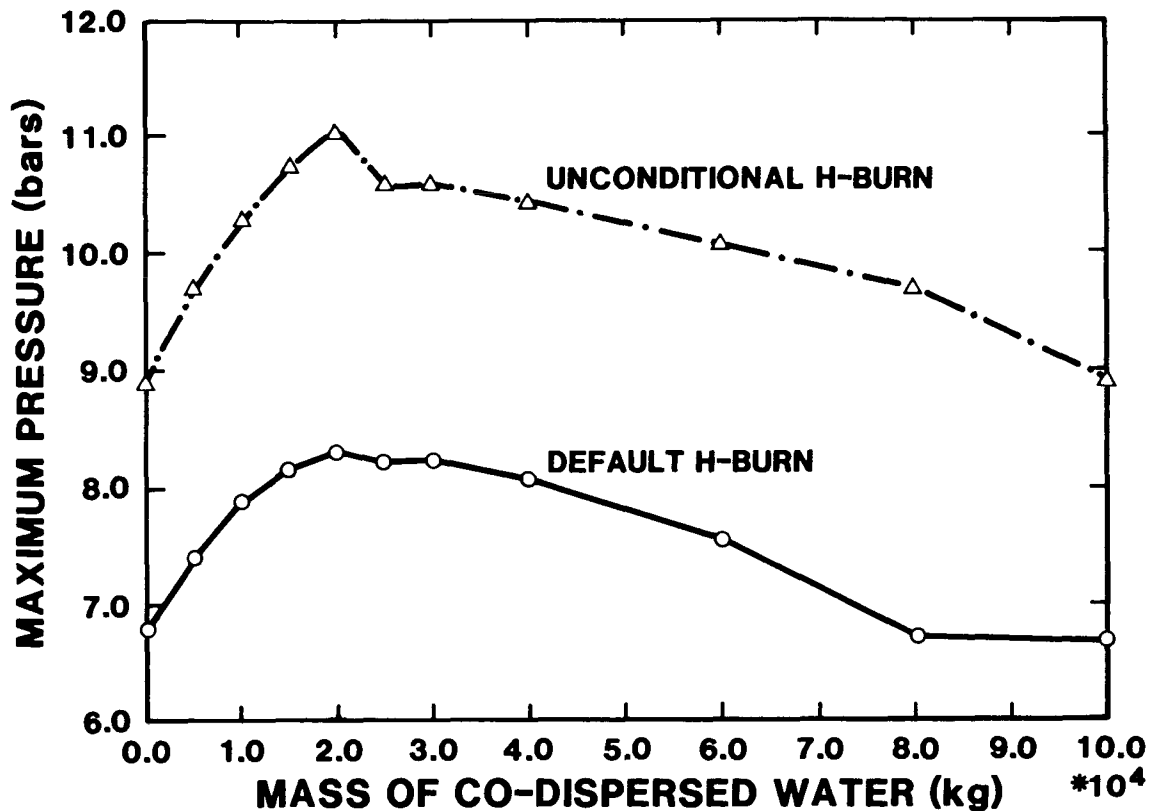


Fig. 3.8 Maximum DCH pressures generated as a function of the mass of water co-dispersed with the debris.

given but, in interpreting the latter, the limitations of the present model in tracking debris temperatures must be kept in mind; see Section 2.2.2.

In Fig. 3.9, it is apparent that, for water masses up to and including those yielding the maximum pressures, Cell 3 temperatures are about 800 K, which is at least approaching the temperature regime for which it was suggested in Section 2.2.2 that hypergolic hydrogen combustion behavior should be considered. At the same time, temperatures of the steam-hydrogen mixture entering Cell 3 from Cell 2 are seen to be much higher, but Cell 2 contains no oxygen. However, from the temperatures, it is apparent that, for water masses ≤ 20000 kg, substantial intermixing between the Cell 2 and the Cell 3 gases

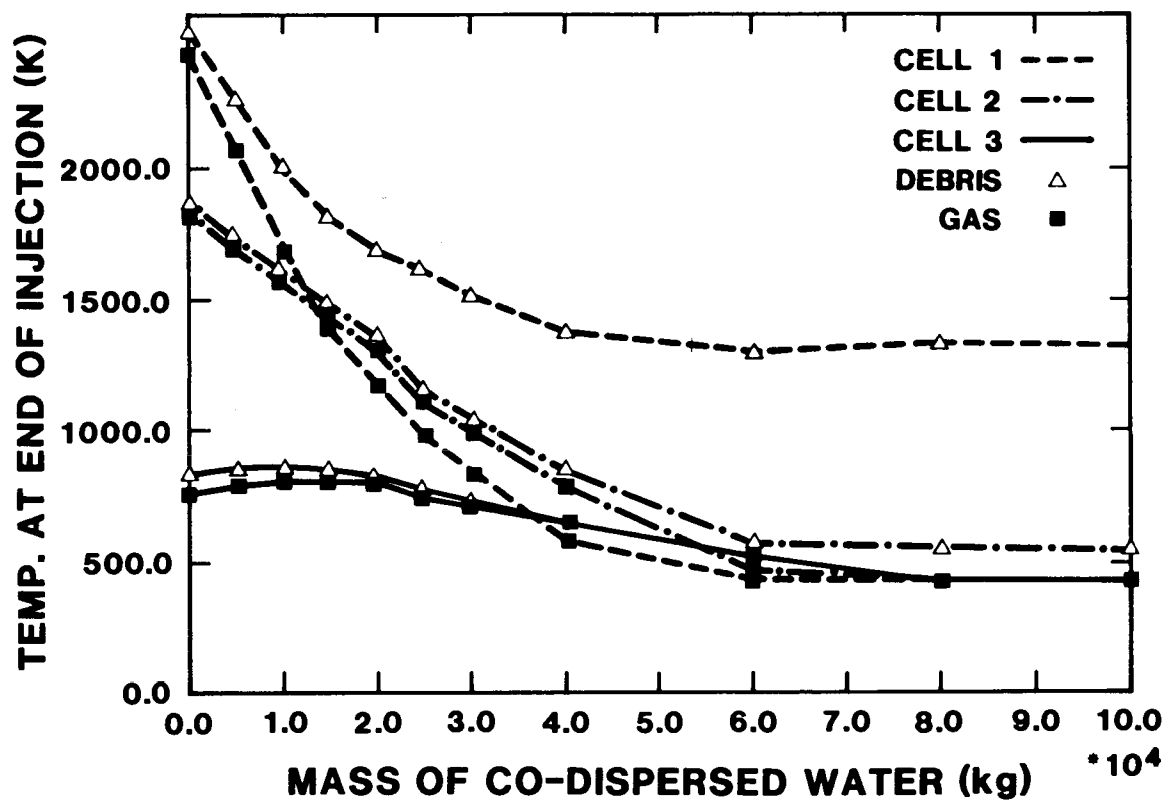


Fig. 3.9 Atmospheric gas temperatures and bulk debris temperatures as a function of the mass of co-dispersed water, calculated assuming the default burn model.

can occur with the mixture temperatures remaining at values for which spontaneous reaction may be plausible, even not allowing for any enhancement of reaction associated with possible catalytic action of the hot oxide particulate.

Given that reaction does occur, the resulting energy release might aid in continuing the reaction as more mixing occurs. In the unconditional burn scenarios, the Cell 3 temperatures vary from about 1100 K to 1200 K for water masses in the range 0-30000 kg, illustrating that the energy available is sufficient to heat the entire volume well into the temperature regime for which spontaneous reaction should be considered as a possibility. Although

this fact does not prove combustion would occur in these scenarios, it does show that the unconditional burn hypothesis is at least internally consistent for co-dispersed water masses in this range.

For the larger water masses, Cell 3 temperatures decline substantially and the temperature of the material entering from Cell 2 declines still more rapidly, falling below 1000 K for water masses above 30000 kg. Under these conditions, the unconditional burn scenario rapidly loses credibility, with the default burn parameters becoming much more plausible. These predict steam inerting by wide margins (Cell 3 steam fractions of 75% - 80% are typical of the scenarios with co-dispersed water).

Even if the arguments given here are correct, it must be remembered that the unconditional burn scenario is undoubtedly an extreme case, since virtually total consumption of the limiting reactant is postulated, which is unlikely to arise in reality. Nonetheless, the preceding arguments do suggest that a more complete model might predict realization of a considerable portion of the pressure enhancement implied by the unconditional burn scenario for water masses ≤ 20000 kg, which would in turn still represent a very serious threat in some instances. On the other hand, it is also likely that the results from such a model would approach those of the default burn scenario at the larger water masses. Thus it is at least possible that the actual sensitivity of the DCH loads to water mass would be considerably greater than suggested by Fig. 3.8, with a maximum at masses ≤ 20000 kg followed by a decline at higher masses that might be considerably steeper than what is implied by either of the curves in Fig. 3.8.

Hydrogen Production. Because of short residence times in Cell 1, the bulk debris temperatures calculated by the present model remain above the postulated 1200 K reaction threshold for all values of the water mass. Zirconium reaction is largely complete in this cell, but a large fraction of the iron is swept into Cell 2 before it can react. Fig. 3.9 shows that calculated debris temperatures in this cell drop below the specified reaction threshold for water masses ≥ 25000 kg, in which case the present model postulates an abrupt cessation of chemical reaction, which in turn leads to an abrupt drop in hydrogen production. This behavior is illustrated in Fig. 3.10, which gives the hydrogen inventory in the inert lower cells (1 and 2), the oxygen-bearing upper containment (Cell 3), and the net hydrogen produced by chemical reaction

during DCH. Although the drop in production is substantial, much of it is seen to be at the expense of the inventory in the lower cells, which is not eligible to burn even in the unconditional burn scenarios due to oxygen depletion in these cells. Nonetheless, the Cell 3 inventory drops sufficiently to produce the drop in peak pressures for the unconditional burn scenario which was noted previously in connection with Fig. 3.8.

The abruptness of the onset of quenching effects in these calculations is, of course, an artifact of some of the simplifications of the present model. However, the potential impact of such quenching is very real and may, in fact, be larger than suggested by Figs. 3.8-3.10. This impact will be treated further in Section 3.3.3.

For water masses too small to induce quenching of reactions in Cell 2, it is seen that the calculated hydrogen production does not depend strongly upon

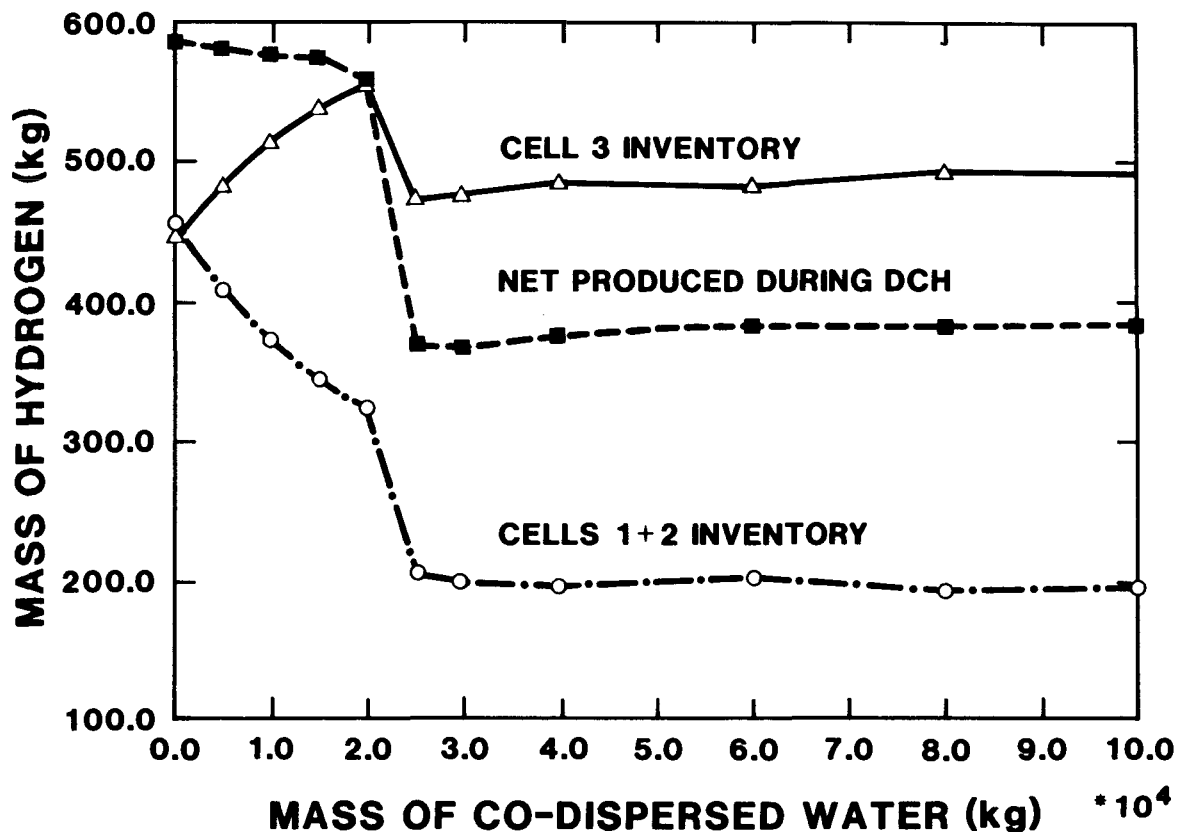


Fig. 3.10 Hydrogen distribution and net hydrogen production as a function of the mass of co-dispersed water.

the water mass, but that the hydrogen inventories in Cell 3 increase while the inventories in the lower cells decrease as the water mass is increased. This behavior reflects the improved transport to the upper containment associated with the additional steam generation, and it augments the impact of hydrogen in the unconditional burn scenarios.

3.3.3 Additional Sensitivities in Co-Dispersed Water Scenarios.

Some additional sensitivities involving co-dispersed water will be discussed in this section, based upon results summarized in Table 3.4. Case 1 in this table is the present base case (20000 kg water), while Case 2 gives the results for no water (it is the same as Case 31 of Table 3.3). The first 9 cases give results for default burn parameters, while Cases 11-18 give results for scenarios analogous to Cases 1-8, respectively, except that the unconditional burn parameters were specified. Cases 1, 2, 11, and 12 are analogous to Cases 18, 1, 19, and 7, respectively, in Table 3.3 except for the differences in the code versions. The net effects of both the unconditional hydrogen burns and of the water are very similar for the two code versions, even though the actual pressures calculated with the more recent code version are somewhat lower. As noted previously, correction of the energy accounting error and the switch from the Cess-Lian to the Modak emissivity model for steam contribute about equally to this reduction, with other differences appearing to have considerably smaller impact.

Effect of Timing of Water Injection. If, as some experimental observations suggest [Ta84b], any water in the reactor cavity is blown out of the cavity at the very start of debris injection, it is reasonable to assume that the effects of cavity water could be reduced. Calculations were therefore run with the 20000 kg of water injected into the problem during just the first second of debris injection, with results given as Cases 3 and 13 in Table 3.4. As suggested, the aggravating effect of the water is considerably reduced. (It is interesting to note that the possibility of early ejection of the water from the cavity has been more usually offered as a reason for questioning the importance of mitigation due to co-dispersed water!)

Location of Water Injection. It has also been suggested that, even if water is absent in (or blown out of) the cavity, it could be resuspended from the floors of intermediate compartments and/or the upper containment in the

Table 3.4

Sensitivity Study for the Effect of Water in DCH Scenarios

Run	Variation From Base Case	$P_{\max}$ (bars)	$T_{\max}$ Cell 2	(K) Cell 3	H_2 After Injection Cells 1 + 2	Cell 3	Net Produced
1	Base Case*	8.3	1310	810	320	550	560
2	No Water	6.8	1840	770	460	440	590
3	1-sec Water Expulsion	7.2	1660	660	360	480	530
4	Water Injected in Cell 2	7.8	991	740	250	500	450
5	Water Injected in Cell 3	6.0	1880	440	395	500	580
6	Baker Drop Diffusivity	7.3	1000	680	40	310	~ 6
7	Quench Trapped Debris-Cell 2 ⁺	8.4	1570	870	330	560	590
8	As Case 7, but $\lambda_{tr} = 0^+$	7.5	1850	800	480	460	630
9	Quench in Cells 2 and 3 ⁺	8.4	1570	870	330	560	590
11	Base Case* with UCHB**	11.1	1330	1220	380	-	-
12	No Water, with UCHB	8.9	1830	1110	520	-	-
13	1-sec Expulsion, UCHB	9.9	1620	990	410	-	-
14	Cell 2 Injection, UCHB	10.5	990	1110	320	-	-
15	Cell 3 Injection, UCHB	8.2	1870	770	480	-	-
16	Baker Drop Diff., UCHB	8.7	890	1000	60	-	-
17	As Case 7, UCHB ⁺	10.9	1580	1280	420	-	-
18	As Case 17, but $\lambda_{tr} = 0^+$	9.1	1840	1120	560	-	-

+ No co-dispersed water, other than quench in pool.

* In the base case, 20000 kg of water is injected at the same time and location as the debris; i.e., it is injected in Cell 1 over a 5-second period.

** UCHB = Unconditional hydrogen burn option used.

turbulent DCH environment [Po86]. In compartments other than the cavity, it is not clear whether sufficiently vigorous flows will actually be directed toward the surfaces upon which the water rests in order to realize this scenario. In order to address its implications if it does arise, calculations were run with 20000 kg injected over a five second period in Cell 2 and in

Cell 3. Cases 4 and 14 give the results for Cell 2 injection, while Cases 5 and 15 give results for Cell 3 injection. It is apparent that dispersal of water in Cell 2 is calculated to lead to aggravating effects similar to Cell 1 dispersal, though somewhat smaller in magnitude. On the other hand, dispersal in Cell 3 yields significant mitigation, relative to the no-water cases. The latter result reflects the fact that introducing the water directly into Cell 3 does little to enhance transport from the lower cells to the upper containment, and it does act to quench the high temperatures, and hence the pressures, that would otherwise develop in the upper containment. The lower Cell 3 temperatures given for Case 5 also reduce the plausibility of the analogous unconditional burn scenario (Case 15), although material entering Cell 3 from Cell 2 continues to be very hot in this instance, since it has suffered no cooling due to the water.

Drop-Side Reaction Rate Limits. Calculations otherwise identical to Cases 1 and 11 in Table 3.4 were run with drop-side reaction rate limits given by the diffusivity expression based upon Baker's work, Eq. 3.1. Results are summarized by Cases 6 and 16 in Table 3.4. In striking contrast to the minor effect found in the absence of cavity water (Case 22 of Table 3.3), substantial reductions in peak pressures are obtained (compare Cases 6 and 16 with 1 and 11, respectively). The reason is that debris temperatures even in Cell 1 are low enough so that chemical reaction is greatly slowed when this representation of the drop-side reaction rate limit is assumed. The resulting absence of the zirconium reaction energy leads to debris temperatures that are 200-300 K lower than those implied by Fig. 3.9. As can be seen by comparing Cases 1 and 6 in Table 3.4, the gas temperatures in the lower cells are substantially lower in Case 6, which correspondingly reduces driving forces for transport to the upper containment. In addition, net hydrogen production is now calculated to be trivial. The combined impact is especially large for the unconditional hydrogen burn variation, even without taking into account the implications of the reduced temperatures for the plausibility of the unconditional burn scenario.

It should be noted that these calculations are expected to over-estimate the potential impact of drop-side reaction rate limitations for at least two reasons: first, the rate limitations with diffusivity based upon Eq. 3.1 are likely nonconservative, and secondly, the present single-field debris model requires that debris freshly introduced into any cell, and energy-generating

reacting debris, all be lumped in with the relatively cool bulk debris field of that cell, with zero equilibration time. Errors introduced by the latter effect can be quite serious, as is illustrated in the Appendix. Nonetheless, the present results do indicate that the large potential energy release associated with zirconium oxidation (even oxidation by steam) can indeed be important. (It did not show up strongly in the sensitivity study no-water case treated in Section 3.2.3 for reasons that were noted there, e.g., thermal saturation effects and the very high gas temperatures that were calculated to exist in that scenario.) This result also suggests that there will be substantial additional uncertainties involved in calculations for DCH scenarios that involve potential quenching effects, until such time that more detailed chemical reaction and heat transfer modeling is available in the CONTAIN DCH treatment.

3.3.4 Water Quench of Trapped Debris.

In all calculations discussed so far, debris assumed to be trapped was in effect removed from the problem, with the energy remaining in this debris having no further effect upon the calculation. This treatment is probably reasonable for debris that is trapped by adhering to solid structures, or which falls on floor areas not covered with water, since heat transfer from thin debris layers into the solid is expected to be rapid in comparison with heat transfer back to the gas in this geometry, and heat transfer from thicker debris layers to the gas is expected to be relatively slow due to the low surface-volume ratio. However, if the debris falls into pools that may exist in various locations within containment, the energy remaining in this debris may reasonably be expected to go into steam generation, which can contribute both to direct pressurization and also to the transport effects that have been discussed previously.

In the CONTAIN IDHM, trapped debris can be accumulated in a so-called "lower-cell layer" which, in turn, can be overlain by a water pool. By specifying artificially enhanced heat transfer from the lower-cell layer to the pool, while the lower boundary of the lower-cell layer is kept adiabatic, direct quenching of the debris in the pool may be simulated. Heat transfer was assumed to be sufficiently rapid so that the rate of steam generation was limited only by the trapping rate: while this assumption could prove incorrect, it is not obviously in error for small hot particles falling in water.

Calculations were run using this treatment in Cell 2, and again using it in both Cells 2 and 3. Debris trapped in Cell 1 was not treated in this fashion because it was judged unreasonable to assume quiescent pools of water could remain in Cell 1; i.e., any Cell 1 water is more reasonably assumed to be dispersed as in the scenarios treated above. Debris trapped in Cells 4 and 5 was not so treated for reasons of convenience; these cells receive only a minor fraction of the total debris. (Any error introduced by neglecting quench of this debris is likely less than the opposing error introduced by assuming all debris trapped in Cell 2 and/or Cell 3 ends up in pools.) Chemical reaction between the debris and the pool water during quench is not included in this calculation but would be a minor effect in the cases treated, because chemical reaction was much more rapid than trapping and most of the metal was therefore reacted prior to the quench.

Some results obtained are summarized in Cases 7-9, 17, and 18 in Table 3.4. In all five cases, no co-dispersed water was assumed. Case 7 gives results obtained assuming quenching of trapped debris in Cell 2 only. Relative to the analogous case without quench (Case 2 of Table 3.4), pressures are substantially higher, 8.4 bars versus 6.8 bars. The debris was calculated to boil about 13000 kg of water from the pool in this scenario, which was added to the Cell 2 atmosphere as saturated steam in the calculation. In itself, this amount of steam would be sufficient to produce a pressure rise of no more than about 0.6 bars in the Surry containment volume. Since the actual pressure increase in the quench scenario is 1.6 bars, relative to Case 2, it is evident that the dominant effect is the accelerated transport of energy from Cell 2 to the upper containment, not just the direct impact of adding more steam to the atmosphere.

In the quench scenario, steam generated in Cell 2 improves hydrogen transport to the upper containment relative to Case 2 even though hydrogen production is virtually unaffected (last three columns, Table 3.4). Temperatures in the Cell 3 atmosphere are very high, up to 870 K, and material entering from Cell 2 is at temperatures exceeding 1500 K. Hence, hypergolic hydrogen behavior in Cell 3 is plausible. Case 17 was run under assumptions identical to Case 7 except that the unconditional burn option was used instead of the default burn model. As expected, a very severe scenario results, with peak pressures approaching 11 bars.

Case 9 was run assuming debris trapped in Cell 3, as well as Cell 2, would also be quenched in water pools. Though substantial quantities (about 27000 kg) of debris were deposited in the Cell 3 pool, this debris was much cooler than in Cell 2 and generated much less steam; furthermore, steam generated in Cell 3 does not contribute to the improved transport effect. Hence, results differed little from Case 7. The analogous scenario with unconditional hydrogen burn was not run.

Cases 8 and 18 were run to provide one more illustration of a point deemed very important in this work: that great caution must be exercised when generalizing as to whether a given effect will be mitigating or aggravating, and hence, whether its neglect will be "conservative" or "nonconservative." In past discussions of DCH, few phenomena have been more unqualifiedly accepted as being a mitigator than the de-entrainment of debris by interaction with structures, represented in the present work by "trapping". All cases discussed above were run with the base case trapping rates (Section 3.2.1). In Section 3.2.3, it was found that deleting trapping from the base case increased pressures by less than a bar, considerably less than the aggravating effect calculated here for the quenching of trapped debris. However, the latter effect depends for its existence upon trapping. Hence, it is reasonable to expect that deleting trapping in this scenario would reduce the calculated loads.

Cases 8 and 18 were run with input identical to Cases 7 and 17, respectively, except that the trapping rate λ_{tr} was set equal to zero in all cells. Eliminating trapping reduced peak pressures by almost 1 bar with the default burn model assumed, and by almost 2 bars with the unconditional burn option. Clearly, if the base case had been defined to include water quench of trapped debris, the neglect of trapping would have been "nonconservative" indeed!

Given that water quench of trapped debris occurs, it is evident that the loads are not a monotonic function of λ_{tr} , which in turn implies that there must exist a "worst case" value of λ_{tr} such that the loads are maximized, for a given choice of the other parameters of the problem. No effort has been made to determine this value of λ_{tr} or the associated loads. It must be expected, however, that the water quench effect may be somewhat larger for some other values of the trapping rate, although it is considered unlikely that much larger effects will result for any value of λ_{tr} .

3.4 Thermal Loads Associated with DCH.

The high temperatures calculated for DCH scenarios have naturally raised some concerns as to whether threats to containment integrity could arise due to overheating of critical containment structures, with either purely thermal damage or reduced pressure capabilities resulting from overheating and/or thermal stresses. In the present work, the emphasis has been heavily upon containment pressure loads, and thermal effects will be considered here only to a very limited extent. In general, analysis of containment vulnerabilities to thermal loads would require identification of specific locations at which the containment might be vulnerable, followed by detailed evaluation of the thermal environment and its consequences at those specific locations. Such tasks would require a much more detailed description of the containment than the 5-cell representation of Fig. 3.2 which has been used in the present work.

The upper dome would constitute one of the regions of interest in an analysis of thermal loads. The geometry of this region is sufficiently simple so that the rather generalized representation of the containment used in this work may give a reasonable representation of this structure. Case 33 of Table 3.3 was selected for more detailed thermal analysis; this is the base case with unconditional hydrogen burn, run on CONTAIN 1.06. The dome is modeled as concrete lined with 1.28 cm steel.

In Fig. 3.11, the gas temperature in Cell 3 is plotted as a function of the time since vessel breach. Though peak temperatures are extreme, they decline rapidly with time. The thermal response of the dome is indicated in Fig. 3.12, in which the temperature histories of various nodes in both the steel and the concrete is plotted. The depth below the inside surface (z) and the material in which each node is located are indicated on the figure. In the steel, and in the concrete at the steel/concrete interface, temperatures initially rise rapidly, but they level out at moderate values and have begun to fall by the time the calculation was terminated. Temperatures at greater depths are still rising when the calculation was terminated, but they are quite moderate and would never rise to levels exceeding those given for the surface. At a depth of 0.07 m, which is still under 10% of the total dome thickness, the temperature rises are negligible.

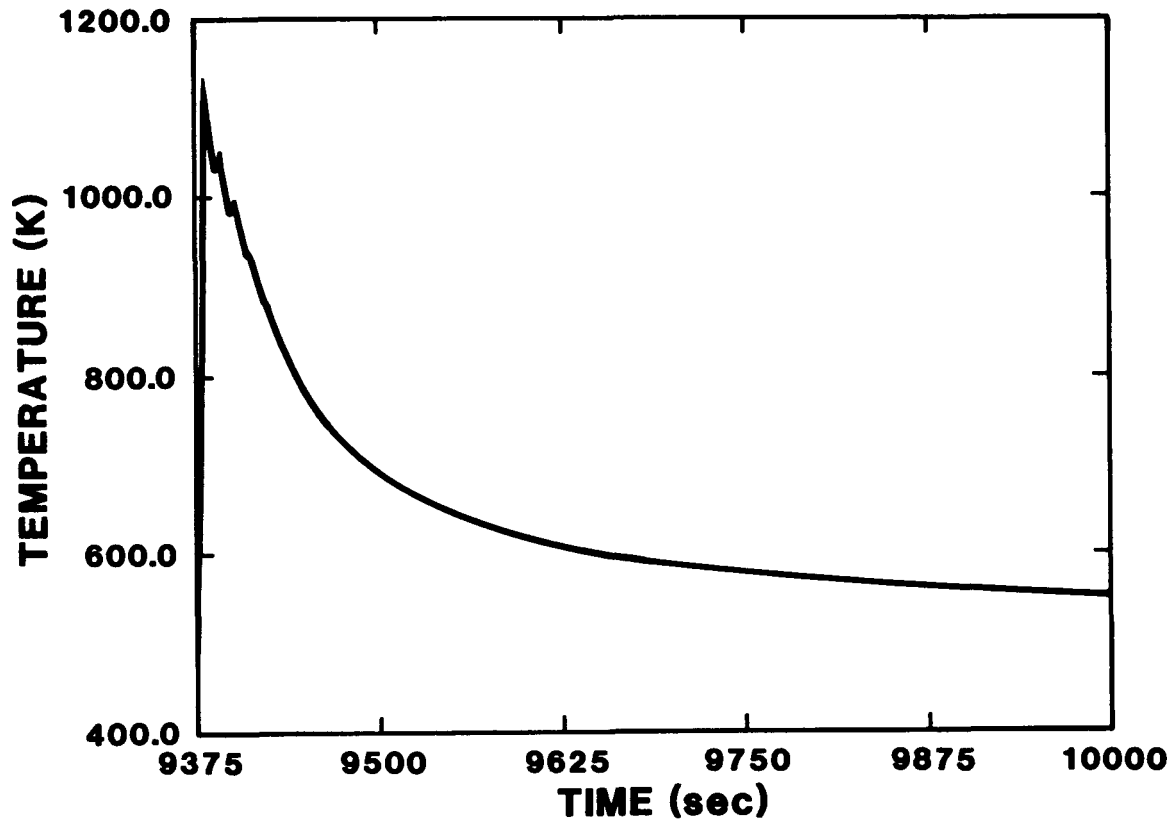


Fig. 3.11 Temperature history of the upper containment atmosphere for the Surry base case DCH scenario with unconditional hydrogen burn.

In assessing thermal stresses, temperature gradients are of greatest interest. In Fig. 3.13, temperature profiles are given in the form of histograms for the times indicated in the figure. Gradients are never truly extreme, and the strongest gradients affect only relatively thin layers of the dome structure.

From the results presented here, it does not appear that the thermal threat is severe for the case analyzed. It must be remembered, however, that the present model gives only a representation of structure temperatures averaged over the structure surface. Thermal environments at specific locations of interest may be either more or less severe than those calculated.

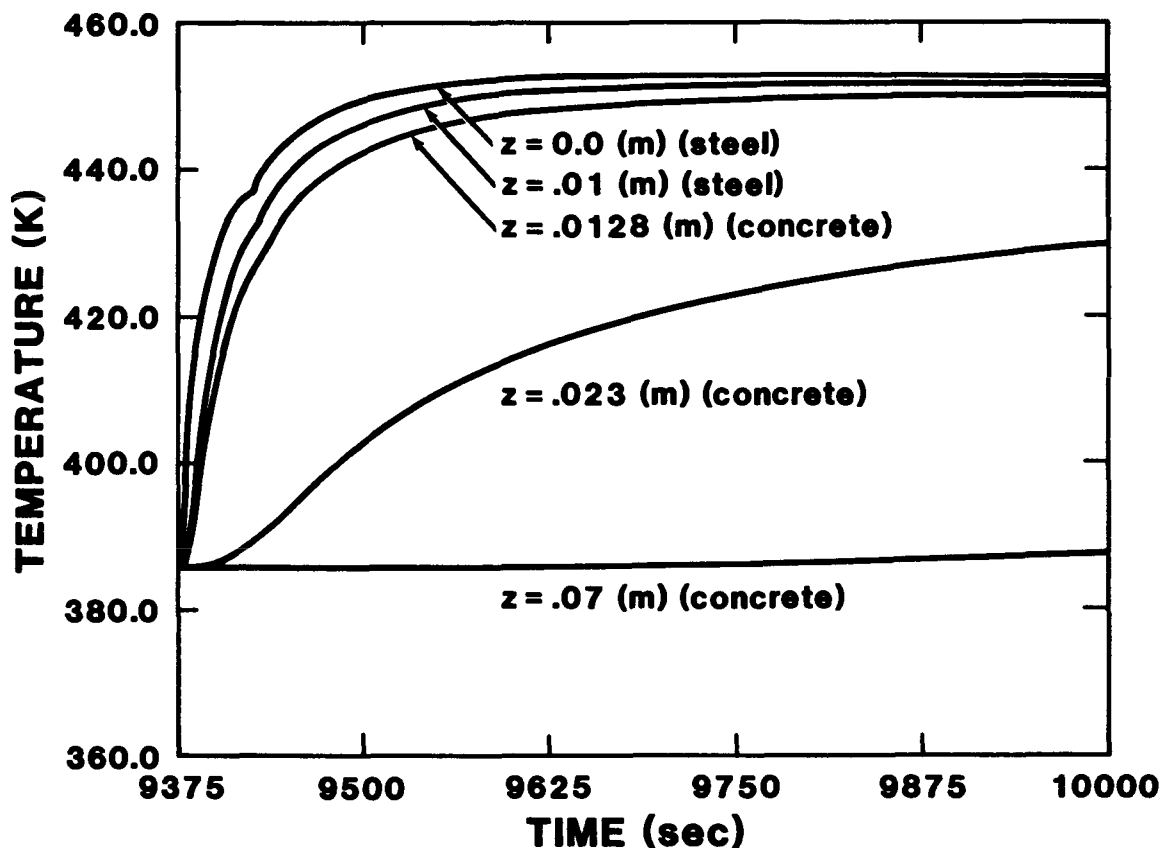


Fig. 3.12 Temperature histories at selected depths within the containment dome wall for the base case with unconditional hydrogen burn.

In parts of the lower containment, the thermal environment during DCH is calculated to be much more severe. In Cells 1 and 2, for example, calculated temperatures of unlined concrete structures rose above 1500 K and to almost 800 K in the cavity cell (Cell 1) and in the basement (Cell 2), respectively. Quantitatively, these numbers mean little, because concrete would undergo spalling and even gross decomposition at such temperatures, and these effects are not modeled. These extreme temperatures lasted only for seconds or tens of seconds, and affected only the immediate surface; at depths greater than 1-2 cm, thermal response was no more severe than indicated in Figs. 3.12 and 3.13. Furthermore, even the surfaces of lined concrete structures in Cell 2 did not get substantially hotter than the dome surfaces (no lined concrete surfaces were modeled in Cell 1). Thus, nothing in the available results

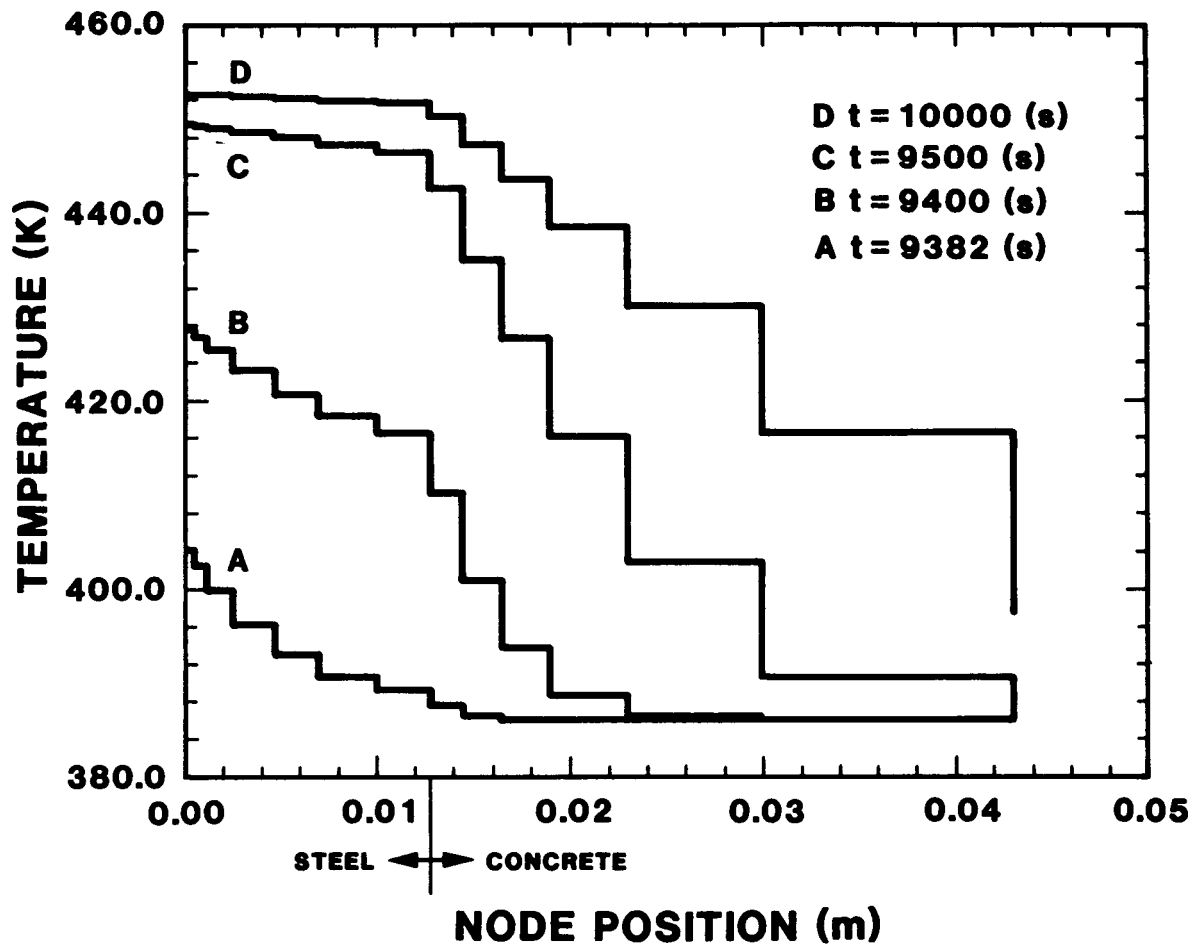


Fig. 3.13 Histograms of the thermal profile within the containment dome wall at selected times in the base case with unconditional hydrogen burn.

suggests that a serious thermal threat to massive structures exists even in the lower containment. Penetrations and other vulnerable points could, of course, be affected; even for these, detailed analysis would be required in order to determine whether the thermal environments calculated here are at all applicable to the relevant locations. Pathways to these locations may be much more tortuous than is implied by the simple containment model used here, for example.

The present study has emphasized pressure loads rather than thermal loads partly because the available analysis tool is better suited to the analysis of pressurization than to the analysis of thermal response. However, it also has

been based upon a belief that DCH is primarily a pressure threat to containment integrity, due to the rapidity of the introduction of energy into the atmosphere and the short duration of the extreme atmospheric temperatures. Results of the present calculations lend some limited support to this belief, although much more detailed analysis would be needed to offer firmer conclusions. It should also be obvious that nothing in this discussion is intended to apply to scenarios hypothesized for some plants, in which the debris itself is assumed to come into direct contact with vulnerable locations on the containment boundary [Pi86b]. In that event, the thermal threat could be severe, and the present analyses are not relevant to that scenario because only structure heating by contact with the hot gases has been considered here.

4. ANALYSIS OF DCH IN ICE CONDENSER PLANTS

In this section, some results obtained by applying the CONTAIN IDHM to ice condenser plants are presented. Detailed discussion of the results will emphasize phenomenologies peculiar to ice-condenser plants. Other features of the calculations will be discussed in less detail than was done in Section 3 for DCH phenomena in the Surry plant.

4.1 Problem Definition.

Using the Station Blackout (TMLB') scenario in the Sequoyah plant as a model, three distinct series of calculations were performed in order to investigate DCH scenarios in ice condenser plants:

- Series I. A series of calculations designed to illustrate important features of DCH scenarios that are governed by the ice condenser and by hydrogen phenomenology in these plants. This series was actually performed the most recently, and utilized the developmental version of CONTAIN 1.06 which was used in some of the later Surry analyses discussed in Section 3 of this report.
- Series II. A series of calculations investigating the response as a function of the core fraction which participates in DCH, performed using CONTAIN 1.04.
- Series III. A series intended to explore sensitivity to some of the uncertainties which were found to be important in the Surry DCH scenarios discussed in Section 3, performed using essentially the same code as was used for Series 2.

The first series of calculations is discussed in Section 4.2 while the second and third are discussed in Section 4.3. The three series of calculations were performed at different times with somewhat different purposes in mind, and thus involve different code versions and different input choices. These variations complicate quantitative comparisons of the results obtained in different series (see Section 4.3.1 for some examples). Calculations within a series involve consistent modeling and consistent input other than the parameters specifically varied. The discussion in the present subsection is limited to features common to all three series, with series-specific features being discussed in Sections 4.2 and 4.3 as appropriate.

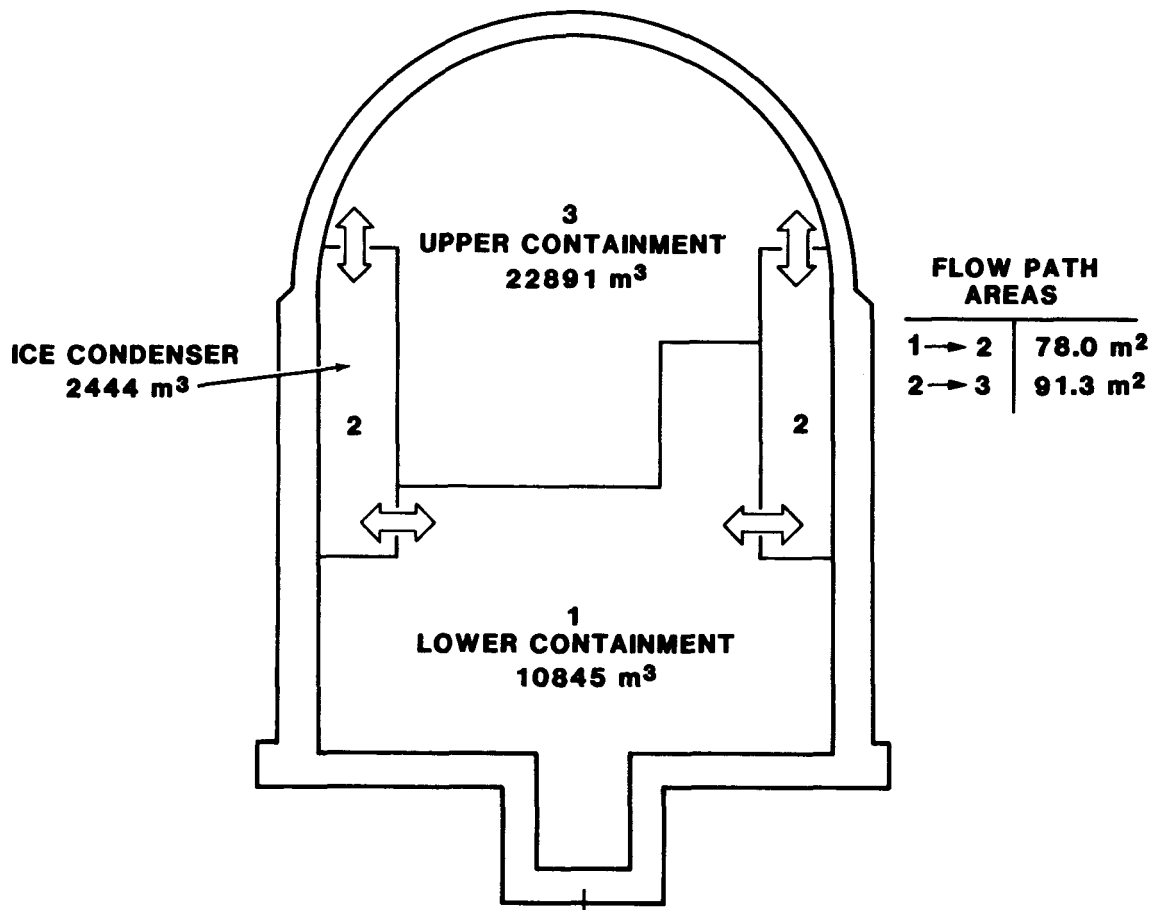


Fig. 4.1 Nodalization of the Sequoyah containment used in the CONTAIN DCH calculations.

In all the studies, the simple three-cell nodalization diagrammed in Fig. 4.1 was used. Cell volumes and flow path areas are indicated in the figure. It should be noted that the interconnections between the compartments include doors which open under low pressure differential in the forward direction and the flow areas given correspond to the doors-open state. In the present work, it was assumed that the doors would not completely reclose under reverse pressure; a minimum flow area equal to 25% of the maximum was assumed to be always present. Air return fans can normally produce a return flow from Cell 3 to Cell 1 in Fig. 4.1. Since the present analyses are based upon station black-out scenarios in which these fans would be unavailable, the fans are not modeled in these calculations.

The simple nodalization used here is realistic in that ice condenser plants typically have distinct lower-containment and upper-containment volumes (Cells 1 and 3, respectively) with flow from the former to the latter being constrained to pass through the ice condenser. However, the actual geometry is far more complex, with the lower containment volume, in particular, being crowded with plant equipment in addition to having a much more complex geometry than considered here. The sensitivity of the calculations to realistic geometric complexities has not been investigated. This fact must be kept in mind in interpreting the results to be presented; in particular, it dictates that great caution is required in making any inferences as to whether any particular ice condenser containment may or may not fail in any particular DCH scenario.

The plant-specific parameters for the present calculations were based upon the Sequoyah plant, but the important phenomena revealed by the calculations should be at least qualitatively applicable to other ice-condenser plants. Furthermore, the Watts Bar plant is very similar to the Sequoyah plant at the level of detail considered here, and the loads calculated would therefore be equally applicable (or inapplicable) to either of these plants.

Watts Bar and Sequoyah do differ substantially with respect to estimated failure pressure for the containment, a fact which considerably widens the parameter space of interest in a practical sense. In the SARRP study, the failure pressure for Sequoyah used in the "central" risk estimate was 4.5 bars [Bh87]. The expert review group convened to aid in the SARRP evaluation of uncertainties chose an uncertainty range of 4.1 to 6.2 bars, with a median value of about 5.2 [Bn87c]. Watts Bar was not treated in SARRP, but estimates of failure pressures for this plant made in other work [Ju84, Gr84] span a considerably higher range, from about 7.8 bars to over 10 bars. Thus, a wide range of pressure values is of direct practical interest, even without allowing for additional uncertainties such as those associated with the previous caveats concerning the simplified representation of containment geometry.

In all cases, the CONTAIN DCH analyses were started at the time of vessel breach. Containment conditions existing at that time were taken from a CONTAIN calculation of the preceding portion of the accident sequence using primary system steam sources taken from the MARCH-HECTR analysis of Sequoyah [Ca84]. With a few exceptions in Section 4.2, these conditions were not

varied in any of the present calculations. The steam source following vessel breach was based upon a postulated blowdown of a primary system initially filled with saturated steam at the system operating pressure. The blowdown was taken to be uniform over the assumed blowdown time (30 seconds in the base case).

Hydrogen associated with in-vessel Zr oxidation was treated in a way that may not be fully realistic. Half this hydrogen was assumed to be released from the primary system along with the steam blowdown following vessel breach. It was assumed that the other half had been released prior to vessel breach and had been burned off; the oxygen inventory available at the start of the DCH analysis was correspondingly reduced but this half of the hydrogen was not otherwise assumed to have any effect upon the problem. Since ice condenser containments are equipped with igniters for the controlled burning of hydrogen, this treatment might be reasonable for some scenarios. In a station blackout, however, operation of igniters would require availability of a dedicated power supply independent of the power supplies whose postulated failures led to the accident. (Unlike the situation in large dry containments, steam condensation in the ice condenser prevents steam inerting of the upper containment, even during a station blackout scenario.)

The reason for this treatment of hydrogen is that a major purpose of the present study is to explore DCH phenomenology rather than to make best-estimate calculations of loads for containment failure analysis or risk assessment. It is well known that, in the absence of igniters, hydrogen released prior to and during blowdown at the time of vessel breach can pose a significant threat to the integrity of ice condenser containments [Ca84, Bn87c], without any additions associated with DCH phenomena. It therefore seemed reasonable to investigate the DCH phenomena in the absence of the already-significant threat posed by pre-existing hydrogen in the containment. In addition, the results may be of some value in assessing the utility of safety options such as independent dedicated power supplies for igniters or catalytic igniters.

The three series of calculations were performed by defining a base case for each series and varying one or more parameters (or modeling assumptions) in various sensitivity studies. Some of the most important parameters of the base cases include: total in-vessel corium inventory involving 101000 kg of

UO₂ and 23000 kg total Zr of which about 49% was assumed to be oxidized in-vessel based upon BMI-2104 analyses of the Sequoyah TMLB' sequence [Gi84]; steel contents differed among the three series. The corium injection fraction was 75% in the base cases with a temperature of 2550 K, and the duration of debris injection was 5 seconds as in the Surry analyses. Also as in Surry, the trapping rate, λ_{tr} , was assumed in Series I and III to be equal to the estimated fall velocity (taken to be 6 m/sec) divided by the cube root of the cell volume given in Fig. 4.1 except for the ice compartment. In the latter compartment (Cell 2), it was judged that this prescription gives unrealistically low trapping rates. Hence, a value based upon an effective volume an order of magnitude smaller than the Fig. 4.1 volume was used, which yielded $\lambda_{tr} = 0.96 \text{ s}^{-1}$ for the ice compartment. Even this value does not seem especially large, in view of the common argument that debris trapping in the ice chest will be very efficient.

These and other parameters of the base case for each series are summarized in Table 4.1. Where the entry "varied" appears, the parameter was varied in so many of the calculations that defining a "base case" value is not useful; many other parameters were varied in one or a few sensitivity runs. It must be remembered that the code versions used in different series were not the same and thus runs in different series would not be identical even if all the parameters listed in Table 4.1 were identical.

4.2 Some DCH Phenomenology in Ice Condenser Plants (Series I Calculations).

In striking contrast with the SARRP Surry results, DCH did not rank as a major contributor to either the risk or the uncertainty in risk that was estimated for the Sequoyah plant in the initial phase of SARRP [Bn87c]. There are several reasons for this result. Some of these are due to the fact that some scenarios significant to the Sequoyah risk profile involve features believed to preclude DCH; an example would be scenarios in which the lower containment is so heavily flooded that the vessel itself is largely submerged at the time of vessel breach. In addition, there were a number of scenarios in which important threats to containment integrity existed independently of DCH, e.g., scenarios involving hydrogen burns at vessel breach; in Surry, scenarios threatening early containment failure which did not involve DCH were of considerably lower probability. Issues of this type will not be considered further here, since the purpose of the present study is to address the effects

Table 4.1

Base Case Parameters
for Sequoyah DCH Calculations

Input Parameter	Series I	Series II	Series III
CONTAIN Version	1.06	1.04	1.04
In-vessel corium composition			
UO ₂ (kg)	100992	100992	100992
Zr (total, kg)	23097	23097	23097
fraction oxidized	0.49	0.49	0.49
Steel (as Fe, kg)	21892	49840	21892
Initial corium temperature (k)	2550	2550	2550
Corium fraction injected	0.75	Varied	0.75
Duration of melt injection (s)	5.0	5.0	5.0
Duration of blowdown (s)**	30.0	30.0	30.0
Debris trapping rate (s ⁻¹)	Eq.2.1*	0.1 & 3.33	Eq.2.1*
Debris drop diameter (mm)	0.5	0.5	0.5
Drop diffusivity (m ² /s)	10 ⁻⁸	∞	10 ⁻⁸
Chem. reaction cutoff temp. (K)	1200	1000	1200
Debris-gas blackbody multiplier, α_g	0.8	0.8	0.8
Debris-wall blackbody multiplier, α_w	0.0	0.0	0.0
Hydrogen Burn Model	Varied	Default	Varied
Ice fraction remaining	0.8	0.8	0.8

* (V/10) used in Eq.2.1 for ice compartment

** Blowdown was at the primary system saturation temperature in Series I; somewhat higher energy contents were assumed in Series II and III.

of DCH phenomenology in scenarios in which it can occur. This study does not address the overall importance of DCH scenarios in the risk profile of Sequoyah or any other plant.

The initial SARRP analysis (including the uncertainty study) did include one assumption that is very much part of the issues to be addressed here. In

SARRP, it was assumed that the ice condenser would so heavily mitigate DCH loads (even with a dry cavity) that DCH would pose no threat to containment integrity except insofar as the ice were to be bypassed, or unless the ice were largely depleted at the time of vessel breach. At the time the initial SARRP analyses were performed, no mechanistic calculations of DCH phenomena in ice condenser plants were available. Hence, there was little choice in this phase of the SARRP study but to rely upon expert opinion and include a strong recommendation that the potential impact of DCH be investigated further in future studies, such as the one reported here. Results to be cited below show that the ice condenser does indeed have the potential to greatly reduce direct loads from DCH (even without assuming very rapid trapping of the debris in the ice beds), but phenomena associated with hydrogen generated by metal-steam reactions also have the potential to largely defeat the mitigating action otherwise expected of the ice condenser. In addition to the obvious impact of hydrogen combustion events, the enhanced noncondensable gas fractions within the ice condenser due to the hydrogen generated can also play a role. (Despite these findings, it does not follow that SARRP's initial results for either the overall risk profile or the assessment of the role of DCH are in significant error: no attempt to evaluate the impact of the present study upon the risk profile for any plant has yet been made. In any case, the final SARRP results will reflect recent findings concerning issues such as DCH.)

Base case parameters for the series of calculations to be discussed in the present subsection are summarized in Table 4.1 (Series I). The purpose of these calculations is partly pedagogical, i.e., to illustrate some of the important phenomena involved. Some of the sensitivity cases presented are therefore quite unrealistic. The results obtained are, however, important as an aid to understanding the uncertainty studies presented in Section 4.3. In addition, some variations in scenario description outside the base case scenario are considered, in order to illustrate a few of the many variables that would require study in making a complete assessment of the potential contribution of DCH to the risk profile of an ice condenser plant.

Some results obtained in this series of calculations are summarized in Table 4.2. The first column gives the case number used in the following discussion, and the second column specifies the parameters which were varied from the base case values given in Table 4.1. The third column reports the maximum pressure calculated. The remaining three columns give the gas

Table 4.2

Results of Phenomenological Study of Sequoyah
DCH Scenarios

Case	Parameter(s) Varied	Max ^P (bars)	T _{gas} at End of Injection (K)		
			Cell 1	Cell 2	Cell 3
1	Steam blowdown only	2.3	390	380	340
2	Thermal en. only, no H ₂	2.9	1830	1320	480
3	Thermal + chem. en., no H ₂	3.1	2230	1550	520
4	Base case w/o H-burn	4.3	2280	1080	680
5	Air in lower containment, no H-burn	5.1	2290	1250	810
6	No ice and no H-burn	6.7	2230	2280	970
7	No ice, no H-burn; P _o =3 bars	8.6	2150	2130	790
8	Base case, default* H-burn	7.0	2280	1080	680†
9	Base case, UCHB**	5.8	2280	1050	770†
10	Pre-existing H ₂ included	7.0	2280	1020	810†
11	Pre-existing H ₂ , UCHB	6.5	2280	1010	980†

† Not the maximum temperatures reached; the maxima occurred later due to hydrogen burns.

* Minimum flammable hydrogen mole fraction = 0.08.

** UCHB - Unconditional hydrogen burn option used.

temperatures at the end of debris injection. The temperature information provides some guidance as to when significant uncertainty may be introduced by the limitations in CONTAIN's ability to model the temperature dependence of chemical reaction rates.

4.2.1 Cases Without Hydrogen Combustion.

DCH loads in ice condenser plants can be influenced by a number of phenomena in addition to hydrogen burns, but the importance of these phenomena can

be difficult to derive from calculations which include hydrogen combustion events. Hence, in this section, the influence of these phenomena will be considered in the absence of hydrogen burns, even though the resulting scenarios may not be realistic in some cases.

Case 1 in Table 4.2 summarizes the results obtained for a steam blowdown only (no DCH and no in-vessel hydrogen), and Fig. 4.2 portrays the pressure-time history calculated for this case. Of all the scenarios to be considered here, only this case bears any resemblance to accidents within the design basis envelope, and the small pressure rises calculated only illustrate the well-known effectiveness of ice condensers in controlling pressurization due to blowdown of the primary system.

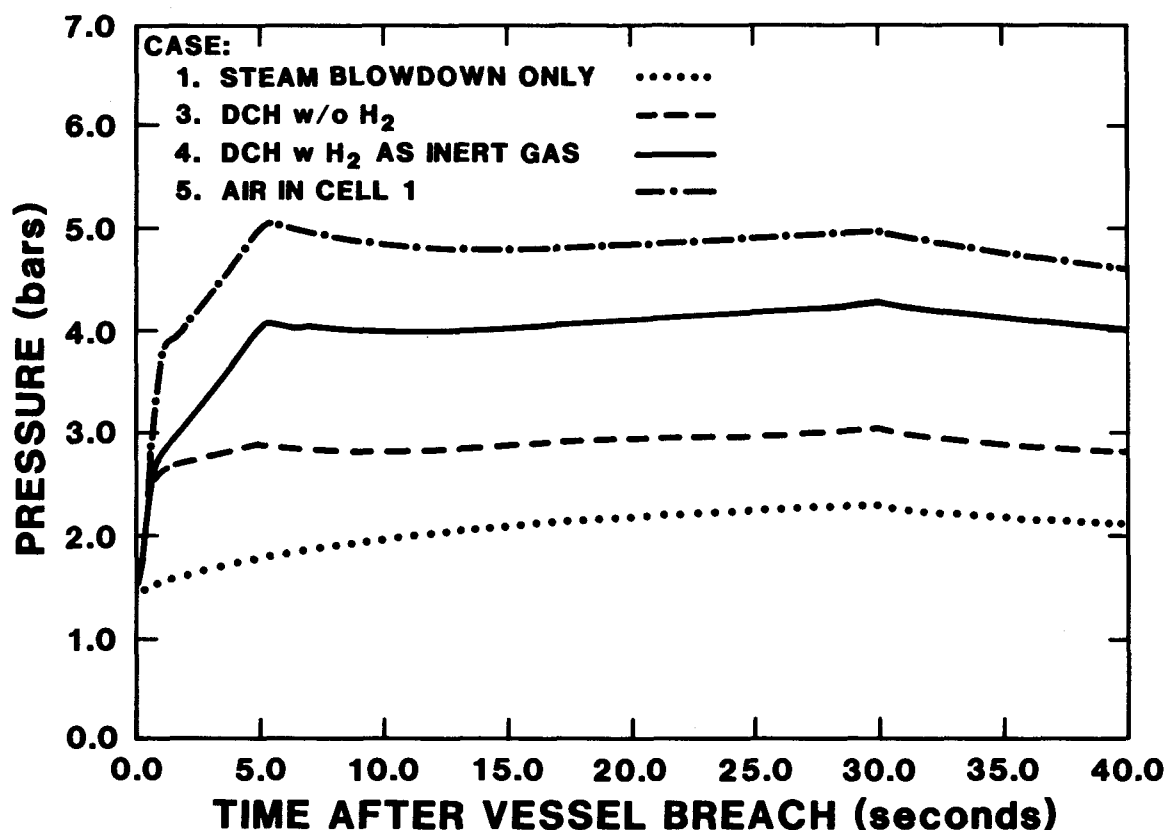


Fig. 4.2 Pressure-time histories calculated for various scenarios in the Sequoyah plant, with hydrogen burns artificially suppressed. Case numbers indicated in the legend refer to the case numbers of Table 4.2 in the text.

Case 2 in Table 4.2 summarizes results obtained for "thermal DCH" only; i.e., with hot corium injected as specified in Table 4.1 (Series I) except that all chemical reaction was switched off; in-vessel hydrogen was also deleted. Case 3 gives results for a calculation in which energy equivalent to total reaction of all metal (with steam) is introduced to Cell 1 via CONTAIN's source table options, with the calculation otherwise identical to Case 2; Fig. 4.2 also gives the pressure-time history for this case. It may be seen that adding the full DCH thermal and chemical energy to the system still results in a surprisingly small pressure rise. The peak pressure calculated, about 3.1 bar, is only about 0.75 bar higher than what was calculated for the blowdown-only case. Furthermore, adding the debris reaction energy (6.7×10^{10} J) increased the maximum pressure by less than 0.2 bar (compare Case 2 with Case 3 in Table 4.2).

For comparison purposes, it is interesting to note that adiabatic, single-cell DHEAT2 calculations for the scenarios of Cases 2 and 3 yield, respectively, peak pressures of 11.7 and 14.9 bars. The extreme differences between the DHEAT2 results and the CONTAIN results show that earlier optimism concerning the effectiveness of ice condensers in controlling DCH loads did have some physical basis, even though calculations to be presented below indicate that this optimism was sometimes substantially overstated due to the inadequate consideration given to hydrogen produced during DCH. These results also show that simple DHEAT2-type calculations are even less useful for ice condenser plants than they are for PWR large dry containments, in terms of making realistic estimates of DCH loads.

Effect of Noncondensable Gas. In the station blackout scenario used in the present study, primary system steam released prior to vessel breach largely purges the lower compartment of air; hence, the calculated steam mole fraction in Cell 1 at the time of vessel breach was 0.85. Since the introduction of hydrogen into the problem was artificially suppressed in the preceding calculations, noncondensable gas fractions in the flow entering the ice condenser were quite low throughout the period of debris injection and primary system blowdown. Under these conditions, the efficiency of the ice condenser in removing steam and energy from the gas entering the ice compartment was calculated to be high, since the rate of diffusion of water vapor through the non-condensable boundary layer at the ice surface is an important limitation on the rate of steam condensation.

In the base case DCH calculations using the standard IDHM chemical reaction model, large amounts (~ 800 kg) of hydrogen are produced during and immediately after the 5-second period of debris injection, with another 50 kg entering from the primary system during this time. This hydrogen greatly increases the noncondensable gas fraction in the ice condenser during and after the time of debris injection. For example, at the end of the debris injection period, the mole fraction of hydrogen was about 0.85 in both the lower containment and the ice condenser itself.

In order to investigate the implications of the noncondensable gas effect, calculations were run equivalent to the base case scenario of Table 4.1 (Series I) except that hydrogen combustion was switched off. Thus, hydrogen was present but it was only allowed to act as a chemically inert, noncondensable gas. Results are summarized as Case 4 in Table 4.2 with the pressure-time history also being given in Fig. 4.2. In this calculation, reaction of Zr was virtually complete and reaction of Fe was considerably more than 50% complete; reaction was almost entirely with steam. Energetically, this case is therefore very similar to Case 3 above. Nonetheless the peak pressure is now about 4.3 bars, which is well over 1 bar higher than the Case 3 pressure and is within the lowest portion of ranges cited above for the failure pressure. This difference is believed to be almost entirely due to the effect of the noncondensable gas in reducing the efficiency of the ice condenser in removing steam and, especially, energy from the gas mixture flowing through it.

There is considerable uncertainty in the magnitude of the noncondensable gas effect in these calculations. DCH scenarios involve unusual conditions in the ice compartment, including extreme temperature gradients, high flow rates, and hydrogen-rich atmospheres, all of which have important implications for the rates of mass and heat transfer to the ice surfaces. Although the CONTAIN ice condenser model does include some simplified representations of these effects, high accuracy is not expected and model validation for such conditions is non-existent. Hence, uncertainties are believed to be significant, although no detailed study of these uncertainties has been undertaken. Nonetheless, it remains clear that the effect of hydrogen as an inert, noncondensable gas would be important in DCH analyses of ice condenser plants even if the potential for combustion of this hydrogen could be ignored, e.g., by inerting the containment atmosphere. More importantly in the context of

analysis of noninerted plants, the noncondensable gas effect substantially raises the base pressure at the start of any subsequent hydrogen burn.

Effect of Air in the Lower Containment. As noted previously, air was calculated to be largely expelled from the lower containment in the TMLB' scenario chosen for analysis here. The Sequoyah risk profile also includes some core-melt scenarios in which the air return fans are operating and the vessel also fails while under high pressure. In some of these instances, spray operation will have resulted in heavy flooding of the cavity, presumably precluding DCH, but this is not always the case. It is therefore of some interest to consider the implications of scenarios in which fan operation mixes the contents of Cell 3 and Cell 1. Case 5 was run with the same total atmospheric masses in containment as in Case 4, but with the distribution being uniform between Cell 1 and Cell 3. (This treatment is not totally realistic, since fan operation would alter the total steam content of the atmosphere as well as its distribution, but the treatment is in keeping with the spirit of the present calculational series as a phenomenological sensitivity study.)

Some results for Case 5 are summarized in Table 4.2 and Fig. 4.2. It is apparent that the presence of air in the lower compartment does have a significant effect, increasing the calculated maximum pressure to about 5.1 bars, which is about 0.8 bars higher than in Case 4. Reasons for this difference include both the extra energy release associated with the oxygen reactions and the increased noncondensable gas effect, which results from both increased noncondensable gas mole fractions and also from the fact that nitrogen has poorer heat transfer properties than does hydrogen (the CONTAIN model includes an approximate treatment of this effect). The relative importance of these contributions has not been determined. It should be noted that realization of a considerable part of the extra energy associated with oxygen reactions is a consequence of the postulated recombination of hydrogen produced by metal-steam reactions so long as bulk oxygen is present in the cell atmosphere. Even in Case 5, the initial mole fraction of steam in Cell 1 (0.31) is considerably higher than the initial oxygen mole fraction (0.12) and this difference rapidly increases as oxygen is consumed. Hence, most of the metal reaction will be with steam, with the recombination reaction then providing the full oxygen reaction energy, until bulk oxygen in the cell is exhausted. Oxygen exhaustion occurs at slightly over 1 second into the calculation due to

the combined effects of reaction and very rapid flow out of the lower containment. Nonetheless, the extra energy released during this time is significant; note the rapid initial pressure rise for Case 5 in Fig. 4.2.

More extensive analysis of the effects of high air concentrations in the lower containment is beyond the scope of this study. Clearly it would need to be considered in more detail in any complete study of the potential contribution of DCH to the overall plant risk profile. The contribution of nitrogen to the noncondensable gas effect would likewise require more consideration in any evaluation of the efficacy of containment inerting for controlling DCH loads.

Effect of Depletion of Ice. In Section 3 of this report, it was found that containment compartmentalization effects in PWR large dry containments could substantially reduce DCH loads relative to what would be calculated using the simpler models of the CLWG, or even relative to single-cell CONTAIN calculations. In the case of Sequoyah, it is therefore of some interest to consider how much of the very large differences between the DHEAT2 and the CONTAIN results noted above might be associated with compartmentalization effects and how much is due to the ice condenser. The question is also of some practical concern, since SARRP identified a number of scenarios in which the ice condenser was rendered partially or totally ineffective, either by ice depletion or by the development of bypass paths.

Two cases were considered, both with hydrogen burns suppressed. In the first (Case 6 in Table 4.2), the calculation was run with ice depleted from the ice condenser but with the initial conditions otherwise the same as in Case 4. This case is unrealistic (and nonconservative) because, if the ice were depleted at the time of vessel breach, containment pressures would be higher at the start of DCH. Both the higher starting pressure and the increased mass of gas available for debris/gas heat transfer would contribute to developing higher pressures. Case 7 was therefore run with enough additional steam added to the containment atmosphere to bring the total pressure to 3.0 bars at the time of vessel breach.

Results are summarized in Table 4.2. The resulting maximum pressures, 6.7 and 8.6 bars for Cases 6 and 7 respectively, are considerably higher than the 4.3 bars calculated for the equivalent scenario with ice present, illustrating

the importance of the direct effects of the ice condenser. On the other hand, these pressures remain far below the extreme values cited above for DHEAT2, indicating that compartmentalization effects are important even in the absence of ice. No doubt this effect would also be subject to the various sensitivities that were investigated in connection with Surry in Section 3. In particular, the high Cell 3 atmospheric temperatures noted for these cases in Table 4.2, together with the extreme temperatures of the material entering from Cell 2, indicate that hypergolic hydrogen behavior is likely if not certain, which would substantially increase the expected loads.

4.2.2 Effect of Hydrogen Combustion.

In the calculations cited above, mole fractions of hydrogen in the upper containment reached values exceeding 0.13 by the end of the 30-second blowdown period in Case 4, and approached 0.09 in Case 5. These values are well above the ignition thresholds in the CONTAIN default burn model (0.08 and 0.07 in CONTAIN 1.04 and 1.06, respectively). Furthermore, the concentrations of steam and oxygen satisfied the flammability criteria by wide margins, and it does not seem very likely that ignition sources will be lacking during and immediately after a DCH event.

Case 8 was run using the same parameters as Case 4 except that a hydrogen burn was permitted to initiate once the hydrogen mole fraction reached 0.08, with the burn parameters otherwise being those of the default burn model. Case 8 is the "base case" of Table 4.1 (Series I). Some results are summarized in Table 4.2 and the pressure-time history is given in Fig. 4.3, which also repeats the pressure-time history of Case 4 for comparison purposes. As would be expected, the hydrogen burn seriously adds to the DCH threat, with a maximum pressure of about 7.0 bars being calculated.

The point at which the curves for Cases 4 and 8 diverge in Fig. 4.3 represents the time of burn initiation, which is seen to be well after the time at which debris injection terminates. Although most of the hydrogen in containment is produced during the 5-second injection time, the amounts transported to the upper containment are insufficient to meet the minimum flammable concentration criterion at this point. However, the continuing blowdown of steam into the hydrogen-rich lower containment forces additional

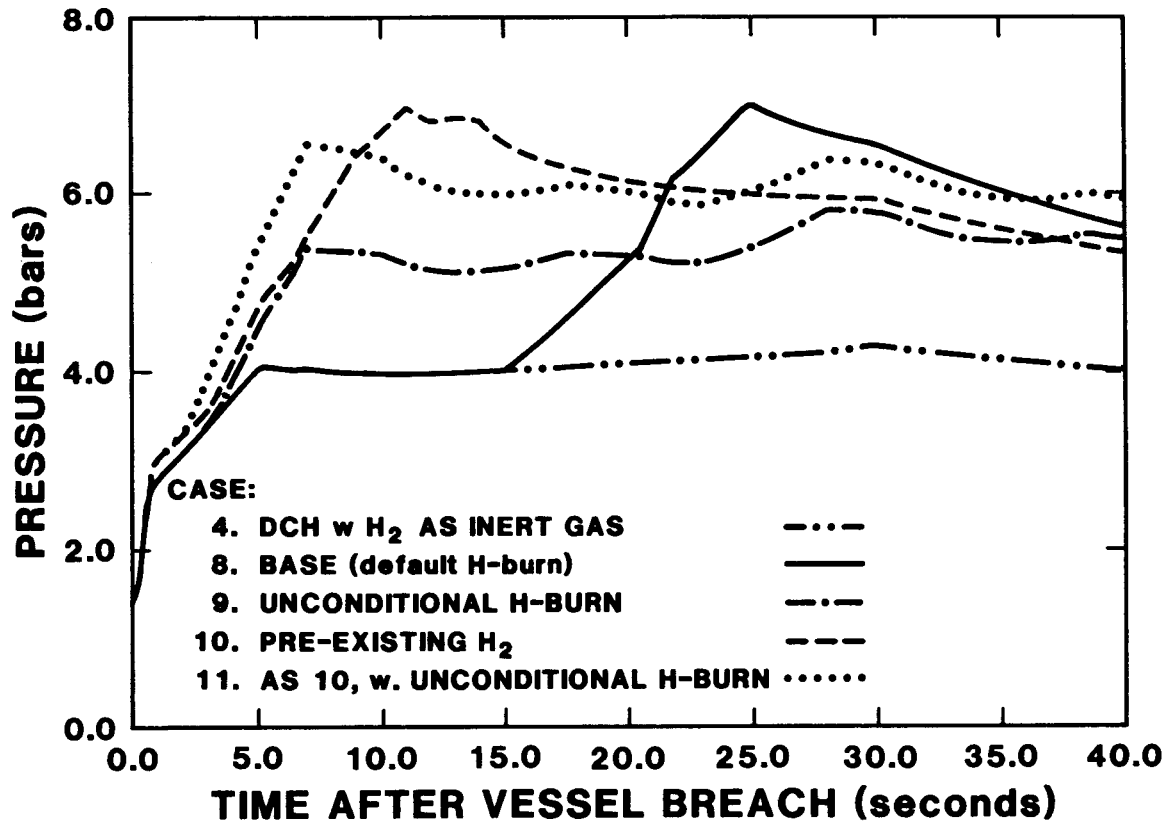


Fig. 4.3 Pressure-time histories calculated for various scenarios in the Sequoyah plant, with alternative assumptions concerning hydrogen combustion.

hydrogen into the upper containment, and the flammability criteria are met well before the blowdown ceases at 30 s in Fig. 4.3.

The temperature histories of the three cells are plotted for the base case in Fig. 4.4. As in Surry, extreme temperatures develop in the lower containment during debris injection. After debris injection ceases, temperatures fall rapidly due to rapid heat loss and the continuing inflow of relatively cool steam from the primary system. Temperatures in the ice condenser compartment are less extreme but still very high during debris injection, and then fall rapidly after injection ceases. The second abrupt temperature rise

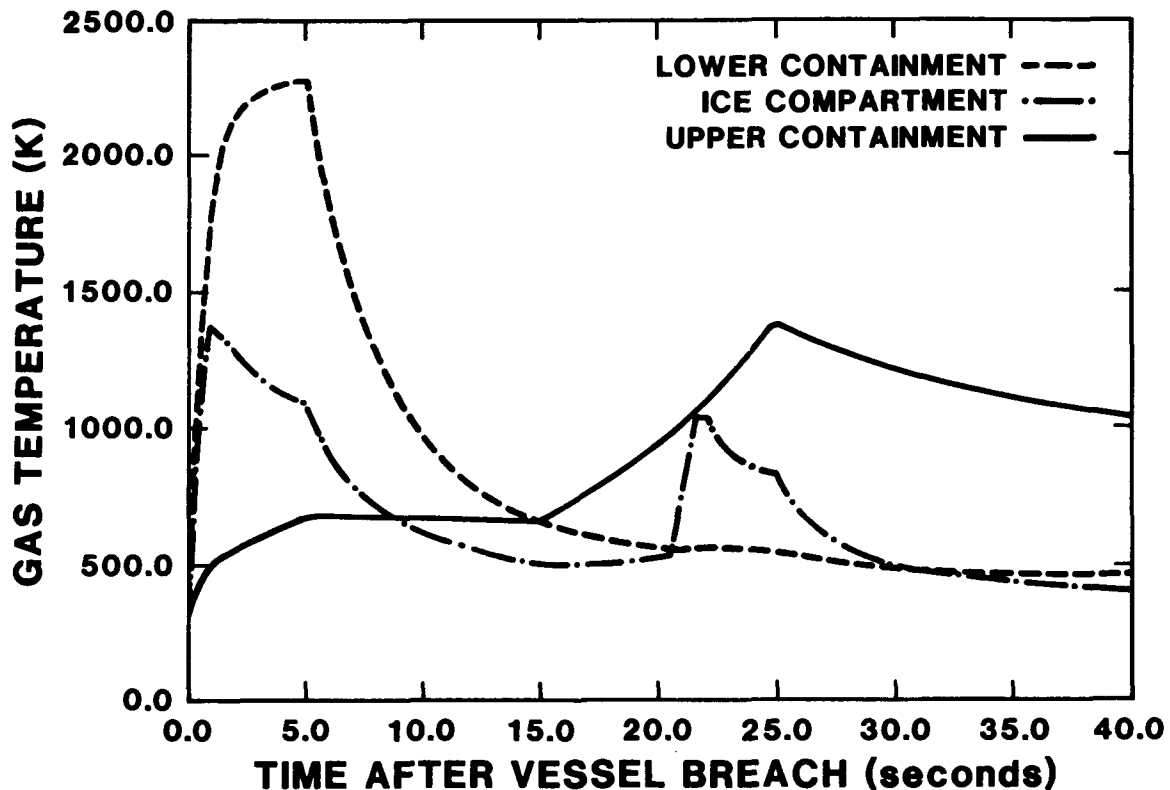


Fig. 4.4 Atmospheric temperature histories for the base case DCH scenario in the Sequoyah plant.

in the ice compartment at about 21 s reflects a hydrogen burn that begins after the pressure rise in the upper containment (due to the burn there) forces enough oxygen to flow back into the ice compartment to meet the default flammability criteria. The temperature history of the upper containment itself may be understood in terms of, first, the immediate response to debris injection and, second, the hydrogen burn initiating at about 15 seconds after vessel breach.

Effect of Unconditional Hydrogen Burns. From Table 4.2 and Fig. 4.4, it may be seen that, in the base case, gas temperatures in the upper containment at the end of debris injection are calculated to be about 680 K, while the gas entering the upper containment (which is 85% hydrogen) is almost 1100 K. No

burn has occurred up to this point, in the base case calculation. Although these temperatures are not quite as extreme as in the Surry base case, they are much higher than the temperatures for which the default burn model's flammability correlations were developed. Hence, hydrogen behavior similar to the hypergolic behavior discussed in connection with Surry should be considered here also. Indeed, it is not necessary to postulate true hypergolic behavior in order to obtain a similar result: since the upper containment contains less than a third of the steam required for inerting, even by the default criteria, it is only necessary to assume that the entering hydrogen plume ignites at some point and then continues to burn as a self-sustaining plume or jet flame.

In Case 9, the calculation was repeated with the burn parameters being prescribed so as to give an unconditional burn, as was done in Surry in order to simulate hypergolic behavior. Results are given in Table 4.2 and Fig. 4.3. Peak pressures, about 5.8 bars, are now significantly less than in the base case. The reason is that in Case 9 the hydrogen tends to burn off as it enters the upper containment, while it accumulates until the flammability threshold is met in the base case. The latter therefore gives a stronger burn once combustion does initiate. Nonetheless, even the unconditional hydrogen combustion adds about 1.5 bars to the maximum pressure calculated for the equivalent DCH scenario without burns (i.e., Case 4). The resulting threat is still very substantial, at least in the context of some of the failure pressures that have been estimated for the Sequoyah plant as cited above.

Effects of Igniters and Pre-Existing Hydrogen. In themselves, the hydrogen burns calculated here are not extremely severe. Even in the base case, the pressure rise due to the burn is only about three bars, which would pose only a moderate threat were it not for the high starting pressure at the time of burn initiation. At this time, the total hydrogen inventory in the containment is very large, about 920 kg, but only 30% of this has been been transported to the oxygen-bearing upper containment, with the remainder still residing in the inert lower containment and ice condenser. Once the burn initiates, no more hydrogen enters the upper containment because pressurization of the latter causes flow reversal. The large inventory of hydrogen remaining in the lower compartments suggests that severer burns would be possible given more efficient transport of the hydrogen to the upper containment.

Indeed, the ultimate limit on burn severity would be set by the available oxygen inventory, not the hydrogen inventory.

Postulating the availability of igniters could not greatly mitigate the scenario considered above. Full credit for burning off any hydrogen released to containment prior to vessel breach has already been taken. Igniters could, at most, reduce the ignition threshold from the base case value of 8% hydrogen to 6-7%. This effect would cause only a minor reduction in peak loads, considerably less than the reduction obtained in the unconditional burn case.

Even given operational igniters, the assumption used here that there would be no hydrogen present in the containment at the time of vessel breach is not fully realistic. In a station blackout scenario with existing igniter design (i.e., igniters dependent upon AC power availability), it is quite possible that all the hydrogen released prior to vessel breach would still be present in the containment.

Sensitivity to these assumptions was investigated in two calculations in which it was assumed that the hydrogen released prior to vessel breach was still present in the containment. This hydrogen, almost 250 kg, was assumed to be distributed equally between the three cells of Fig. 4.1. In the first of these calculations (Case 10), the base case burn parameters were used, while the second calculation (Case 11) employed the unconditional burn option, starting two seconds after the onset of debris injection.

Results are summarized in Table 4.2 and Fig. 4.3. When base case burn parameters are assumed, including the pre-existing hydrogen in the calculation does not increase the peak loads calculated; instead, the burn merely initiates earlier, during debris injection. With the unconditional burn option, the pre-existing hydrogen does increase the peak loads, though they are still somewhat less than those calculated for the base case. Thus, the presence of the pre-existing hydrogen substantially reduces the difference between the base case and the unconditional burn results.

These results suggest that the presence of additional hydrogen in containment at the time of vessel breach does not necessarily lead to a more severe scenario. However, these results are little more than suggestive and must not be overgeneralized. There are large uncertainties in the amount of hydrogen

produced by in-vessel zirconium oxidation, the fraction of this hydrogen released prior to vessel breach, and how this hydrogen will be distributed within containment at the time of vessel breach. The assumptions made here concerning these parameters are largely arbitrary, and quite different results could be obtained if different assumptions were made. Furthermore, previous analyses have shown that, if enough hydrogen is released, detonable gas compositions may develop in parts of the ice condenser and/or the upper plenum [Ca84, Bn87c]. If the onset of debris injection triggers an actual detonation, the ability of the ice condenser to mitigate the subsequent DCH loads could be compromised (e.g., through the formation of bypass paths), even if the detonation itself did not directly fail the containment [Bn87c].

Effects of Limitations of the CONTAIN Reaction Model. No calculations have been performed for the specific purpose of investigating uncertainties associated with the various limitations of the CONTAIN reaction model, but there are at least two such limitations that should be kept in mind. The first concerns the inability of the single-field debris model to provide detailed tracking of the temperature history of the reacting debris and, hence, the inability to give a good description of the temperature dependence of the drop-side reaction rate limits. Sensitivity studies performed for the Surry plant indicated that these uncertainties could become important in scenarios in which the bulk gas temperatures were below the values at which rapid reaction is expected, but were not important when the temperatures remained sufficiently high. In the latter case, the debris does not cool greatly and reaction rates remain high for any reasonable rate expression. From Fig. 4.4 and Table 4.2, it is apparent that the second situation prevails in Cell 1, where most of the reaction is calculated to occur. Hence, it is not believed that drop-side reaction rate limits introduce major uncertainty into the specific scenarios treated here.

Another limitation of the reaction model is that all reactions are assumed capable of going to completion, while in reality the steam-iron reaction can not proceed if the steam/hydrogen ratio falls too low, e.g., below ~0.5 for pure Fe in equilibrium with pure FeO. Since the calculated steam/hydrogen ratios do fall to levels below 0.5 in these analyses, it is likely that the calculated hydrogen production is being overestimated somewhat.

4.3 Sensitivity Studies for the Sequoyah TMLB' Scenario (Series II and III Calculations).

In Section 4.2, results of calculations using the most recent version (1.06) of CONTAIN were presented. In the present section, results of some of the earlier sensitivity studies performed using the CONTAIN 1.04 version of the IDHM will be summarized.

4.3.1 CONTAIN 1.04 / CONTAIN 1.06 Differences.

Since the calculations discussed in Section 4.2 were made with a different version of the code from the one in the Series II and Series III calculations, and some of the input parameters also differed, a brief discussion will be given of the impact of these changes upon the results. The more important of these differences are as follows:

- 1). CONTAIN 1.04 versus CONTAIN 1.06 modeling changes, of which the most important is believed to be treatment of atmosphere/structure radiative heat transfer by the improved Modak model in CONTAIN 1.06 versus the Cess-Lian model in the older version.
- 2). Correction of the inconsistency in the energy accounting scheme which existed in the CONTAIN 1.04 version of the IDHM (this inconsistency did not affect non-DCH calculations using version 1.04); see Section 3.2.3.
- 3). In the CONTAIN 1.06 calculations of Section 4.2, the blowdown steam and hydrogen were assumed to be at the steam saturation temperature for the primary system pressure. In the earlier calculations, the blowdown enthalpy was somewhat higher. The difference in enthalpies is about equal to that required to heat the steam by 90 K, after blowdown.

A calculation was run on CONTAIN 1.04 using the same input deck as used in the base case (Case 8) of Table 4.2. Peak pressures were 7.33 bar, about a third of a bar higher than in the base case. This result reflects the combined effects of both the modeling changes and the energy accounting error noted above.

The effect of the difference in blowdown enthalpy was explored by running a case on CONTAIN 1.04 with the higher enthalpy, but otherwise identical to Case 8 of Table 4.2; this calculation closely resembles the base case for the Series III calculations (Table 4.1). The peak pressure was 7.68 bar, about 0.35 bar higher than the pressure calculated using CONTAIN 1.04 assuming the

saturation enthalpy. The extra energy introduced into the lower containment during the 30-second blowdown period is about 10% of the DCH chemical reaction energy, and effects were trivial during the debris injection stage itself. However, the somewhat higher steam temperatures in the lower containment after the cessation of debris injection were sufficient to improve hydrogen transport to the upper containment, which appears to be the principal reason for the increased maximum pressure calculated.

There is significant uncertainty associated with the actual energy of the blowdown steam, as well as substantial uncertainties concerning the quantity and the timing of the blowdown. The response to this difference in blowdown enthalpies is an indication of the sensitivity of the results to the blowdown details: the difference between the two values of the enthalpy assumed are believed to be well within the uncertainty range for this parameter.

4.3.2 Containment Loads as a Function of Corium Mass Participating and Debris Trapping Rate.

Using the CONTAIN 1.04 version of the IDHM, a series of calculations was performed in which the fraction of the total corium inventory injected was systematically varied from 0 to 1.00. The trapping rate was not scaled to the cell size as in other calculations; instead, the entire series of calculations was performed twice, once using a value of $\lambda_{tr} = 3.33 \text{ s}^{-1}$ for all cells and once using $\lambda_{tr} = 0.1 \text{ s}^{-1}$ for all cells. The intent was to span a wide range of possible values of the trapping rate. No claim is made that these values are bounding, although it does seem very unlikely that trapping could be slower than implied by the value of 0.1 s^{-1} .

Other parameters for these calculations are summarized in Table 4.1, Series II. The default hydrogen burn model was used. A noteworthy variation from other calculations discussed in this report is the assumption of a considerably larger iron content of the corium, almost 50000 kg as compared with about 22000 kg in Series I and III. The larger value is based upon the melt composition at vessel breach cited in BMI-2104 analysis of the Sequoyah TMLB' sequence [Gi84]. (These calculations were performed in support of the NUREG-1150 effort, which relied heavily upon the BMI-2104 work.) In addition, no drop-side reaction rate limits were assumed, other than the assumption of a reaction threshold temperature of 1000 K. As in previous calculations, it was

assumed that 50% of the hydrogen due to in-vessel zirconium oxidation was released to containment along with the steam during blowdown, while the remainder was assumed to have been released and burned off prior to vessel breach.

The maximum pressure calculated as a function of corium participation fraction is plotted in Fig. 4.5 for both values of λ_{tr} . The abrupt rise in

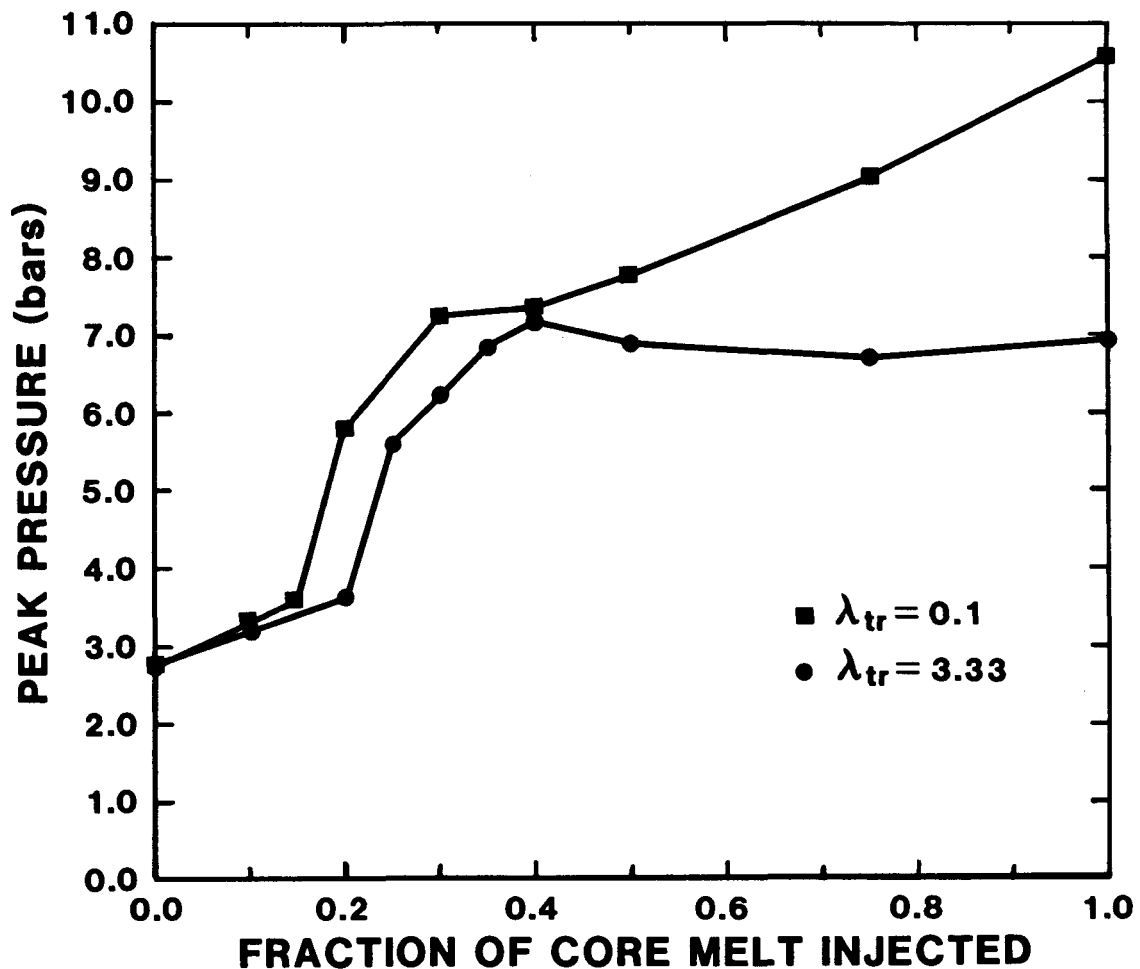


Fig. 4.5 DCH pressures in Sequoyah as a function of core participation fraction for two different values of the trapping rate.

peak pressure at about 20% core injection corresponds to the onset of hydrogen combustion; i.e., for smaller participation fractions, hydrogen mole fractions in the upper containment do not meet the minimum value (0.08) required for flammability in the CONTAIN 1.04 default correlations.

Some of the most interesting features of the results displayed in Fig. 4.5 include the following:

1. Development of containment-threatening loads does not require large injection fractions, provided only that hydrogen concentrations in the upper containment do meet the flammability criteria.
2. Once the flammability criteria are met, further increases in the corium mass participating do not result in significant increases in the peak pressure calculated for the rapid-trapping case. For the case with slow trapping, there is a gradual increase with injected corium mass.
3. For low to moderate corium injection fractions, there is relatively little sensitivity to the large variations in trapping rates investigated here. At larger core injection fractions (≥ 0.5), sensitivity to the trapping rate does increase.

The lack of sensitivity to trapping rate at the lower corium injection fractions may be explained in terms of the rapid reaction rates and debris-gas heat transfer rates, as was discussed in connection with Surry (Section 3.2.3). The insensitivity of the pressure to the debris mass injected in the rapid-trapping case appears to reflect several influences:

- 1). At corium injection fractions greater than about 0.3, the metal-steam reaction becomes steam-starved; i.e., insufficient steam is available during the injection period to oxidize all the metal. Thus, additional increases in the injected mass do not lead to large additional increases in the hydrogen produced.
- 2). Given that total hydrogen production is relatively independent of injected corium mass, peak pressures could still increase if the driving force for transport to the the upper containment were to increase. Since the moles of total gas injected (steam plus hydrogen) is independent of corium mass in these calculations, increased driving forces would require increased lower-containment temperatures. In Fig. 4.6, maximum temperatures in the lower containment are plotted as a function of corium injection fraction. It is seen that there is a rapid initial rise at low injection fractions but that, for fractions ≥ 0.3 , there is a tendency toward thermal saturation, with only moderate additional temperature rises being calculated at large injection fractions because most of the additional energy remains in the debris. (This is not a consequence of the steam starvation noted above: the energy production is primarily due to the zirconium reaction, and zirconium oxidation is not seriously steam starved, because of the reaction hierarchy assumed in the CONTAIN IDHM.)

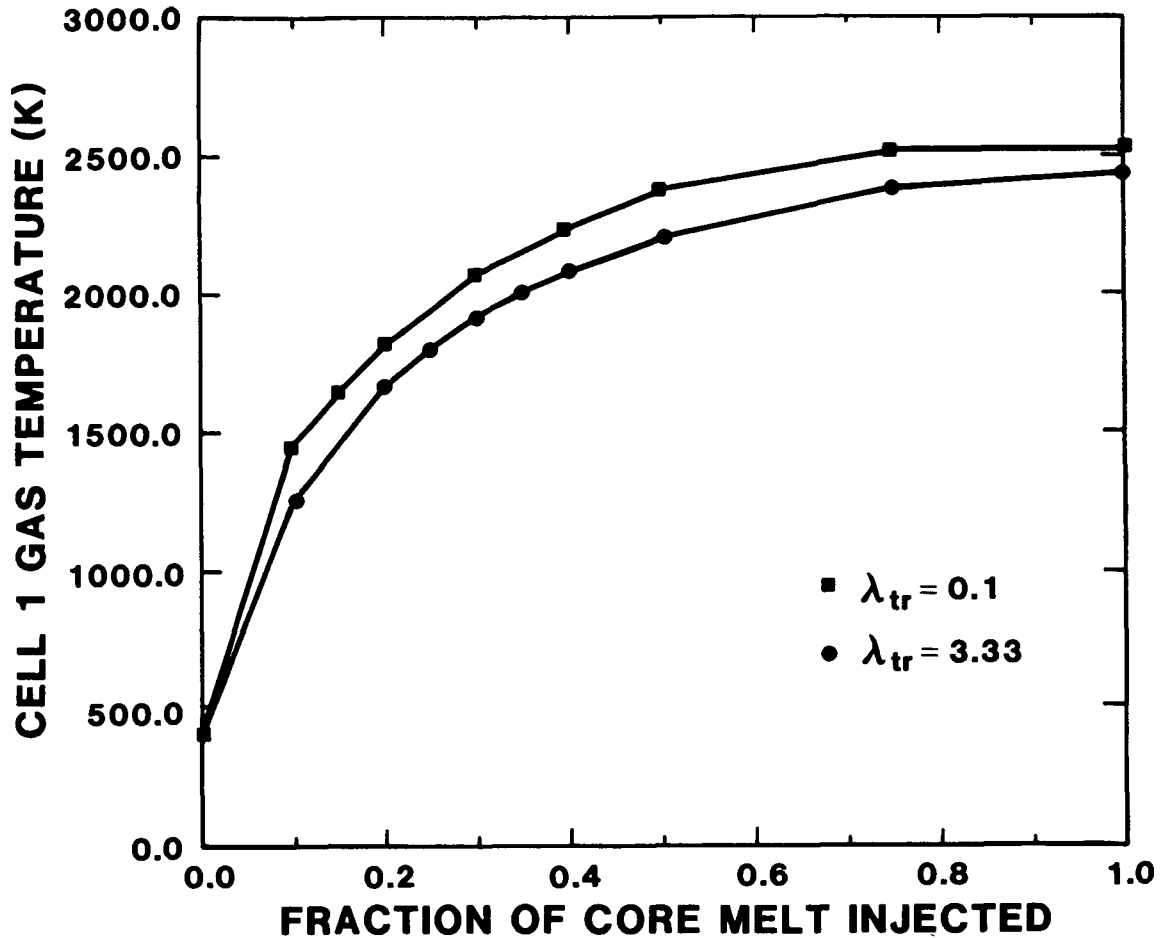


Fig. 4.6 Lower containment temperatures at the end of debris injection, calculated as a function of core participation fraction for two different values of the trapping rate.

- 3). In cases with low injection fractions (≤ 0.35), the burn does not initiate until well after debris injection is over, and the steam blowdown is complete by the time the burn is complete. At higher injection fractions, the reverse is true: the burn initiates at about the time debris injection is complete, and only about half the blowdown steam has been added by the time the burn is complete. Hence, in the latter, the effects of the blowdown and the burn are not completely additive, and rapidly-falling temperatures in the lower containment permit substantial backflow to partially compensate for the pressurization due to the burn. These effects are smaller in the cases with lower injection fractions, which tends to compensate for the lower hydrogen production and smaller energy releases associated with the latter cases.

At low trapping rates, the maximum pressures do increase with injected corium mass, leading to a significant sensitivity to λ_{tr} at high injected masses. There are at least two reasons for this effect. First, significant amounts of debris, including some unreacted iron, reach the upper containment when the trapping rates are low. Second, at low trapping rates, debris remaining airborne in the lower containment substantially increases the heat capacity of the debris-gas system which, in turn, reduces the rate of cooling of the lower containment. This effect, in turn, reduces the extent of the backflow from the upper containment during the hydrogen burn and, hence, increases the degree to which the burn can pressurize the containment. Both effects increase with increasing injected mass.

Neglect of drop-side reaction rate limitations no doubt causes some overestimate of the rates of hydrogen production in these calculations. However, this effect is unlikely to be large once bulk gas temperatures in the lower containment rise above the melting point of steel and its oxides, ≤ 1700 K; from Fig. 4.6, it is apparent that this condition is satisfied even for rather low injection fractions, ≤ 0.2 . Likewise, the neglect of chemical equilibrium in the iron-steam reaction can lead to overestimation of hydrogen production at higher injection fractions, > 0.3 . Neither effect is likely to reverse the conclusion that substantial threats to containment integrity can arise at moderate injection fractions due to the combined impact of DCH pressurization and combustion of the hydrogen produced by metal-steam reactions. Indeed, it is questionable as to whether the tendency of the CONTAIN model to overestimate the extent of reaction is enough to compensate for the neglect of pre-existing hydrogen in containment at the time of vessel breach.

The use of the default burn model also neglects the possibility that hydrogen entering the upper containment may burn as a plume, more or less as it enters. Although this effect might reduce peak combustion loads somewhat, it would also lower or eliminate the threshold effect for the onset of hydrogen combustion as a function of corium injection fraction.

Finally, it must be emphasized that all DCH calculations for ice condenser plants are expected to be sensitive to parameters governing the generation of hydrogen and its transport to the upper containment. Some examples of such sensitivities will be given in the next subsection of this report. Given

different values of the parameters governing hydrogen generation and transport, the sensitivity to the injected mass and the trapping rate could be rather different from that which has been found here.

4.3.3 Comparison of Some DCH Sensitivities in Surry and Sequoyah.

In this section, we compare results obtained in some sensitivity studies performed for the TMLB' DCH scenarios in both Sequoyah and Surry. Many of the Surry results are the same as some of the cases discussed in Section 3.2.3 and will be described here only in the context of considering the differences (or similarities) in the response of the two different types of containment to the various parameters considered. For both plants, the CONTAIN 1.04 version of the IDHM was used.

Base case parameters are those of Table 4.1, Series III for Sequoyah and those given in Section 3.3.1 for Surry. The parameters were chosen to be similar (with corium masses scaled to core size) except for the treatment of hydrogen released prior to vessel breach and the treatment of the blowdown at vessel breach. In Surry, about 75% of the hydrogen produced by in-vessel zirconium oxidation was assumed to be released prior to vessel breach (based upon a MARCH calculation). This hydrogen was assumed to be still present in the containment atmosphere at vessel breach, since the default flammability criteria were not approached and containment temperatures prior to vessel breach were in a regime for which these criteria should apply. In Sequoyah, 50% of the in-vessel hydrogen was assumed to have been released and burned off prior to vessel breach, as discussed in Section 4.1. For both plants, in-vessel hydrogen not released prior to vessel breach was assumed to enter along with the blowdown steam.

In Surry, the blowdown was based upon a MARCH calculation and included both dead-ended primary system water and superheated steam, with about two thirds of the total mass being injected into containment during the first half of the blowdown period. In Sequoyah, the blowdown was assumed to be uniform over the specified blowdown time, with the total mass taken to correspond to the primary system filled with saturated steam at system operating pressure, though the actual blowdown enthalpy specified was somewhat higher than saturation, as noted in Section 4.3.1. The Surry blowdown may be somewhat the severer of the two in the present context, in that the higher injection rates

at early times are expected to be more favorable to the transport of DCH energy to the upper containment.

Although other parameters defining the base cases were similar for the two plants, this does not mean that the values chosen are actually equally realistic for the two plants. For example, more detailed analysis might show that the assumed 75% corium injection fraction was less plausible in one plant than in the other, or that the use of Eq. 2.1 to estimate trapping rates introduces greater error in one case than in the other. No claim is made that the base case constitutes a "best estimate" scenario for either plant.

The parameter variations considered here and the maximum pressures obtained are summarized in Table 4.3. Since hydrogen phenomenology has been shown to be of such great importance to DCH scenarios, all parameter variations were run using both the default burn model and the unconditional burn option for both plants.

Effect of Hydrogen Combustion Behavior. In Surry, the unconditional burn assumption uniformly gives substantially more severe results in all cases, for the simple reason that steam inerting prevents the occurrence of significant burns in the default model. In Sequoyah, the default burn usually (not always) gives the more severe response because the upper containment is not inert and the default model allows hydrogen to accumulate until the ignition threshold is reached. Since both models predict the occurrence of a burn in the ice condenser plant for most of the scenarios, the choice between the models is generally less significant than in Surry. Also, in Sequoyah, the default burn model gives a less regular variation in the peak pressure as a function of the other parameters considered. This irregularity appears to be due to the fact that the peak pressures are somewhat sensitive to accidents of timing between burn initiation and other important events of the calculation; in two calculations (Cases 6 and 9), burns did not occur at all under the default criteria.

It should be remembered that the behavior designated "unconditional burn" here may involve rather different combustion conditions which have quite different criteria for their occurrence in the two plants. In Surry, the unconditional burn involves gas mixtures with high steam contents and rather low oxygen contents, with the reaction energy insufficient to heat the mixture

Table 4.3

Comparison of sensitivity study results for Surry and Sequoyah.
Peak pressures are given in bars (10^5 Pa).

Case	Variation	Surry Plant		Sequoyah Plant	
		Default	Unconditional	Default	Unconditional
		<u>Burn</u> <u>P_{max}</u>	<u>Burn</u> <u>P_{max}</u>	<u>Burn</u> <u>P_{max}</u>	<u>Burn</u> <u>P_{max}</u>
1	Base case	7.2	9.3	7.6	6.6
2	No trapping: $\lambda_{tr} = 0$	7.9	9.8	7.4	7.4
3	Fast trapping: $\lambda_{tr} = 10\lambda_{tr}$ (base)	6.4	8.5	6.4	5.5
4	Change drop diam. from 0.5 to 1.0 mm	6.9	9.0	6.4	5.8
5	Change steam blowdown from 30 to 10 sec.	9.5	12.3	8.5	8.8
6	Change core injection fraction from 0.75 to 0.25	5.9	7.7	3.4	4.6
7	Change Zr oxidation from 0.5 to 0.30	7.4	9.1	7.6	6.6
8	Add 2.0E4 kg co-dispersed water	8.8	11.6	8.1	7.7
9	Add 1.0E5 kg co-dispersed water	6.9	9.5	3.6	4.2

greatly (more than a few hundred degrees K); an "unconditional burn" requires that the mixture temperature before reaction must be fairly close to the temperatures for rapid reaction at the start. In Sequoyah, "unconditional burns" may merely involve an entering plume of hydrogen which ignites at some point and then continues to burn as a conventional self-sustaining plume flame, since the upper containment is not inert.

b. Effect of Trapping; Cases 1, 2, and 3. The fractional trapping rate in the base case was based upon Eq. 2.1, as noted previously. Sensitivity to

trapping rates does not differ greatly for the two plants, though it may be somewhat greater for Sequoyah. Possible reasons include greater dependence upon hydrogen produced during DCH for the generation of high loads (much of the hydrogen in the upper containment in the Surry analysis was released prior to vessel breach, while all such hydrogen is assumed burned off in the Sequoyah treatment). The fact that the Sequoyah default burn calculation with no trapping actually gives a lower pressure than the base case may be taken as an illustration of the somewhat irregular behavior of the default burn model as a function of other parameters that was noted above.

In both plants, the two extremes of no trapping ($\lambda_{tr} = 0$; case 2) and very fast trapping ($\lambda_{tr} = 10 \lambda_{tr}(\text{base})$) show that the sensitivity to debris de-entrainment is considerably less than has generally been assumed in previous assessments of DCH (see, for example, the discussion of DCH for Sequoyah in [Bn87c]). A major reason for this relative insensitivity is that a significant fraction of the potential threat to containment integrity resides in the chemical potential of the hydrogen generated in the vicinity of the vessel breach, relative to the oxygen which resides in more distant parts of the containment. The reaction rates are so rapid (for the parameters explored here) that large changes in the trapping rate do not dramatically affect the quantity of hydrogen produced. The trapping rate does affect the intercell transport and exchange of thermal energy, however, and this effect is reflected in the sensitivity seen in these three cases, but the size of the sensitivity indicates that the resulting effects are of secondary importance compared to others discussed here. From a calculational viewpoint, this is fortunate, because an accurate prediction of the extent of de-entrainment at each location in the debris flow pattern is beyond the capability of any existing computer code.

c. Effect of Droplet Diameter; Cases 1 and 4. Experimental results from tests at Sandia [Ta86a] and Argonne [Sp86] indicate that debris particles will typically be around 0.5 mm in diameter, which is the value assumed here in the base case. However, there is a wide distribution of particle sizes, and moreover, the mean size will doubtless change with different debris injection conditions. The effects seen here are slight for Surry, but moderate for Sequoyah. The principal reason for the sensitivity is the reduction in the rates of heat and mass transfer from the drops due to the larger surface-to-volume ratio. Since these energy injection and chemical reaction rates are

competing with rapid removal rates such as heat transfer to heat sinks and debris de-entrainment, the result is reduced peak pressure. Again, the greater sensitivity found for Sequoyah may reflect a greater sensitivity to any factor which alters the rates and amounts of hydrogen generation during DCH.

d. Effect of Steam Blowdown Timing; Cases 1 and 5. There is considerable uncertainty about the configuration and condition of the debris residing in the lower head region at the time of vessel failure. There is also uncertainty about the interaction between the debris flow out the breach and the flow of the steam/hydrogen mixture driving the debris out. Finally, there is uncertainty concerning the time dependence of the size and shape of the vessel breach while melt is being ejected from the vessel. All of this translates into a high degree of uncertainty regarding the relative timing of melt ejection and steam blowdown. As seen in Case 5 of Table 4.3, the effect on peak pressure is very significant for both plants and both burn models. In all cases, the reasons are essentially as discussed previously for Surry (Section 3.2.3), i.e., enhanced transport of energy and hydrogen when the blowdown is more rapid. In Sequoyah, the effect of the rapid blowdown is greater in the unconditional burn calculation than in the default burn calculation. The reason is that, when the hydrogen is delivered more rapidly, less benefit results from burning it off as it is delivered, and the difference between the two models is reduced.

e. Effect of Core Injection Fraction; Cases 1 and 6. The importance of the quantity of debris which is injected into the containment has long been recognized as a key uncertainty in DCH analysis. Case 6 demonstrates that the present analysis also indicates that this sensitivity is important. However, the effect is not as large as predicted by earlier, simplified, analyses, such as the DHEAT calculations presented in NUREG-1079. While one should avoid over-simplification of these complex processes, the reduced sensitivity can generally be attributed to the saturation effects discussed in Sections 3.2.3 and 4.3.2. There is no obvious difference in the sensitivity of the two plants to the injected mass in the unconditional burn case. In the default burn case, the apparent sensitivity in Sequoyah is larger because, at the low injected mass, the default burn criteria were not met. Different results might be obtained for this case if hydrogen released to containment prior to vessel breach were included in the calculation. (In comparing these results

with those of Section 4.3.2, the considerably smaller iron content of the corium assumed here leads to somewhat higher injection fractions being required in order to meet the default burn criteria.)

f. Effect of In-vessel Oxidation Fraction; Cases 1 and 7. In conventional degraded core accident progression analysis, the fraction of Zr which is oxidized in-vessel is an important uncertain parameter, since it can affect the hydrogen concentration at the time of vessel failure, and therefore determines the potential size of burns which occur then. By contrast, in these DCH analyses the sensitivity is quite small. Reasons for this result include a tendency for the impact of enhanced zirconium content of the melt to be compensated for by the effect of reduced production of hydrogen prior to vessel breach. In addition, the thermal saturation effect discussed in connection with the Surry plant (Section 3.2.3) appears to play an important role for Sequoyah also. For both plants, it is likely that the latter arguments will break down in any scenario for which the lower cell gas temperatures do not rise to levels approaching the debris temperatures. When atmospheric heating is not so extreme, it is likely that the energy release associated with zirconium oxidation can play a more important role, as discussed in connection with the Surry water quench scenarios (Section 3.3.3).

g. Effect of Co-Dispersed Water; Cases 1, 8, and 9. In many hypothetical accident sequences, a substantial amount of water may be present in the reactor cavity at the time of high pressure melt ejection. There is a great deal of uncertainty regarding the interaction between the core debris jet and this water. One scenario is that one or more steam explosions will occur after only a fraction of the debris has been injected into the cavity, and that the cavity water will then be dispersed ahead of the bulk of the injected debris. Another possibility is that the relatively cold water will be co-dispersed with the debris, exiting the cavity region as small droplets intimately intermixed with the debris, steam, and hydrogen. Reality would no doubt be a mixture of these two alternatives; i.e., some fraction of the cavity water would be co-dispersed, but it is at present very difficult to predict with confidence what that fraction is. Experiments with water-filled cavities have been somewhat inconclusive, in part because of the tendency of the reinforced concrete cavity structures to be disassembled by the debris-water interactions [Ta84b].

The response of Surry DCH scenarios to co-dispersed water was discussed in some detail in Section 3.3. Cases 8 and 9 show a qualitatively similar behavior for Sequoyah in that moderate quantities (2×10^4 kg) yield a scenario more severe than the base case while very large quantities (10^5 kg) lead to mitigation. Quantitatively, there is a distinct difference, with the aggravating effect of moderate amounts being less for Sequoyah and with the mitigating effect of large amounts being much greater. In Surry, the aggravating effects of moderate amounts was associated with the increased steam supply improving the transport of thermal DCH energy to the upper containment, with an additional increase in severity due to improved hydrogen transport in the unconditional burn case. In Sequoyah, the ice condenser is expected to prevent as large an increase in the direct transport of DCH thermal energy, and it is therefore reasonable that the total effect be less.

A major reason for the mitigation observed in the Sequoyah calculation with 10^5 kg of co-dispersed water is that the water cools the bulk debris temperature below the input reaction threshold temperature (1200 K) during much of the debris injection period, thereby shutting off the generation of hydrogen. The result is that the default flammability criteria are never met and no burn occurs using the default model; even the unconditional burn is substantially reduced. In addition, containment conditions are so cool and wet in this scenario that the unconditional burn assumption loses its credibility. Again, rather different results might be obtained for this scenario if hydrogen released to containment prior to vessel breach were to be included.

The CONTAIN single-field debris model is, of course, incapable of giving a quantitative representation of the degree to which quenching can reduce the generation of hydrogen in this kind of scenario. However, there is little reason to doubt that the effect is potentially important in ice condenser DCH scenarios if substantial water is present in the cavity. Indeed, it may manifest itself at considerably smaller quantities of water than the 10^5 kg assumed here, e.g., if less conservative parameters are chosen for the drop-side reaction rate limits (see Section 3.3.3).

5. COMPARISON OF DCH SENSITIVITIES IN THE SURRY AND BELLEFONTE PLANTS

In this section, we compare results obtained in some sensitivity studies performed for the TMLB' DCH scenarios in the Surry and the Bellefonte plants. Bellefonte is a PWR plant with an atmospheric large dry containment having a very large capacity, about 96000 m³ volume with an estimated failure pressure of at least 10 bars [Ju84]. The calculations to be discussed were performed at a relatively early stage of the CONTAIN IDHM application program. The model used was essentially the CONTAIN 1.04 version of the IDHM discussed previously except that modeling for drop-side reaction rate limits (other than the reaction threshold temperature) had not yet been incorporated. The results obtained have been described in some detail previously [Ga86], and are included here partly for the sake of completeness. The present discussion will be limited and will emphasize the differences and similarities in the response of the two different containments to the various parameters considered.

Base case parameters for these calculations are summarized in Table 5.1. They differ substantially from those used in many of the preceding calculations. The corium injection fraction was taken to be 50%, not 75%, of the total inventory, duration of injection was 10 seconds rather than 5, and there was no trapping in the base case (i.e., debris remains suspended in the atmosphere indefinitely). The base case debris drop size was 1 mm, rather than 0.5 mm, and no drop-side reaction rate limits were included. These differences tended to compensate for one another and in the case of Surry, at least, the base case peak pressures differ only slightly (0.15 bar higher) from the CONTAIN 1.04 base case result of Section 3.2.3. Despite this similarity, caution is required in making any comparisons between the results of these calculations and those discussed previously.

Containment nodalization assumed for Surry was the same as in the other calculations considered in this work (Fig. 3.2), while the nodalization used to represent Bellefonte is illustrated in Fig. 5.1. As in Surry, debris is assumed to be injected into the relatively small Cell 1 representing the cavity and immediately adjacent volumes, and the principle transport paths to

Table 5.1

Base Case Parameters for the
Surry-Bellefonte Study

Input Parameter	Surry	Bellefonte
CONTAIN Version	1.04	1.04
In-vessel corium composition		
UO ₂ (kg)	80000	106000
Zr (total, kg)	16500	25900
fraction oxidized	0.5	0.5
Steel (as Fe, kg)	16500	45360
Initial corium temperature (k)	2550	2550
Corium fraction injected	0.5	0.5
Duration of melt injection (s)	10.0	10.0
Duration of blowdown (s)	30.0	30.0
Debris trapping rate (s ⁻¹)	0.0	0.0
Debris drop diameter (mm)	1.0	1.0
Chem. reaction cutoff temp. (K)	1200	1200
Debris-gas blackbody multiplier, α_g	0.5	0.5
Debris-wall blackbody multiplier, α_w	0.0	0.0
Hydrogen Burn Model	Default	Default

the upper containment (Cell 7) involve passage through intermediate compartments. Unlike the Surry representation used, however, much of the total volume below the upper containment is bypassed by the main flow: little transport through Cells 4, 5, and 6 occurs, and only Cells 2 and 3 play a role similar to that of the "basement cell" (Cell 2) of Surry in Fig. 3.2. The combined volume of these cells in Bellefonte is considerably smaller than the analogous volume in Fig. 3.2, especially in comparison with the total volume; i.e., 5600 m³ out of 96000 m³ in the Bellefonte nodalization versus 9300 m³ out of 49200 m³ in the Surry nodalization. The effect of this difference has

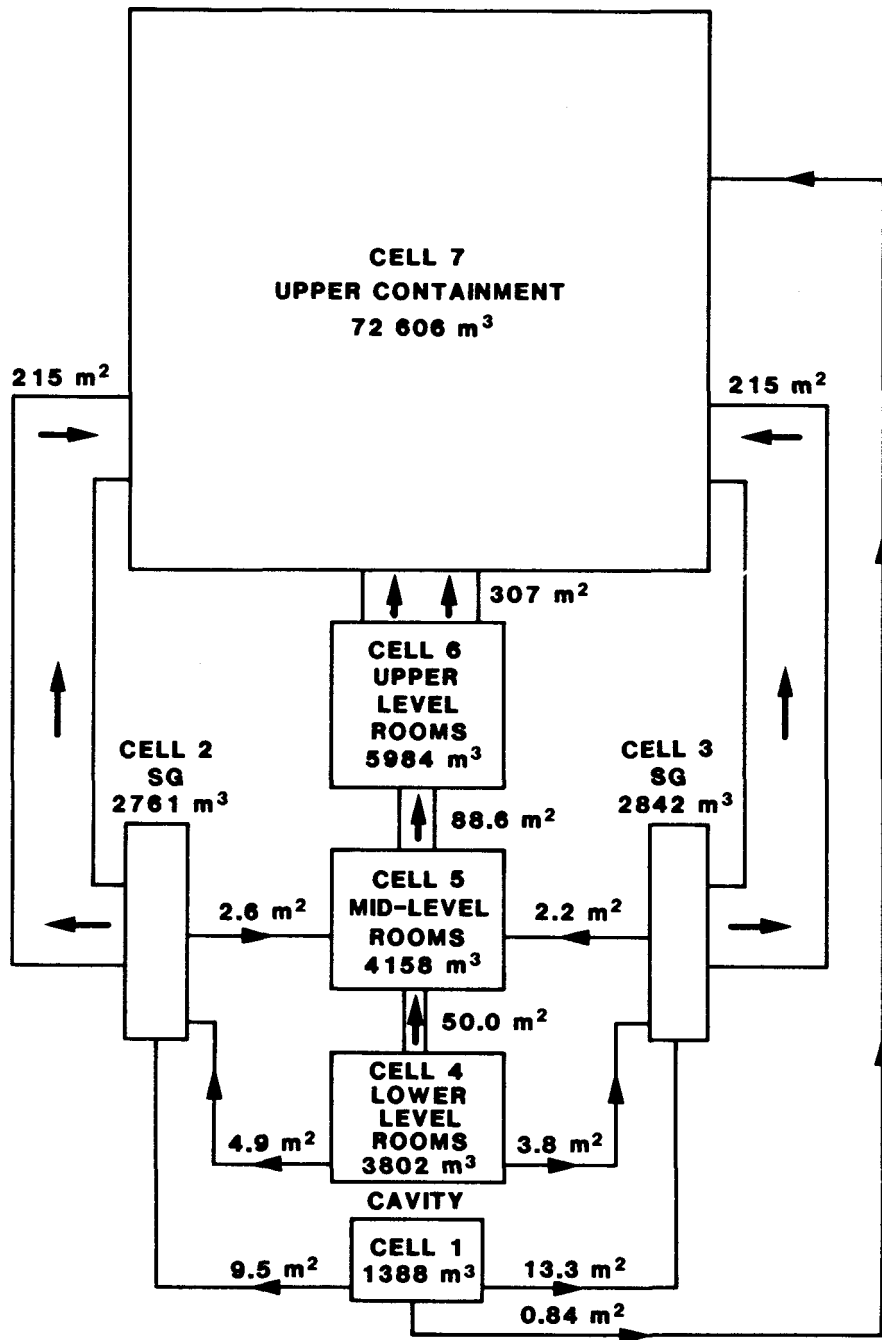


Fig. 5.1 Nodalization used for CONTAIN calculations of DCH scenarios in the Bellefonte plant.

not been studied in detail. It is plausible, however, that the competition between transport of debris and energy through the intermediate compartments, versus loss in those compartments, may be somewhat more favorable to transport in Bellefonte than in Surry. In this case, Bellefonte might be expected to show somewhat less sensitivity to effects which increase the rate of energy transport to the upper containment. Conditions existing within containment at the time of vessel breach were based upon CONTAIN calculations using primary system sources calculated by the RELAP code prior to core degradation, and by the MARCH code after the onset of core degradation.

Results of the calculations are summarized in Table 5.2. The first column gives the case numbers; the number refers to the parameter set used and the letter indicates the plant (S for Surry, B for Bellefonte). The next two columns give, respectively, the duration of debris injection and the duration of the primary system blowdown assumed. The fourth column indicates any other differences with respect to the base case input parameters. The last two columns give the maximum pressures calculated for Surry and for Bellefonte, respectively. A blank in one of these columns indicates that the particular parameter set was not run for that plant; only a few of the parameter sets were run for both plants. Some points of interest in these results include the following:

Effect of Hydrogen Combustion Model: Cases 1S, 2S; 1B, 2B, 14B. In Surry, hydrogen burns were insignificant when the default model was used because of steam inerting. In Bellefonte, the hydrogen mole fraction in the upper containment reached the flammability threshold, 0.08, at a time the steam mole fraction was about 0.45, which is somewhat less than the inerting threshold, 0.55. Hence, a burn occurred even with the default model. However, under steam-rich conditions, the flame speed correlations (taken from the HECTR code [Di86]) used in the CONTAIN default model predict a very slow burn, so that the burn adds relatively little to the total DCH pressure in this instance. Case 14B was run with all burns suppressed and with parameters otherwise the same as the base case, with a peak pressure of 6.3 bars as opposed to 6.6 bars in the base case. It must be emphasized that the data base for the flame speed correlations in steam-rich atmospheres is very limited and was taken at relatively low pre-combustion temperatures. Flame speeds may be underestimated in the base case calculation, perhaps by significant factors.

Table 5.2

Summary of Results,
Surry-Bellefonte Study

Case No.	Parameter Variations			Peak Pressure (bar)	
	Δt_{deb}^* (s)	Δt_{stm}^* (s)	Other	Surry	Bellefonte
1S, 1B	10	30	Base Case	7.4	6.6
2S, 2B	10	30	Unconditional Burn	9.7	8.3
3S, 3B	10	60	--	6.3	6.2
4S, 4B	10	20	--	8.0	7.0
5S, 5B	10	10	--	9.5	7.7
6S	5	30	--	7.1	-
7S	10	30	0.5 mm Debris Drop	7.3	-
8S	10	60	$\lambda_{\text{tr}} = 1.0 \text{ s}^{-1}$	5.5	-
9S	5	30	**	6.5	-
10B	5	20	--	-	6.9
11B	10	30	$\lambda_{\text{tr}} = 1.0 \text{ s}^{-1}$	-	5.7
12B	10	30	$\alpha_w = 0.5$	-	5.9
13B	10	30	34000 kg water	-	6.1
14B	10	30	No H-burn	-	6.3

* Δt_{deb} = duration of debris injection

Δt_{stm} = duration of primary system blowdown

** λ_{tr} from Eq. 2.1, $\alpha_g = 0.8$, $\alpha_w = 0.2$

The unconditional burn option was used to investigate the implications of postulating hypergolic behavior (Cases 2S and 2B). Results are similar to those observed in previous calculations, with little difference between the responses of the two plants. In Bellefonte, temperatures calculated for the

upper containment rose above 1000 K in the base case (even with burns suppressed), while the temperatures of the material entering from Cells 2 and 3 (Fig. 5.1) were as high as almost 2000 K. Hence, there can be little doubt that the hypergolic behavior is highly credible in this scenario and that its implications must be considered.

Effect of Blowdown Duration: Cases 1S, 3S-5S; 1B, 3B-5B. These cases explore the effect of the rate of blowdown from the primary system, with results for Surry closely resembling those discussed previously (Sections 3.2.3, 4.3.3). In Bellefonte, the effect appears to be somewhat less, perhaps reflecting a reduced sensitivity to factors increasing the rate of energy transport to the upper containment as suggested above. The comparison is somewhat complicated by the fact that, with the fastest blowdown (Case 5B), steam concentrations rose fast enough to prevent hydrogen burns in the default model, while a slow burn did occur in the base case as discussed above. Nonetheless, a comparison between Case 5B and 14B (base case with burn suppressed) still indicates somewhat less sensitivity to blowdown rate than in the analogous Surry calculations.

Effect of Trapping: Cases 3S and 8S; 1B and 11B. These cases permit comparisons between results obtained with no trapping and results obtained assuming $\lambda_{tr} = 1.0 \text{ s}^{-1}$. Results are in line with the degree of sensitivity to trapping observed in Sections 3.2.3, 4.3.2, and 4.3.3. No gross differences between Surry and Bellefonte are evident in the degree of sensitivity to trapping. However, the blowdown rates assumed for the Surry and Bellefonte plants were different in these cases, and more precise conclusions concerning this point cannot be drawn.

Effect of Debris Injection Duration: Cases 1S and 9S; 4B and 10B. These results indicate that injecting the debris more rapidly, without assuming a more rapid blowdown also, actually reduces the peak pressure calculated slightly. This result may seem counter to what one might intuitively expect, but it is in keeping with the concepts which have emerged from the analyses presented in earlier sections of this report. Reducing the debris injection time while holding the blowdown rate constant reduces the amount of steam which can be heated by the debris, and the temperatures reached by this steam are not correspondingly increased because of the thermal saturation effect,

i.e., most of the heat remains in the debris even if local thermal equilibrium is achieved (see Section 3.2.3).

Effect of Particle Size: Cases 1S and 7S. This effect is trivial here, since there is no trapping and hence no competition between the rate of debris-gas heat and mass transfer and the rate of debris removal. Results cited in Sections 3.2.3 and 4.3.3 show the drop size effect may not be large even for the trapping rates given by Eq. 2.1. It could be more important for more rapid trapping, or for scenarios other than the base case scenarios for which the drop-size effect was studied.

Effect of Debris-Structure Radiation: Cases 1B and 12B. In all other calculations discussed in the present report, it was assumed that aerosol clouds accompanying DCH would render the atmosphere opaque, and that all thermal radiation from the debris particles would be absorbed by the gas, not the structure surfaces. In Case 12, it was assumed that direct debris-structure radiative heat transfer could occur to a substantial degree, i.e., at half the rate calculated for a perfect black body radiator. This distinction is important because energy radiated directly to the surface of the structures at no time resides in the gas and, hence, is ineffective in contributing to DCH loads. (By heating the structure surfaces, this energy does have a slight impact upon gas-structure heat transfer but the effect is usually minimal.)

Comparison of Cases 1B and 12B shows a significant reduction in pressure, about 0.6 bars, when substantial debris-structure radiation is assumed. However, the amount of direct debris-structure radiative transfer assumed here is probably unrealistic in view of the experimental data which indicate that very dense aerosol clouds having high opacity accompany high pressure melt ejection events. Given a more realistic estimate of the debris/structure radiation, it is likely that the effect would be smaller. Nonetheless, it is possible that the pressures calculated totally neglecting the effect may be high by up to a few tenths of a bar.

Effect of Cavity Water: Cases 1B and 13B. Case 13B is identical to Case 1B except that 13B was run assuming 34000 kg of cavity water would be co-dispersed with the debris. (The amount of water was based upon a MARCH calculation indicating that this quantity could be present in the cavity.) For

Surry, the results given in Section 3.3 suggest that this quantity of water might be expected to yield somewhat higher pressures than the base case. However, the results of Table 5.2 show that, for Bellefonte, a moderate mitigating effect, about 0.5 bar, is calculated. It is tempting to speculate that this difference reflects a somewhat reduced sensitivity of Bellefonte (relative to Surry) to factors which increase the rate of energy transport to the upper containment: since the aggravating effect of co-dispersed water is due to increased transport, a reduced sensitivity to this factor would tend to permit the mitigating effect of debris quench to dominate. However, there are many differences between the parameters governing the calculations of Section 3.3 and those discussed here, in addition to the difference in containment geometry. Hence, it is not possible to draw definitive conclusions as to whether the factors governing the differences in the results are indeed plant specific. The results do serve as another reminder of the caution needed in extrapolating a sensitivity found for one scenario to another, whether the second scenario is defined by different plant parameters, different accident parameters, or simply different modeling assumptions applied to the same physical accident situation.

Effect of Containment Capacity. Although the parameter variations studied here did not include those found to generate the most severe threats in Sections 3 and 4 (e.g., rapid blowdown with unconditional burn), it is obvious that none of the cases considered for Bellefonte come close to the estimated failure pressure of at least 10 bars, while two of the scenarios treated for both plants (the base case with unconditional burn and the rapid blowdown case) do lead to pressures that would be a serious threat to Surry. It is by no means clear that assuming any given set of parameters in these calculations is actually equally plausible for both plants; hence, no conclusions should be drawn from just the results cited here as to whether DCH is in reality a greater threat to one plant than to the other. Nonetheless, it is clear that one would have to postulate much more pessimistic combinations of input assumptions and/or modeling assumptions in order to calculate a severe threat for Bellefonte than for Surry. A large, strong containment is perhaps the most general of all the potential "mitigators" of DCH threats considered in this work: unlike so many of the other potential effects that have been suggested as mitigating DCH, we have found no scenarios and no phenomenological uncertainties suggesting that a tough containment could actually make the problem worse!

6. SUMMARY AND CONCLUSIONS

The goal of the CONTAIN Interim Direct Heating Model has been to treat the highly uncertain phenomena affecting DCH parametrically in a context where the better-understood phenomena are simultaneously being treated with the state-of-the-art models incorporated in the standard released version of CONTAIN. Though many refinements are desirable, the work has progressed to the point where interesting results can be obtained. The model has been applied to station blackout accidents in PWR plants representing the three main types of PWR containments: Surry, a subatmospheric large dry containment; Sequoyah (or Watts Bar), an ice condenser plant; and Bellefonte, an atmospheric large dry containment.

Results of applying the IDHM to DCH scenarios in the Surry plant suggest that compartmentalization effects do have substantial potential to reduce the chemical and thermal interaction between the debris and atmosphere, and thereby to mitigate DCH loads. Thus the Surry base case scenario yielded peak loads of only 7 bars when the five-cell representation of the containment was used, while 11-12 bar pressures were calculated for a single-cell representation of an otherwise-equivalent scenario. However, the degree and even the existence of this mitigation has been found to be quite sensitive to many scenario details and phenomenological uncertainties.

In the Surry base case, loads were mitigated by reaction of metals with steam rather than with oxygen, and by the fact that the cavity was assumed to be dry and the primary system blowdown time (30 seconds) was assumed to be long compared with the debris injection time (5 seconds). The last two factors result in there being relatively limited atmospheric mass in the lower containment to which the debris may transfer energy, and consequently relatively limited rates of transport of energy to the upper containment. Since the limited masses of gas available are heated to extreme temperatures, 1500-2500 K, radiant heat loss to lower-containment structures can compete effectively with energy transport to the upper containment, where the main reservoir of atmospheric mass (and oxygen) is located.

Since limited rates of energy transport played an important role in mitigating the base case loads, these loads were rather sensitive to factors which could accelerate energy transport to the upper containment. These factors were found to include more rapid blowdown of the primary system, and steam generated by rapid quench of debris trapped by interactions with structures in the lower containment, provided this debris is deposited in pools rather than being retained by relatively dry surfaces. Even water co-dispersed with the debris can have a similar effect due to the steam generated. The effect of co-dispersed water was found to be sensitive to the amounts of water involved, the timing and location of its dispersal, and uncertainties in the chemical reaction rates. In the cases considered, DCH loads at Surry were enhanced by 1.5-2.5 bars by the various factors noted here as leading to accelerated energy transport. (Since the factors which accelerate transport also reduce lower-containment temperatures, reduced rates of heat loss also play a role in producing these results.)

The base case was found to be rather insensitive to such parameters as the extent of in-vessel zirconium oxidation, debris drop size, and uncertainties in the chemical reaction rate. Even sensitivity to the mass of corium participating was only moderate. These results are also related to the limited mass of gas available in the lower containment. Much of the total energy remains in the debris until it is lost to lower-containment structures under these conditions. Hence, variations in the total energy released in the lower containment produce relatively small variations in the energy actually transferred to gas, unless there are also significant effects upon energy transport.

Results obtained in this study imply a very important role for uncertainties concerning hydrogen combustion in atmospheres which are steam inert by normal criteria, but which are also characterized by high temperatures and the presence of hot particulate. Both of the latter conditions are likely to favor hydrogen-oxygen reaction. Indeed, at some of the temperatures calculated, it is plausible to assume that the hydrogen-oxygen reaction will occur spontaneously, without need for ignition and flame propagation in the usual sense. The consequences of hydrogen combustion were bounded by overriding the CONTAIN default burn model to specify that combustion occur unconditionally whenever hydrogen was present in a cell containing any oxygen. Results indicated that hydrogen combustion could add 2 to 3 bars to the maximum

pressures in typical cases. The large quantities of hydrogen produced by metal-steam reactions during DCH contributed to this effect, as did hydrogen produced by in-vessel zirconium oxidation and released to containment prior to vessel breach.

There is synergism between the effects of unconditional hydrogen combustion and the various factors accelerating energy transport to the upper containment, in part because the latter also improve transport of hydrogen to the upper containment. Very severe loads, typically 10-12 bars, were calculated for these scenarios. Since the improved transport minimizes energy loss in the lower containment, and the hydrogen combustion permits recovery of much of the full metal oxidation energy, it is not surprising that these scenarios are characterized by loss of much of the mitigation associated with compartmentalization in the base case.

It is extremely important to recognize that the key to understanding the results obtained in this work is to consider the effects of the various parameters upon the transport of energy to the upper containment, not just the effect upon the transport of debris. Totally eliminating trapping in the base case increased peak pressures only moderately, by less than a bar, because energy still was rapidly lost to structures in the lower containment even though the debris itself remained airborne indefinitely with no trapping, and much of it eventually did reach the upper containment. On the other hand, factors increasing the steam flow may effectively increase the energy transport, even if much of the debris itself is trapped. Energy can also be transported effectively in chemical form (i.e., via the generation of hydrogen), if hydrogen combustion can occur in the upper containment. For these reasons, the base case scenario showed only a moderate sensitivity to trapping rates, although it is obvious that trapping will eliminate DCH threats if one can postulate arbitrarily large trapping rates. Unless trapping rates are very large ($\lambda_{tr} \gg 1 \text{ s}^{-1}$), trapping does not appear to totally dominate DCH scenarios as has been widely assumed in the past.

In the other plants studied (Sequoyah and Bellefonte), the same phenomenological principles apply in a qualitative sense, but significant quantitative differences arise due to the different boundary and initial conditions imposed by plant parameters. In Sequoyah, sensitivity to factors governing energy transport to the upper containment was reduced (but not eliminated) by

the ice condenser, while hydrogen phenomenology was very important. The dominant impact of the latter was the obvious one of hydrogen combustion, but the effect of hydrogen as a noncondensable gas, which increases energy transport through the ice condenser, was also quite significant.

In Sequoyah, the choice of hydrogen burn model (i.e., default versus unconditional) matters less than in Surry because the ice condenser prevents steam inerting and, in most (but not all) cases considered, the default flammability criteria were met and both models therefore yielded burns. Furthermore, the default model typically gave somewhat severer loads, since it allows hydrogen to accumulate until the threshold concentration is met, yielding a larger burn. Using the default model, there was only limited sensitivity to the injected corium mass, provided only that sufficient corium was injected so that the hydrogen produced and transported to the upper containment was sufficient to meet the default burn criteria. The corium injection fraction required was about 25%, depending upon the metal content. (In the Sequoyah calculations, it was assumed that any hydrogen released to containment prior to vessel breach would have been burned off; relaxing this assumption did not greatly affect the base case loads but it would no doubt reduce the corium mass required to meet the hydrogen combustion threshold.)

Based upon a more limited set of calculations, sensitivities exhibited by the Bellefonte plant were qualitatively similar to those found for Surry. Quantitatively, it appeared that differences in plant lay-out and the resulting differences in flow paths reduced the sensitivity to factors affecting the rate of energy transport, though it remained substantial.

The results obtained here suggest an important, albeit tentative, conclusion that may be drawn concerning the role of containment capacity (i.e., volume and failure pressure) in governing the threat to containment integrity associated with DCH. Earlier analyses implicitly downplayed the importance of containment capacity because the simple and highly conservative bounding calculations used indicated that DCH threats had the potential to fail any existing containment. The present work, with its wide spectrum of possible mitigating effects, restores containment capacity as an important discriminant. Thus, the proportion of otherwise-equivalent scenarios which would pose a serious threat varies dramatically as containment capacity is varied over a range typical of capacity estimates for existing plants (e.g., Surry versus

Bellefonte, Sequoyah versus Watts Bar). This conclusion should not be over-interpreted: in particular, it can not be extended to make even a comparison of the relative risks associated with DCH in different plants, since it is not established that "otherwise equivalent" DCH scenarios are equally probable in different plants. Nonetheless, once understanding progresses to the point where such comparisons can be validly made, it seems highly likely that containment capacity will be a dominant determining factor, unless it turns out that DCH risks prove minor for all plants.

All conclusions offered here must be tempered by a recognition of the complexity of the problem. The numerous phenomena involved in DCH interact strongly in a highly nonlinear way, and valid generalizations as to the magnitude or even direction of a given effect are often difficult to make. Effects found to matter little under some conditions may prove very important under others. Uncertainty in chemical reaction rates is a good example: it appeared to be a trivial effect in the Surry base case, but was highly important in the co-dispersed water scenarios and could prove important in the rapid-blowdown scenarios. More generally, the various factors governing total energy release in the lower containment would be expected to be more important when effects yielding rapid energy transport were also present. Except when explicitly stated otherwise, the descriptions of sensitivities given here apply only to the base cases used as starting points.

Even generalizations as to whether neglecting a given effect is "conservative" or "nonconservative" are likely to be in error because many such effects aggravate DCH loads under some circumstances but reduce them under others. Examples include postulating unconditional hydrogen combustion in place of the default model and the effects of co-dispersed water. Even the trapping of debris can aggravate DCH loads relative to the no-trapping case if the trapped debris rapidly generates steam due to quenching in pools of water. Often the impact of various phenomena upon the calculated loads was found to be quite different from what has been widely assumed in the past. The fact that both co-dispersed water and debris trapping can increase the calculated loads under certain circumstances provides good examples.

Another potential limitation of this work is that the severity of DCH environments forces the application of many standard CONTAIN models (e.g., for heat and mass transfer) in parameter regimes far from those for which the

models were designed, let alone those for which the models have been validated. Uncertainties due to this circumstance have been assessed only to a very limited degree. In the particular cases that were examined, the effects were not large, however.

Despite the large numbers of DCH parameter variations and alternative modeling assumptions considered in this work, it is by no means complete. Many possible combinations of parameters have not been treated. Some important uncertainties have not been considered at all, e.g., uncertainties introduced by the highly simplified geometries used to represent containments whose actual geometric configurations are far more complex. The results obtained here are judged most useful for improving understanding of the phenomena governing the DCH loads, and identifying those phenomena which most merit additional theoretical and experimental study. On the other hand, use of these results to judge the threat to containment integrity due to DCH in any specific plant or plants should be done only with great caution: the present studies are limited in important ways, as just noted; in addition, no assessment has been made as to the probability of the various plant/scenario/parameter combinations considered, other than an attempt to eliminate some obvious impossibilities.

The preceding caveats notwithstanding, very rapid progress has been made in understanding the DCH threat. The capabilities and analyses described here represent a major advance over the ultra-conservative calculations upon which the Containment Loads Working Group was forced to rely in its discussions of DCH. Further progress is expected as the results of ongoing experimental and analytical programs sponsored by the NRC are incorporated into systems codes such as CONTAIN. In the meantime, it is apparent that the incorporation of even the simple and partially parametric models now available into a well-developed containment systems code can yield generous dividends in terms of improved understanding of the phenomena governing DCH.

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APPENDIX

Examination of Selected Uncertainties and Approximations in the CONTAIN Interim Direct Heating Model

In this Appendix, a number of uncertainties and approximations involved in the CONTAIN Interim Direct Heating Model (IDHM) will be examined in somewhat more detail than was done in the main text. Some additional details concerning certain features of the IDHM itself will also be given. Topics to be discussed include heat and mass transfer between debris and gas, treatment of the surface area available for reaction, modeling of drop-side reaction rate limits and choice of the diffusivity used in the model, chemical equilibrium effects and chemical reactions neglected in the IDHM, and agglomeration of debris drops. Examples are given for some of the reaction rate uncertainties, using a simple test problem.

A.1 Heat Transfer Rates and Gas-Side Reaction Rate Limits.

A.1.1 Transport Properties.

The rate of debris-gas heat transfer and chemical reaction calculated using Eqs. 2.2 and 2.3, respectively, will depend upon the values of gas transport quantities including the thermal conductivity k , the kinematic viscosity ν , and the diffusivity, D_j , of the j th reacting species in the bulk gas mixture. In CONTAIN, transport properties for pure species are calculated using simple algebraic expressions, and those for gas mixtures are estimated using simple mixing rules. These representations have been adequate for most past applications, but may not always be adequate for the conditions characterizing DCH. The CONTAIN property library is in the process of undergoing a general upgrade, and the present discussion is restricted to examining limitations in the current treatment of gas properties which might have the potential to perturb DCH calculations significantly.

Examination of Eqs. 2.2 and 2.3 shows that heat and mass transfer rates calculated will, at most, show a dependence upon kinematic viscosity of $\nu^{-1/6}$.

This dependence is too weak for uncertainties in ν to introduce significant effects, and only the thermal conductivity k and the diffusivities will be discussed.

Thermal Conductivity. Comparison of the CONTAIN values for the thermal conductivities of pure gas species with literature values [Kr73] has shown that the code's values are sufficiently accurate so as not to introduce significant error in DCH calculations. In the IDHM (and in the ice condenser model), mixture thermal conductivities are calculated using a simple average over mole fraction:

$$k_g = \sum_j X_j k_j, \quad (A-1)$$

where k_g is the conductivity of the gas mixture, and X_j and k_j are, respectively, the mole fractions and the conductivity of the j th species.

This method of averaging is inadequate for high precision work, but the errors involved are not believed to be important for present purposes for most common containment gas mixtures. However, potential exceptions include mixtures involving substantial quantities of hydrogen. In the DCH analyses discussed in the main text, the atmosphere consisted primarily of steam and hydrogen whenever hydrogen concentrations were high; i.e., concentrations of other noncondensable gases were low in these scenarios. Hence, the adequacy of the average over mole fraction will be examined here for binary steam-hydrogen mixtures only.

In Fig. A.1, estimated thermal conductivities of steam-hydrogen mixtures are plotted as a function of hydrogen mole fraction for temperatures of 500, 1000, 2000, and 3000 K. The dashed curves give results obtained using CONTAIN's mole fraction averaging technique, while the solid curves give results obtained using the Lindsay and Bromley (L & B) modification of the Wassiljewa equation as given in [Re77]. (All values in Fig. A.1 are calculated using the CONTAIN expressions for the pure species conductivities and viscosities; only the errors associated with the mixing rules are being considered here.) The L&B method is believed to be considerably more accurate and reportedly gives results that are accurate to within 5% for most cases [Re77]. Fig. A.1 indicates that the CONTAIN values can exceed the L & B values by as much as 30% at 500 K, with the difference decreasing somewhat with increasing

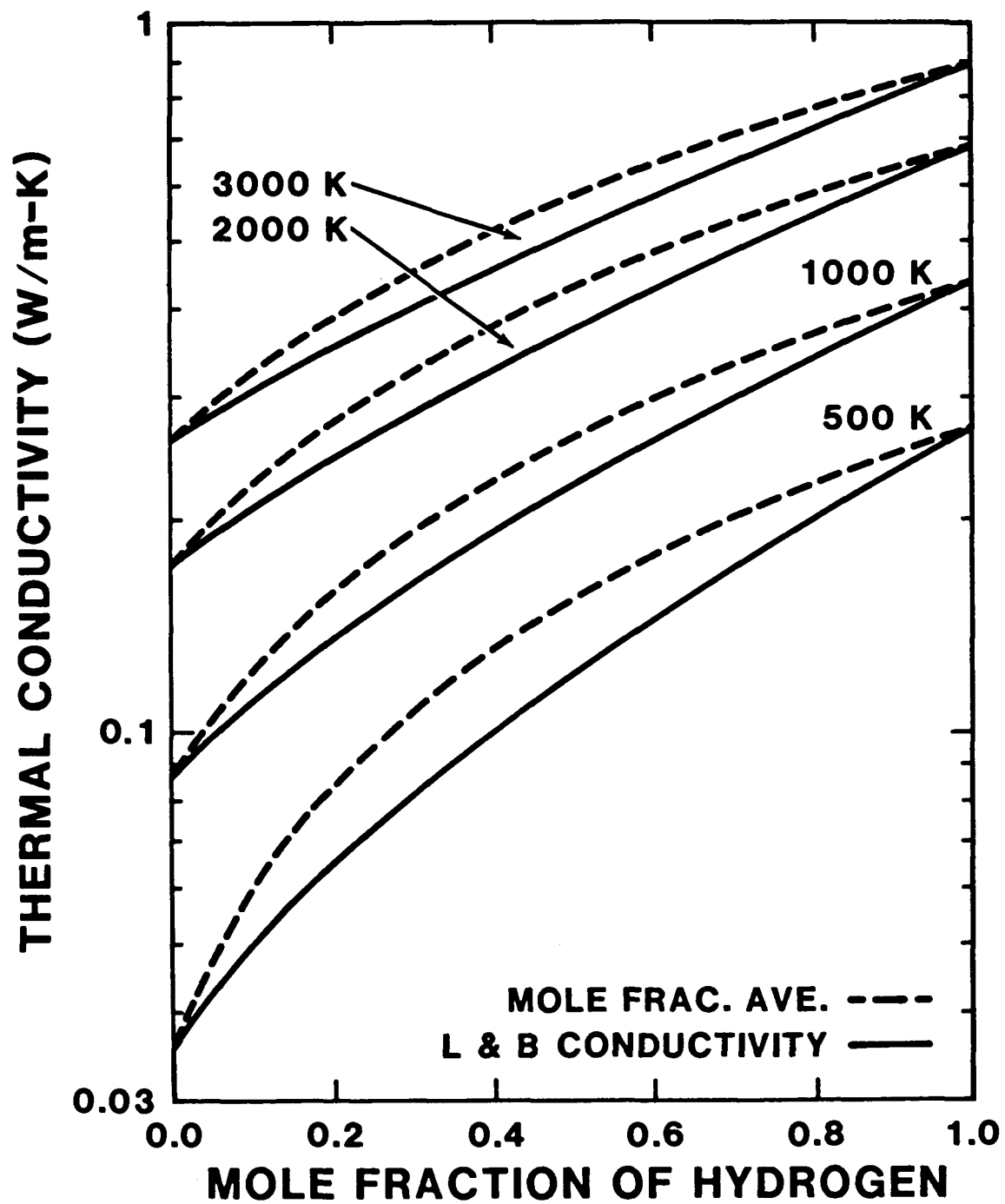


Fig. A.1 Thermal conductivities of steam-hydrogen mixtures as a function of hydrogen mole fraction at the indicated temperatures.

temperature. At the temperatures generally of most interest in DCH ($T > 1000$ K), it appears that errors will not exceed 20%. These errors in the thermal conductivity probably do not significantly affect the results of actual DCH containment calculations, and their impact is certainly small compared with other uncertainties in the analyses. Nonetheless, they can have a substantial effect upon the response of the model in certain special cases, as will be shown in Section A.5.

Fig. A.1 suggests that a somewhat more serious error in certain cases could arise due to the use of the conductivity calculated for the bulk gas mixture in evaluating heat transfer from the drop. Even if the bulk gas is pure steam, the composition at the surface of a reacting metal drop may be almost pure hydrogen, with the composition varying widely through the boundary layer surrounding the drop. The conductivity of hydrogen is several times as large as that of steam, and neglecting the effect of hydrogen upon the conductivity in the drop boundary layer could introduce significant error in such cases; see Section A.5.

Gas Diffusivities. Estimation of accurate diffusivities in complex binary mixtures is a nontrivial task and only binary diffusivities are used in CONTAIN. For oxygen, the IDHM employs the prescription given by Bird, Stewart, and Lightfoot [Bi60] for diffusion in binary nonpolar gas mixtures, evaluated for oxygen diffusing through nitrogen, which gives

$$D(O_2-N_2) = 6.405 \times 10^{-5} T^{1.823}/P, \quad (A.2)$$

where P is the pressure in Pa and D is in m^2/s . For steam, the IDHM uses the prescription given in [Bi60] for polar-nonpolar gas mixtures, evaluated for steam and air, yielding

$$D(H_2O-Air) = 4.40 \times 10^{-6} T^{2.334}/P. \quad (A.3)$$

Eq. A.3 is also used for calculating steam transport rates in processes involving steam condensation and evaporation throughout CONTAIN.

In Fig. A.2, these values are compared with values calculated using the more accurate, but somewhat more complex, Wilke-Lee modification of the Hirschfelder, Bird, and Spotz (WL-HBS) equation as given in [Pe73]. WL-HBS

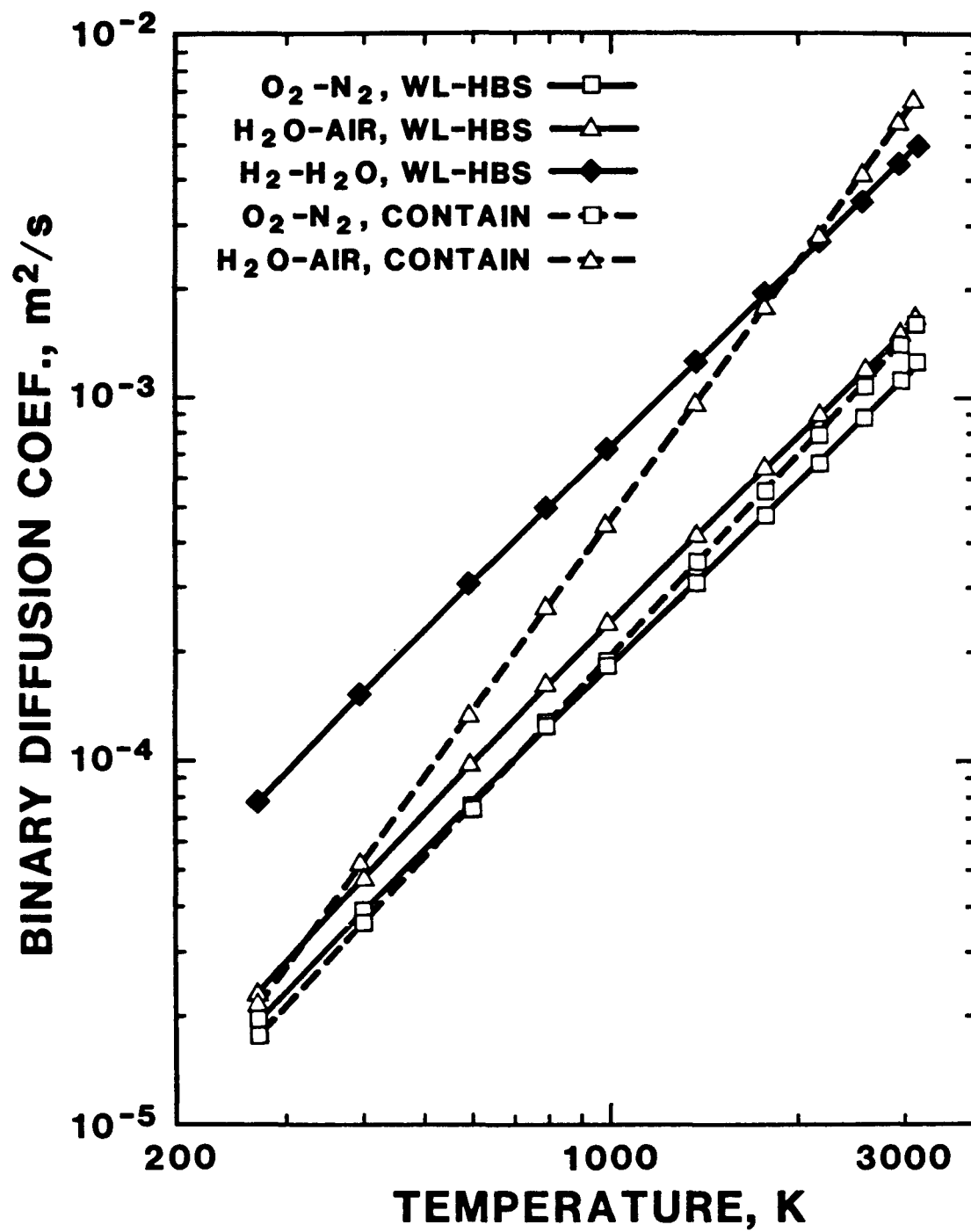


Fig. A.2 Binary diffusion coefficients for the indicated gas pairs at a pressure of 1 bar.

diffusivities for hydrogen in steam are also given. For the O_2-N_2 diffusivity, it is seen that Eq. A.2, though hardly precise, gives results that are probably adequate for present purposes, since realistic DCH scenarios are rarely dominated by reaction with oxygen in atmospheres consisting mostly of air (as opposed to steam). In any case, obtaining significant improvement would require a multi-component formulation, since there is almost always sufficient steam present so that $D(O_2-N_2)$ cannot provide a very accurate representation of the oxygen diffusivity within the gas mixture.

For processes involving condensation and evaporation, the relevant temperatures are generally relatively low (300-450 K), and Eq. A.3 gives values of the steam-air diffusivity close to the WL-HBS values in this temperature range. On the other hand, the temperature dependence of Eq. A.3 is much too steep for high-temperature applications, and it is apparent that Eq. A.3 would substantially over-estimate the diffusivity of steam in air at the high temperatures (1500-2500 K) typically of interest in DCH applications. However, in most DCH scenarios dominated by reaction with steam, the dominant noncondensable gas present is hydrogen, not air. From Fig. A.2, it can be seen that Eq. A.3 actually does yield diffusivities fairly close to the WL-HBS values for steam-hydrogen mixtures in the high-temperature DCH regime. Although this result is entirely fortuitous, it leads to the conclusion that major errors in DCH analyses due to the use of Eq. A.3 are not expected, and that substantial improvements in accuracy are doubtful within the framework of treatments based upon binary diffusion coefficients, since gases other than steam and hydrogen usually are present to at least some degree.

It is concluded that, in the long run, the treatment of diffusivities in the IDHM should be improved, and that the desired improvement cannot be made using binary diffusion coefficients alone. However, the errors associated with the present treatment are unlikely to seriously affect the calculations described in the main text, given the gas compositions and temperatures generally of interest to those calculations.

A.1.2 Estimation of Surface Area of Reacting Debris.

In Section 2.2.2, it was noted that the reaction rate given by Eq. 2.3 was evaluated using an effective surface area for airborne debris, S'_d , which might be less than the full debris surface area, S_d , used in the evaluation of heat

transfer (Eq. 2.2). The means of forming this estimate will be briefly described here. The method used is simple and the justification offered here makes no claims to rigor.

The problem arises because the IDHM tracks only one debris field, but not all debris drops necessarily contain metal. Even in fresh debris, metallic and oxidic constituents may be in separate drops; as reaction proceeds, some of the initially-metallic drops will be converted to oxide by chemical reaction. Hence, crediting the full debris surface area when estimating the rate of mass transport through the gas phase to the reacting debris surface can substantially overestimate reaction rates, when gas-phase transport is the rate-limiting process. The IDHM therefore uses a simple correction procedure to obtain a better estimate of the reaction rate.

For simplicity, consider the case of only one reacting metal, and assume that the metal is introduced in debris drops which have an initial metallic mass fraction f_m^0 ; there may be other debris drops which contain no metal. Let the total mass of debris airborne in a cell be W_d and let its metallic content be W_m . If the mass of debris that actually contains metal is W_{dm} , then $S'_d = sW_{dm}$, where $s = 6/\rho d$ is the specific surface area of the debris, i.e., the surface area per unit mass of debris. In the IDHM's single-field representation of the debris, there is no provision for letting the density ρ or the drop diameter d vary as a function of composition; hence, ρ and d are treated as being the same for all debris drops in the following discussion.

The code does track W_m and W_d as a function of time, but has no direct information concerning W_{dm} . However, given the value of f_m^0 as defined above, an estimate of W_{dm} can be constructed. Let $R(t)$ refer to the rate at which debris is injected as a function of time, and let the subscripts d , m , and dm have the same meaning for R as for W . Let $\delta W_m(t, t')$ be the amount of metal remaining at time t from what was injected on the differential earlier time interval, $(t-t', t-t'+\delta t')$. Referring to Eq. 2.3 of the main text, it is apparent that the rate of reaction for a given parcel of metal-containing debris does not depend upon the amount of metal remaining, so long as reaction rates are controlled by gas-phase transport only. If the other factors controlling reaction rates remain constant, then the reaction rate will remain

constant until the metal is totally exhausted after some characteristic reaction time, t_{rx} , at which time the reaction rate abruptly drops to zero. Hence, if we can neglect trapping during the time interval t_{rx} ,

$$\delta W_m(t, t') = R_m(t-t')(1-t'/t_{rx})\delta t', \quad t-t' < t_{rx};$$

$$\delta W_m(t, t') = 0, \quad t-t' > t_{rx}. \quad \text{Hence,}$$

$$W_m(t) = \int_0^{t_{rx}} R_m(t-t')(1-t'/t_{rx})dt'. \quad (\text{A.4a})$$

If f_m^0 is constant over the interval of interest, $R_{dm} = R_m/f_m^0$ and we may write

$$W_{dm}(t) = \int_0^{t_{rx}} R_{dm}(t-t')dt'/f_m^0. \quad (\text{A.4b})$$

When reaction rates are limited only by gas-side transport, t_{rx} is typically short in DCH scenarios: often ≤ 1 s for any drop size < 2 mm. It is therefore reasonable to consider the approximation of treating R_m (and R_{dm}) to be constant over the time interval $(t-t_{rx}, t)$. With this assumption, Eq. A.4 gives

$$W_m = R_m t_{rx}/2; \quad \text{and} \quad W_{dm} = R_m t_{rx}/f_m^0. \quad (\text{A.5})$$

From Eq. A.5, it is apparent that

$$W_{dm} = 2 W_m/f_m^0; \quad S'_d = 2 s W_m/f_m^0. \quad (\text{A.6})$$

Estimating W_{dm} and S'_d from Eq. A.6 requires only the current value of W_m , which the code has available, and the value of f_m^0 , which can be provided through input. No information about the past injection and/or reaction history is required. This approach is, in essence, what the CONTAIN IDHM uses, subject to the additional rather obvious condition that $S'_d \leq S_d$. At each time step, a new estimate of S'_d is formed using Eq. A.6 and the current value of W_m .

In the DCH calculations discussed in the main text, the condition that debris injection rates not vary substantially over time intervals $\leq t_{rx}$ was satisfied in any calculation in which gas-side transport was rate-limiting, and reaction rates are insensitive to the S'_d estimate if drop-side rate limits govern the reaction rate. Trapping was also generally slow compared with gas-side reaction rates except in a few sensitivity cases. Hence, the assumptions used to derive Eq. A.6 were usually satisfied fairly well. However, errors are not believed to be excessive even when the assumptions given above fail badly. To see why, consider an opposite extreme from the constant injection rate assumed above, i.e., injection as a single pulse over a time interval $\ll t_{rx}$. In this case, W_{dm} will initially be W_m/f_m^0 , not $2W_m/f_m^0$ as in Eq. A.6, and the reaction rate is overestimated by a factor of two. As the reaction proceeds and W_m decreases, S'_d as estimated here will decrease, and the amount of metal remaining will decline exponentially with a time constant $t_{rx}/2$, rather than linearly over a time period t_{rx} . At a time $t_{rx}/2$, the approximation used in the IDHM indicates that 63% of the metal has reacted rather than 50% as given by the linear decrease; at a time $t = t_{rx}$, the IDHM approximation gives 86.5% consumption while the linear decrease would imply 100% reaction. Compared with other uncertainties in DCH modeling, the errors introduced by these approximations appear rather small.

As actually implemented in the IDHM, the approach is complicated somewhat by the need to consider both zirconium and iron. For zirconium, the appropriate reaction surface, $S'_d(Zr)$, is estimated essentially as above, i.e.,

$$S'_d(Zr) = \text{Min}(2sW_{Zr}/f_{Zr}^0, S_d) \quad (\text{A.7a})$$

In estimating the surface area available for iron reaction, it is assumed that the iron and zirconium are initially intermixed. Because of the reaction hierarchy assumed, the surface of drops containing iron is not credited toward iron reaction if these drops also still contain zirconium. Hence,

$$S'_d(Fe) = \text{Min}(2sW_{Fe}/f_{Fe}^0, S_d) - S'_d(Zr). \quad (\text{A.7b})$$

($S'_d(Fe) \geq 0$ required.)

The values of f_{Zr}^0 and f_{Fe}^0 are input to the code and may be chosen completely independently of the bulk composition of the injected debris as determined by the debris source tables. As an example of the use of f_{Zr}^0 and

f_{Fe}^0 , consider a case in which the bulk debris composition upon injection is 10% Zr, 20% Fe, and 70% oxides. If it is assumed that the debris is completely homogenized, so that each drop has the bulk composition at injection, then $f_{Zr}^0 = 0.1$, $f_{Fe}^0 = 0.2$. The assumption of homogenized debris was used in the calculations discussed in Section 5 of the main text. In the calculations discussed in Sections 3 and 4, it was assumed that the iron and the zirconium were intermixed, but that they were totally segregated from the oxides, i.e., were in drops consisting purely of metal. Applied to the present example, that assumption would give $f_{Zr}^0 = 0.333$, $f_{Fe}^0 = 0.667$. Nothing prevents the user from assuming that the metals themselves are segregated, and specifying $f_{Zr}^0 = f_{Fe}^0 = 1.0$. However, the assumption of intermixing is, to some degree, embedded in Eq. A.7, and the calculation would not proceed exactly as desired.

A.2 Drop-Side Reaction Rate Limits.

The model for reaction rates based upon gas-side mass transport limits typically allows for very rapid reaction, even when S'_d is limited as outlined above. In reality, it is at least possible that reaction rates will be limited by mass transport within the debris drop. The method by which drop-side limits are modeled in the CONTAIN IDHM is outlined below, followed by some discussion of appropriate values of the drop-side diffusivity required by the model.

A.2.1 Model for Drop-Side Reaction Rate Limits.

The model to be described is based upon diffusion within a stagnant sphere. Experiments involving metal oxidation studies are often analyzed in terms of a parabolic rate law. However, when the parabolic rate law is applied to spherical geometry, the resulting prediction of extent of reaction as a function of time is quite close to what one calculates for the model based upon diffusion within a sphere, provided the appropriate relation between the numerical value of the parabolic rate constant K and the diffusivity of the spherical debris drop, D_d , is used [Ba86]. A much more serious question concerns whether a model based upon diffusion within a stagnant sphere is appropriate at all. For example, it is possible that internal circulation will reduce the barriers to mass transport within the drop, and thereby reduce or even effectively eliminate any drop-side reaction rate limitations, at least when the debris is molten. This subject will be briefly

discussed at the close of Section A.2.2, but will not be considered further here. The remainder of the present discussion only addresses the representation of the drop-side reaction rate in the IDHM, assuming such a limit does exist.

Many formidable modeling uncertainties would confront any attempt to develop a detailed stand-alone model for the drop-side reaction rate limits. Incorporating such a model in CONTAIN could prove just as challenging. Hence, a simple model was developed, which at least permits the IDHM to acknowledge the potential existence of drop-side limitations and to examine the sensitivity to drop-side reaction rate limits.

We assume that the debris consists of initially homogeneous drops of diameter d , with reaction rate limited only by the diffusion of oxygen atoms into the drop interior and/or diffusion of metal atoms outward, with an effective value of the diffusivity D_d . Let F be the fraction of the initial metallic content which has reacted at time t . Then, solution of the diffusion equation in spherical coordinates gives

$$F(t) = 1 - \frac{6}{\pi^2} \sum_{n=1}^{\infty} e^{-4n^2 \pi^2 D_d t / d^2}. \quad (A.8)$$

Let $y = 4D_d t / d^2$. Two useful (and quite accurate) approximations are

$$F(y) = \frac{6}{\pi^2} y^{1/2} - 3y, \text{ if } y \leq 0.2; \text{ and} \quad (A.9a)$$

$$F(y) = 1 - \frac{6}{\pi^2} e^{-\pi^2 y}, \text{ if } y \geq 0.2 \quad (A.9b)$$

Note that $F(y = 0.2) \approx 0.91$, i.e., reaction is over 90% complete at this point.

In Eqs. A.8 and A.9, $F(t)$ does not depend upon the initial metal concentration, and the time required to react a given fraction of the metal is therefore independent of the initial metal mass in this model. From Eq. A.9a, it is seen that $F \propto t^{1/2}$ at early times, or the reaction rate $dF/dt \propto t^{-1/2}$. Thus, the rate is strongly time-varying, at early times. However, the IDHM

does not keep track of the age of the debris, i.e., the time since a particle was injected. Only the amounts of unreacted metal and total debris are tracked. This being the case, the best that can be done is to define some kind of effective time constant, τ_d , such the W_m/τ_d gives a reasonable measure of the reaction rate. This approach gives an exponential decay in the amount of unreacted metal. From Eq. A.9b, it can be seen that the late-time behavior actually is exponential, with time constant

$$\tau = \frac{d^2}{4\pi^2 D_d} \quad (A.10)$$

However, this exponential decay rate is not achieved until reaction is largely complete; earlier, reaction is faster. Use of $\tau_d = \tau$ would give too slow a reaction rate.

After some numerical experimentation, it was concluded that a more appropriate value is obtained if one chooses τ_d such that one obtains the correct time required to react half the metal in an initially-fresh debris drop. Setting Eq. A.9a equal to 0.5 and solving for y gives

$$\left. \begin{array}{l} y = 0.03055 \\ \text{or } \frac{t}{\tau} = \pi^2 y = 0.3015 \end{array} \right\} \text{ for 50\% reaction}$$

Here, τ is as defined in Eq. A.10. Then, requiring τ_d to be such that $1 - e^{-t/\tau_d} = 0.5$ at this time also leads to the result

$$\tau_d = (0.3015/\ln(2))\tau = 0.435\tau = 0.01107d^2/D_d \quad (A.11)$$

Using this approach, the fraction of metal reacted in a freshly-introduced debris drop is given by:

$$F = 1 - e^{-t/\tau_d} \quad (A.12)$$

The extent of reaction is underestimated at early times and overestimated at late times. Expressed in terms of the total amount of initial metal, the maximum underprediction is -11.7% and the maximum overprediction is +12.6%. In a relative sense, of course, there can be extreme underprediction at early

times. For many purposes, the parameter of greatest interest will be the amount of energy (or hydrogen) introduced into the system at any given time. Even for the extreme case of a pulse of metal introduced instantaneously, the arguments just given show that the maximum error in the amount of energy introduced at any given time never exceeds 12.6% of E_{mx} , where E_{mx} is the maximum possible energy release, corresponding to complete reaction of all the metal. When the debris is introduced over a more extended time period, the error in the energy released, and hydrogen produced, at any given time should be less. This argument suggests that the present approach may not introduce gross error, and in some cases that conclusion is believed to be valid. However, there may be exceptions, particularly when parameters are near threshold values separating positive versus negative feedback effects. For example, the initial reaction rate of freshly-introduced debris can be substantially underestimated. If the debris environment is relatively cool, this underestimate implies that erroneous conclusions can be reached as to whether the initial energy release is greater than or less than the rate of heat loss to the environment, and this error can, in turn, lead to erroneous conclusions as to whether the debris will ignite, versus cooling off after only very limited reaction.

Once τ_d is calculated, it is necessary to combine the drop-side and the gas-side rate limits to obtain the over-all effective time constant for reaction, τ_e . First, a time constant for the gas side reaction rate, τ_g , is calculated by converting the metal masses and reaction rates involved into oxygen equivalents, i.e., the number of moles of metal multiplied by the oxygen/metal stoichiometric ratio in the corresponding oxide. Let N_m be the equivalents of metal present, and let $\dot{N}_g$ be the rate of reaction (equivalents reacted per second) based upon gas-side rate limits only, as calculated from Eq. 2.3 and Eq. A.7. Then τ_g is defined to be

$$\tau_g = N_m / \dot{N}_g.$$

The exact relation between τ_e , τ_g and τ_d can depend upon complex chemical details not considered here, but it is likely that, in most cases,

$$\text{Max}(\tau_g, \tau_d) \leq \tau_e \leq \tau_g + \tau_d.$$

In the IDHM, it is assumed that

$$\tau_e = (\tau_g^2 + \tau_d^2)^{1/2}; \quad (\text{A.13})$$

this assumption satisfies the preceding inequalities and yields the correct asymptotic limits when $\tau_g \ll \tau_d$ or $\tau_g \gg \tau_d$, but is otherwise arbitrary. The final estimate of the reaction rate is then taken to be N_m/τ_e , in terms of chemical equivalents. (Some details needed to preserve the reaction hierarchy and to apply Eqs. 7a and 7b consistently have been omitted in this discussion.)

The diffusivity, D_d , is specified by the user and may be temperature dependent. It is controlled by four input parameters, D_1^0 , e_1 , D_2^0 , and e_2 . Four cases apply:

1). $D_1^0 = D_2^0 = 0$: No drop-side limit (D_d effectively infinite)

2). $D_1^0 > 0$, $D_2^0 = 0$: $D_d = D_1^0 e^{-e_1/T_d}$.

3). $D_1^0 = 0$, $D_2^0 > 0$: $D_d = D_2^0 T_d e^{-e_2/T_d}$.

4). $D_1^0 > 0$, $D_2^0 > 0$: $D_d = \text{Min}(D_1^0 e^{-e_1/T_d}, D_2^0 T_d e^{-e_2/T_d})$.

Here T_d is the debris temperature. The second option above permits representation of the results of metal oxidation studies when these are analyzed in terms of a parabolic rate law with an Arrhenius temperature dependence of the rate constant. The third permits representations of theoretical expressions for liquid diffusivity (see Section A.2.2), while the fourth form permits a transition between the preceding two forms at some desired point (e.g., the solidification temperature), provided the low-temperature form exhibits a steeper temperature-dependence than the high-temperature form. Although these options permit considerable flexibility in specifying the temperature dependence of D_d , their current utility is seriously limited by the inability of the present single-field debris model to provide a detailed description of the debris temperature. The user may also specify a threshold temperature, below which no reaction occurs, independently of any value of D_d .

A.2.2 Diffusivities for Drop-Side Reaction Rate Limits.

Based upon a variety of metal oxidation studies, Baker [Ba86] suggested a value of the diffusivity equivalent to

$$D_d = 1.27 \times 10^{-4} e^{-22647/T} \quad (\text{A.14a})$$

for the oxidation of steel and steel-zirconium mixtures in steam, and a value of

$$D_d = 9.7 \times 10^{-5} e^{-22900/T} \quad (\text{A.14b})$$

for pure zirconium in steam. (Here, we drop the subscript d on T.) Since these values are based largely (not entirely) upon parabolic rate law fits to metal oxidation in the solid state, their applicability to molten droplets has been questioned. Theoretically, liquid diffusivities are expected to vary as T/μ , where μ is the liquid viscosity, which is expected to show an Arrhenius-type dependence upon the temperature. Powers [Pw86] has considered the problem of estimating diffusivities for high-temperature molten metals and metal oxides, and has noted that the Scheibel modification of the Wilke-Chang (SWC) correlation yielded order-of-magnitude agreement with some limited experimental data. Using viscosity estimates based upon information in [Pw86] and [Co84], and the SWC correlation as given in [Pw86], the following estimates of D_d were obtained in the present investigation:

$$\begin{aligned} \text{O in ZrO}_2: \quad D_d &= 3.7 \times 10^{-11} T e^{-4620/T} \\ \text{O in FeO:} \quad D_d &= 2.6 \times 10^{-10} T e^{-14070/T} \\ \text{O in Fe:} \quad D_d &= 5.7 \times 10^{-11} T e^{-4980/T} \\ \text{O in Zr:} \quad D_d &= 2.1 \times 10^{-11} T e^{-3656/T} \end{aligned} \quad (\text{A.15})$$

Values of D_d given by Eq. A.14a and Eq. 15 are plotted as a function of temperature in Fig. A.3. The values obtained from Eq. A.15 cannot be expected to be meaningful over the full temperature range indicated, since the materials involved will freeze at the lower temperatures, even allowing for eutectic formation.

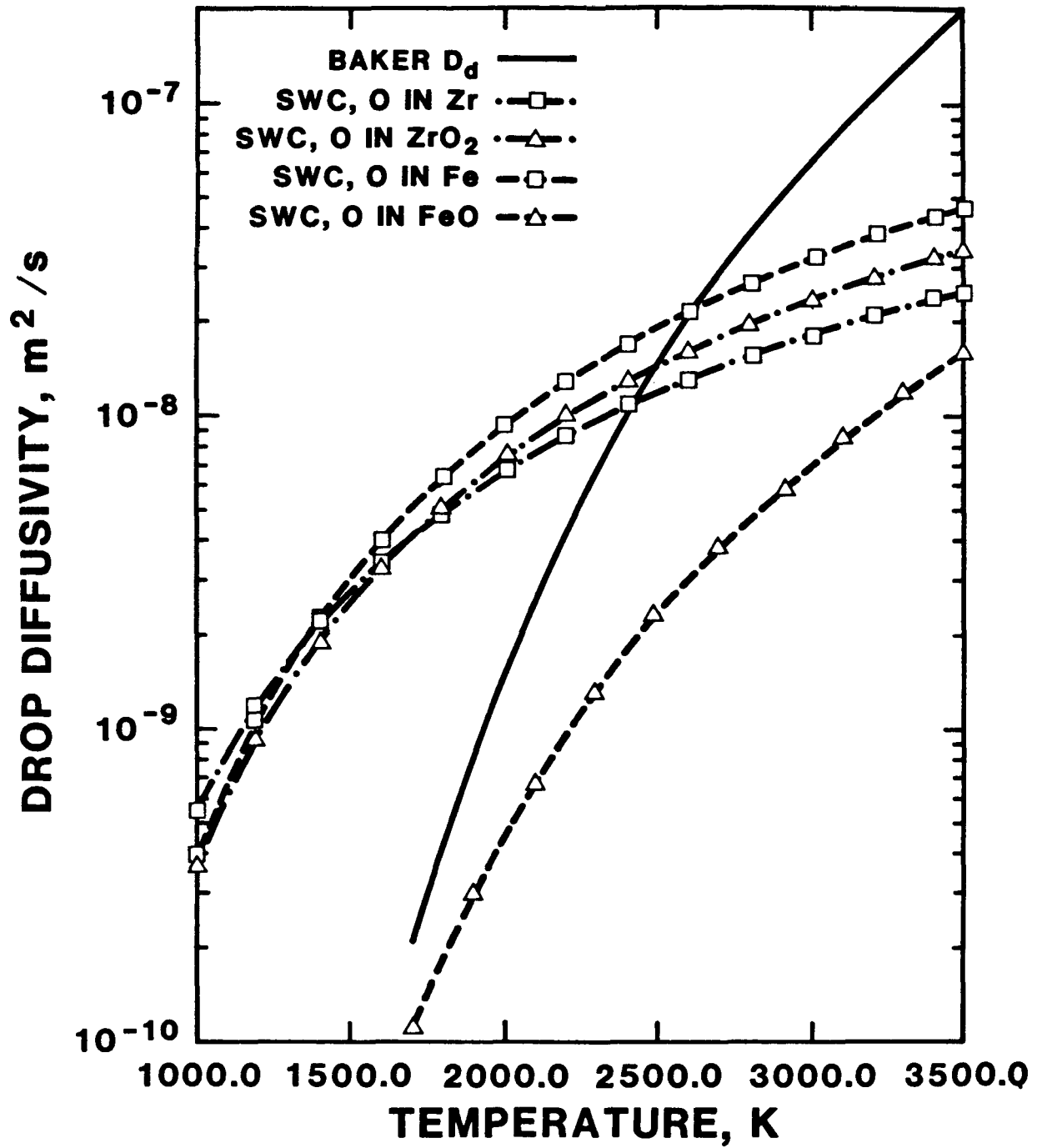


Fig. A.3 Estimates of the diffusivity of oxygen in Zr and Fe metals and their oxides.

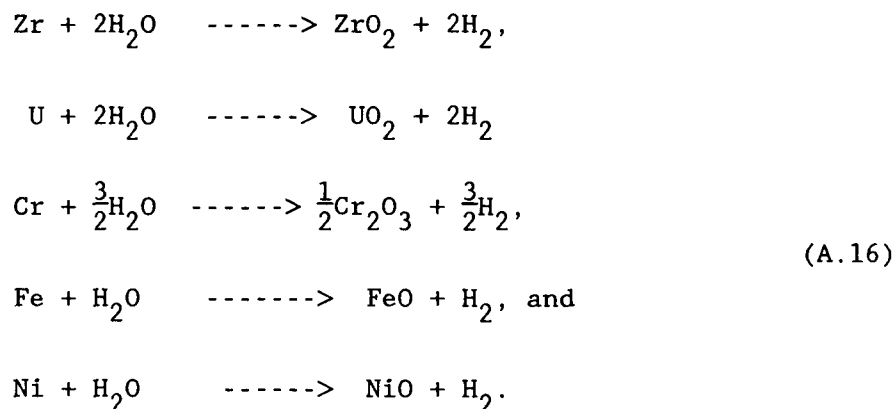
In the DCH calculations discussed in the main text, most of the reaction was calculated to occur in cells with debris at temperatures of 2000-2500 K for many of the scenarios treated, although this was not always the case. In this temperature range, Fig. A.3 indicates that the various relations imply values of D_d within a factor of two to three in either direction of $10^{-8} \text{ m}^2/\text{s}$, except for the relation given for O in FeO.

Since the capability of the IDHM to make use of a detailed temperature-dependent description of D_d is limited, many of the calculations were run with a constant value of $D_d = 10^{-8} \text{ m}^2/\text{s}$, and with the reaction threshold temperature set to a relatively low value (e.g., 1200 K) in order to minimize premature shutoff of reaction due to the limitations of the single-field model's ability to track in detail the thermal history of the reacting debris. Although this treatment may be somewhat conservative given the assumption of reaction rates controlled by diffusion in a stagnant sphere, the validity of that assumption is itself debatable. For example, in studying the reaction of electromagnetically levitated iron spheres in oxygen atmospheres, Robertson and Jenkins observed intense turbulence (probably due to surface tension effects) at the drop surface [Ro70]. The effects of drop-structure impacts and drop shattering could also yield new fresh surface area for continued unimpeded reaction. At present, it would be difficult to make a strong case that the treatment with D_d equal to $10^{-8} \text{ m}^2/\text{s}$ is either "conservative" or "nonconservative," in general.

A.3 Neglect of Chemical Equilibria and Neglect of Chromium.

The present model uses a hierarchical reaction scheme and, furthermore, assumes that all reactions treated are capable of going to completion, given sufficient time. The latter assumption is valid for all practical considerations in the case of the metal-oxygen reactions, and the present discussion is limited to consideration of metal-steam reactions. In addition, the IDHM treats steel as consisting of iron only, but stainless steels used in reactor internals actually contain significant quantities of chromium and nickel as well as iron; e.g., the steel melt in the Surry BMI-2104 analysis for the TMLB' sequence consisted of 80.2% Fe, 12.7% Cr, and 7.1% Ni [Gi84]. Effects related to the neglect of Cr and Ni will be briefly considered here also.

Reactions of the metals potentially present with steam may include the following:



(Other reactions not listed above are also possible.) The reaction of uranium is included because of the possibility that UO_2 may undergo significant in-vessel reduction to the metal by reaction with zirconium [Pw86].

Equilibrium hydrogen/steam ratios were calculated at 2000 K and 2500 K for the above reactions using thermochemical data given in [Pw86]. Results are summarized in Table A.1, expressed in terms of the water mole fraction at equilibrium. Also given in the table are the enthalpies of reaction at 298 K, taken from [Pe73]. The usual thermochemical convention concerning sign is used, i.e., negative values imply an exothermic reaction.

Table A.1
Steam-Hydrogen Equilibria and Heats of Reaction for
Metal-Steam Reactions

Metal	Equilib. H_2O Mole Frac.		$\Delta H_{\text{rx}}(298)$ (MJ/k-mole)
	T = 2000 K	T = 2500K	
Zr	2.5×10^{-6}	5.9×10^{-5}	-598
U	5.5×10^{-6}	6.1×10^{-5}	-590
Cr	0.025	0.072	-200
Fe	0.31	0.33	-28
Ni	0.992	0.988	-2.5

The values given apply for the pure metals in equilibrium with their pure oxides, and constituents of the atmosphere other than steam and hydrogen have been neglected.

Let X_b and X_e be, respectively, the mole fraction of steam in the bulk atmosphere and the equilibrium value in Table A.1. For simplicity of discussion, we neglect atmospheric constituents other than steam and hydrogen, though the inclusion of non-reacting gases (e.g., nitrogen) would not change the equilibrium steam/hydrogen ratios. If equilibrium were treated properly, reaction would stop once X_b decreases to X_e . Furthermore, even when $X_b > X_e$, the concentration in the drop boundary layer would not fall below X_e , while the present model assumes the boundary layer concentration is zero. Hence, the reaction rate predicted by the IDHM (based upon gas-side limits only) should be multiplied by a correction factor C_e approximately equal to

$$C_e = (X_b - X_e)/X_b. \quad (A.17)$$

In the Surry DCH calculations, values of X_b were generally in the range 1.0 to 0.4, neglecting other gases. In the Sequoyah calculations, values of X_b of 0.1 or even lower were sometimes calculated to exist.

From Table A.1, it is apparent that treating the Zr reaction as going to completion introduces negligible error, and that any uranium produced by in-vessel reaction with Zr is thermochemically equivalent to the Zr it replaces, for present purposes. Even for chromium, the neglect of equilibrium would yield only minor error in most cases. Nickel, on the other hand, is inert for all practical purposes, since hydrogen production during DCH invariably reduced X_b below values at which nickel reaction could occur, in the calculations considered.

For iron, the situation is more complex. Even at $X_b = 1.0$, C_e is about 0.7, and it decreases to about 0.36 for the Surry base case, in which $X_b \sim 0.5$ was typical for the lower containment. However, this reduction applies only to the gas-side reaction rate, not the overall reaction rate. For the Surry base case conditions, side calculations indicate that the IDHM formulation would give τ_g equal to about 0.10 s and 0.19 s, respectively, for X_b values of 1.0 and 0.5. Combined with the base case value of τ_d , 0.275 s, the resulting estimates (using Eq. A.13) for τ_e are 0.29 s and 0.34 s, respectively. An

approximate correction for equilibrium effects might be attempted by dividing τ_g by C_e , while leaving τ_d unchanged. If this is done, the resulting estimates for τ_e become 0.31 s and 0.61 s for $X_b = 1.0$ and 0.5, respectively. Thus, sensitivity to equilibrium effects is somewhat less than what would be expected from evaluating the impact upon the gas-side rate limit alone.

For Sequoyah, there were several cases in which the calculated X_b actually became less than X_e , which would obviously terminate iron oxidation. Zr oxidation would be unaffected. Chromium was not treated but, if it were, it would behave almost as the IDHM assumes iron does; thus, its presence would somewhat extend the range of validity of the IDHM estimates of hydrogen production. In any event, it must be remembered that even the iron equilibrium permits conversion of up to two thirds of the available steam to hydrogen. Treatment of equilibrium chemistry is unlikely to yield large reductions in the calculated hydrogen production.

From the last column of Table A.1, it is evident that reaction of chromium with steam releases much more energy than the reaction of iron, and this energy is currently neglected in the IDHM because chromium is not treated. For coriums of the compositions assumed in the calculations of the main text, this energy would range from about 13% to about 27% of the energy available from zirconium oxidation. Thus, it is not a dominant effect, but neither is it entirely negligible.

In hierarchical models such as the IDHM, it is assumed that a more reactive metal such as Zr is completely consumed before oxidation of less reactive metals begins, which is not strictly true. However, the values of X_e in Table A.1 imply that treatment of equilibria would yield insignificant change insofar as Zr is concerned. The separation between the oxidation of Cr and the oxidation of Fe would be less clear-cut, in an equilibrium treatment.

It is concluded that the IDHM limitations discussed here do not introduce major errors; certainly nothing has been identified that could lead to a qualitative change in any of the principal conclusions of the main text. However, quantitative errors that are at least marginally significant could arise in some instances and improvements would be desirable. These would involve treatment of chemical equilibria to at least some degree, and inclusion of chromium in the reaction chemistry.

A.4 Agglomeration of Debris Drops.

Throughout this work, there has been repeated allusion to the limitations of the single-field debris model used in the IDHM. Extending the model to permit treatment of multiple debris fields differing both in terms of initial properties (size, composition, etc., when injected) and in terms of time of injection into the containment has been under active consideration. Schemes for multi-field extensions may involve substantial data-management problems in practice and none have been implemented to date. The problem consists of more than just devising means of multiplying the present single-field model in some manner, in part because the various debris drops can interact in ways that are currently neglected. One of the potential interactions is agglomeration due to collisions between the drops. The purpose of the following brief discussion is to show that this effect is indeed potentially important.

To investigate the agglomeration issue, calculations were performed using a modified version of the WETJET code used in the study of localized deposition from wet plumes [Le86]. The code treats agglomeration due to differential gravitational settling and turbulence, and includes depletion by gravitational settling. Realistic, non-Stokesian fall velocities are used. Various effects which would introduce large errors in standard aerosol codes such as MAEROS when particle sizes and/or turbulence levels are large are included, although with approximations that still leave a significant residual uncertainty. The code solves for the time-dependent behavior of a specified initial distribution of droplet sizes in a single cell which is assumed to be well mixed, as in standard aerosol codes. Introduction of a continuing source during the problem is not allowed for, and thus results obtained are of only limited applicability to DCH scenarios with debris injection spread over a significant time interval.

The problem treated was derived from the Surry DCH base case discussed in Section 3 of the main text, with initial conditions chosen to resemble those calculated to exist in the basement cell (Cell 2 of Fig. 3.2) during debris injection. In the cavity cell (Cell 1), the calculated concentrations of airborne debris were factors of three to four higher, and would give correspondingly more rapid agglomeration. Lognormal size distributions with $\sigma_g = 2$ and mass median diameters (MMD) of 500 μm and 200 μm were assumed. (The CONTAIN calculations assumed 500 μm , which is also close to the MMD yielded in

some DCH experiments; some debris ejection models predict sizes of the order of 200 μm , given ejection from a highly pressurized primary system.) Gravitational depletion was calculated assuming a settling height of 20 meters (approximately the cube root of the cell volume); essentially the same assumption was used in the CONTAIN base case calculations.

Fig. A.4 illustrates how the debris distribution would evolve for the 500 micron MMD case in the absence of agglomeration. The solid curve gives the fraction of the initial mass still remaining airborne as a function of time. It is apparent that about 2 seconds is required to deplete the airborne mass by a factor of two. The other curves give, as a function of time, the drop diameters corresponding to the 10th, 50th, and 90th percentiles by mass; the 50th percentile value is equivalent to the MMD. It is seen that these sizes decline slowly with time as gravitational settling preferentially depletes the larger particles. These sizes apply only to that fraction of the material

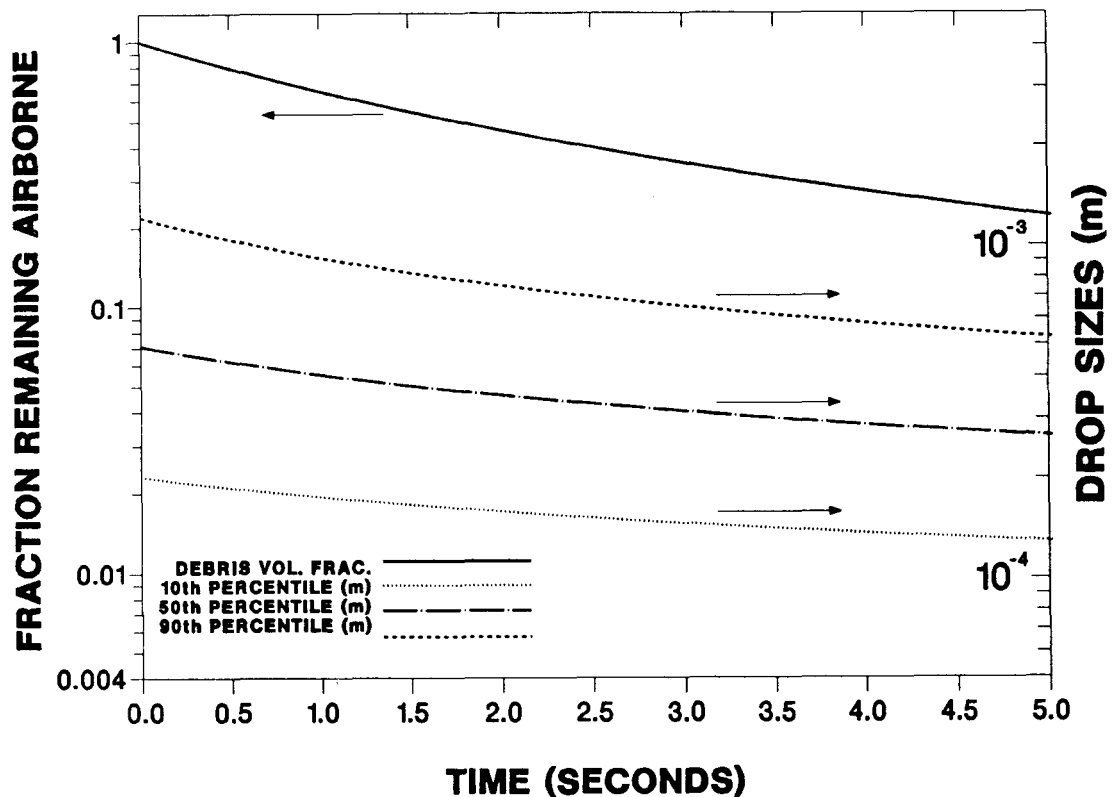


Fig. A.4 Calculated evolution of the debris airborne mass and size distribution for a scenario derived from the Surry DCH base case calculation, with no agglomeration included.

which is still airborne. Since agglomeration is switched off in this calculation, the size distribution of the total debris mass (airborne plus settled) would be time-independent.

Fig. A.5 gives analogous results for the case with agglomeration due to differential gravitational settling treated, but without turbulence. Less than one second is now sufficient to deplete 50% of the initial mass. The size of the material airborne increases rapidly during the first second, with the MMD doubling during the first 0.3 second, despite the fact that the deposition processes are preferentially depleting the airborne material of the larger particles. It is interesting, and potentially significant, to note that the MMD doubling time (0.3 seconds) is about the same as the characteristic time for reaction of a 500 μm drop in the CONTAIN calculations, for the reaction parameters assumed in those calculations. Since the agglomeration

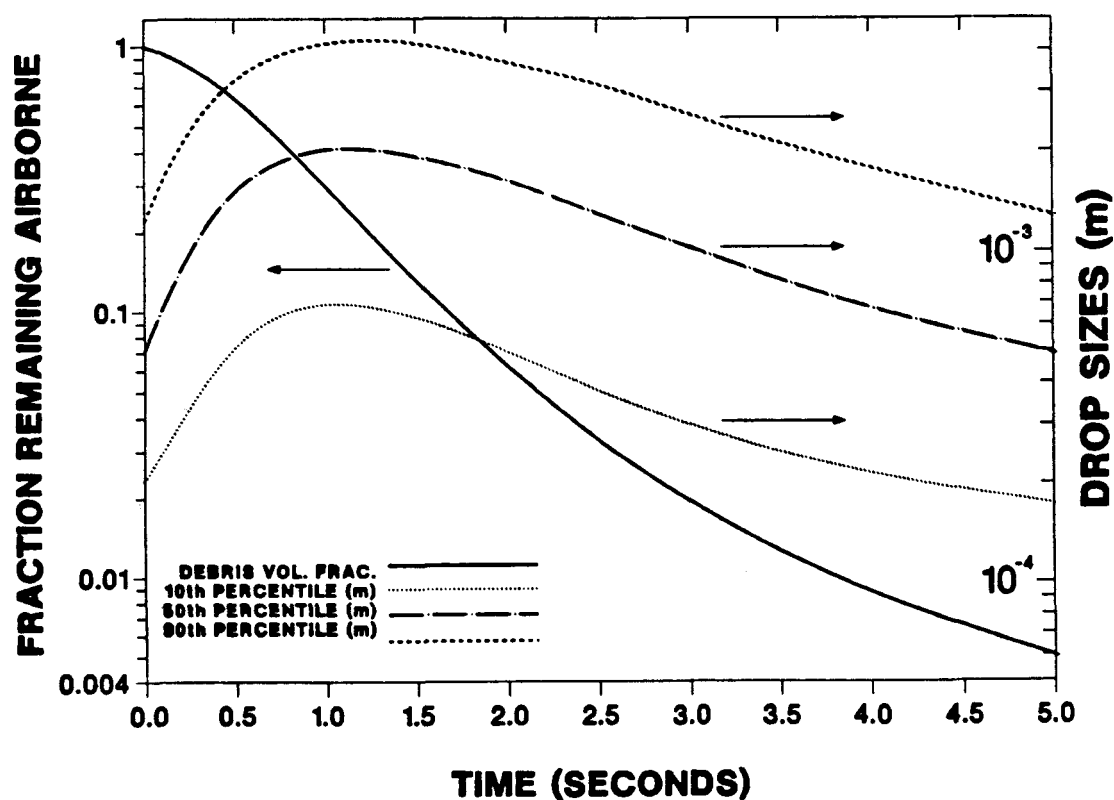


Fig. A.5 Calculated evolution of the debris airborne mass and size distribution for a scenario derived from the Surry DCH base case calculation, with the effects of agglomeration due to differential gravitational settling included.

and reaction processes are occurring on similar time scales, and since reaction rate is a strong function of particle size, it is not at all clear that the effects of agglomeration on reaction will be negligible.

Because the smaller particles are rapidly swept up by the larger, deposition is much more nearly complete after five seconds in Fig. A.5 than in the no-agglomeration case. This rapid sweep-up would not apply to particles of aerosol size, $< 10 \mu\text{m}$, because they interact much less efficiently with the relatively large debris drops.

In analogous calculations for debris with an initial $200 \mu\text{m}$ MMD, the effects of agglomeration, relative to the no-agglomeration case, were even more dramatic than in the $500 \mu\text{m}$ MMD case. Indeed, after the first 0.5 second, the two scenarios with agglomeration did not differ greatly; that is, more rapid agglomeration tended to compensate for the smaller initial size assumed. Nonetheless, initial particle sizes of the order of $200 \mu\text{m}$ might still have an important impact upon the DCH scenario, because of the very rapid chemical reaction and heat transfer to be expected for such small particles.

Turbulence can enhance agglomeration rates [Li85], and calculations were also run for non-zero values of ϵ , the turbulent intensity. The relatively large particles involved here do not respond very effectively to the turbulent eddies, and large values of the turbulent intensity ($\epsilon = 100$ to $1000 \text{ m}^2/\text{s}^3$) were required in order to significantly enhance agglomeration. Meaningful estimates of turbulent intensities in DCH scenarios are not available, and it is therefore difficult to interpret the significance of these results.

Simple hand calculations, based upon particle mean free path arguments, support the qualitative conclusion that agglomeration can be important in DCH scenarios. Quantitatively, there are important uncertainties in these calculations, which will not be reviewed here. It is believed that the calculations are as likely to underestimate the agglomeration rate as to overestimate it, provided the assumption (made in the code) that drops which touch actually do coalesce is valid. It seems plausible that this assumption would be valid so long as the debris is molten, but not once it solidifies.

Rapid agglomeration does not necessarily imply large particle sizes because there also may be fragmentation processes occurring more or less simultaneously, especially in the vicinity of the debris injection point. Thus, the actual debris description may reflect a dynamic interplay between fragmentation and agglomeration processes. Among other things, such behavior could imply a continual re-creation of fresh debris surfaces, which would tend to invalidate the stagnant-drop assumption used in developing the drop-side reaction rate model of Section A.2. As was noted there, it is at least possible that drop-side mass transport will not be rate-limiting, until the drop solidifies.

Calculations were also run for parameters appropriate for the Surtsey experimental program. Although the effects of agglomeration were calculated to be somewhat less than for the Surry DCH scenario discussed here, they were still predicted to be quite significant. Evidently, the possibility of agglomeration also should be considered when interpreting Surtsey experimental results. It is possible that the measured size distributions reflect the net results of the interplay of agglomeration and fragmentation processes, rather than the final results of fragmentation processes acting alone.

In any case, the results discussed here raise questions as to whether it is worth developing a multifield model which attempts to track the time evolution of populations of debris drops unless it can allow for the interactions between the drops. Developing a detailed description for these processes could turn an already-challenging task into a truly formidable problem indeed. It may prove possible to develop somewhat simplified modeling that still treats the dominant effects in at least an approximate fashion. Such means have not yet been developed in any detail, however, and further pursuit of the subject would be beyond the scope of this report.

A.5 Some Examples of Sensitivity to Rate Uncertainties.

In this section, the effects of some of the uncertainties in reaction rates discussed in Sections A.1 and A.2 will be illustrated with some IDHM calculations for a simple test problem. Effects discussed in Sections A.3 and A.4 will not be considered.

Limitations of the model may be divided into two categories. The first involves limitations in the treatment of the various reaction rates, and the second involves limitations inherent in the single-field debris model, i.e., its inability to distinguish debris drops having different compositions and different past histories. In order to study the first category, the effects of the second category may be minimized by defining a test problem in which debris of a single composition is injected "instantaneously", i.e., within a time that is short compared with the characteristic reaction and heat transfer times.

Except where otherwise noted, the test problem involved injection of debris during a 0.002 second pulse, which is "instantaneous" in the above sense. The atmosphere consisted of either steam or a 50:50 steam-hydrogen mixture and was held at a fixed temperature (gas-structure heat transfer was defined so as to be negligible and the injected debris quantity was too small to heat the atmosphere). The model for drop-side reaction rate limits was active, with D_d given by Eq. 14b for pure Zr and Eq. 14a for other debris compositions. In order to permit comparisons with some results given by Baker [Ba86], the gas-drop relative velocity, v_d , in Eqs. 2.2 and 2.3 was assumed to be zero, except as noted below. For simplicity of interpretation, zero trapping was assumed. Cases considered and some results obtained are summarized in Table A.2.

In the table, the second through fourth columns give, respectively, the atmospheric pressure, temperature, and composition (in terms of the steam/hydrogen ratio); the fifth column lists other variations in input. In this column, the entries 'dh2ox' and 'hx' refer to multipliers which the IDHM user can specify to multiply the steam mass transfer rate and the heat transfer rate which the code calculates using Eqs. 2.3 and 2.2, respectively. (Similar multipliers are provided for the rate of oxygen diffusion and the radiative heat transfer rates). The column headed T_d gives the initial temperature of the debris assumed. The last two columns give the results of the calculations, expressed in terms of the percent of the zirconium and the iron that have reacted when the debris cools to the point that reaction ceases for practical purposes. The first six cases involve pure zirconium and a blank therefore appears in the last column; debris composition for the other cases is given in the fifth column. "Surry" refers to the composition of the corium assumed in the Surry calculations of Section 3 of the main report.

Table A.2
IDHM Results for a Simple Test Problem

Case	P_g	T_g (K)	$P(H_2O)$	Other Variations	T_d (K)	% Metal Reacted	
	(bars)		$P(H_2)$			Zr	Fe_
1	1.0	400.0	1.0	----	2273	9.2	---
2	1.0	400.0	2×10^6	----	2273	91.0	---
3	1.0	400.0	1.0	dh2ox = 2.0	2273	13.8	---
4	1.0	400.0	1.0	dh2ox=2, hx=0.7	2273	82.6	---
5	3.0	1200.0	1.0	----	2273	74.0	---
6	5.0	2000.0	1.0	----	2273	94.5	---
7	3.0	1200.0	1.0	$W_{Zr}/W_{Fe} = 0.5$	2273	91.8	27.0
8	5.0	1500.0	1.0	$W_{Zr}/W_{Fe}=0.5, v_d=6.8$	2550	96.2	38.9
9	5.0	1500.0	1.0	Surry corium, $v_d=6.8$	2550	60.1	10.0
10	5.0	1500.0	1.0	Surry; $v_d=6.8$; 5 s inj.	2550	12.6 ^a	0.85 ^a
11	5.0	1500.0	1.0	As #8, with $D_d = 10^{-8}$	2550	99.5 ^b	72.1 ^b
12	5.0	1500.0	1.0	As #9, with $D_d = 10^{-8}$	2550	99.1 ^b	73.3 ^b
13	5.0	1500.0	1.0	As #10, with $D_d = 10^{-8}$	2550	98.0 ^a	92.3 ^a

^aPercent reacted at end of 5-second injection period

^bPercent reacted 0.5 s after injection

The first case gives results for the response of the Zr drop in a 50% mixture of steam and hydrogen at relatively low temperatures (400 K). In this case, reaction energy is insufficient to make up for heat loss, the drop begins to cool, and the strong temperature-dependence of the reaction rates controlled by the drop diffusivity assumed here quickly shuts off the reaction. The second case gives results for the Zr drop in an atmosphere of essentially pure steam. Here, the reaction energy exceeds the initial heat loss rate, and the drop heats up and stays hot long enough for the reaction to be almost complete.

One reason for the difference between Case 1 and Case 2 is that the steam concentration difference driving transport of steam to the drop surface is twice as great in Case 2. However, the lower thermal conductivity of the pure steam atmosphere is a more important effect. The code uses the bulk atmosphere composition to calculate the debris-gas heat transfer. In reality, the

drop boundary layer will not be pure steam, and it might be argued that the thermal conductivity of the 50-50 steam-hydrogen mixture assumed in Case 1 would actually give a value that is more nearly correct for the boundary layer in Case 2. The implications of this assumption are investigated in the third calculation, in which the atmosphere is 50% hydrogen but $dh_{2ox} = 2$, in order to reproduce approximately the mass transfer rates appropriate for a bulk atmosphere consisting of pure steam. The fraction reacted (Case 3) is then little more than in the first case. However, if the rate of heat transfer by conduction is reduced by only 30% ($h_x = 0.7$ in Case 4), the reaction is again largely complete.

One of the cases considered by Baker [Ba86] also involved a 0.5 mm Zr drop, initially at 2273 K, reacting with steam at some relatively low (but unspecified) temperature. He obtained a degree of reaction that was 74% complete, using essentially the same basic model as that employed here except that he was able to implement a time-dependent drop-side reaction rate similar to Eq. A.8, since his model only tracked the history of an individual drop. Depending upon how the uncertainties involved in heat transfer are handled, the results just cited show that the present model can yield either a quite comparable degree of reaction or a substantially smaller amount of reaction. Since the calculation is so sensitive, not too much can be made of this comparison, except to note that the present model does not appear to over-predict the extent of reaction, relative to that described in [Ba86].

The extreme sensitivity exhibited by these results reflects the fact that the initial conditions in this calculation are close to the threshold for zirconium ignition, and the fraction reacted is therefore very sensitive to moderate variations in the parameters which govern the ignition threshold. Many DCH calculations are expected to show much less sensitivity because the gas quickly becomes heated to temperatures approaching that of the debris. Under these conditions, there cannot be much sensitivity to debris-gas heat transfer; furthermore, reaction rates will remain high if the temperature of the debris-gas mixture is high enough. This behavior is illustrated in Cases 5 and 6, which differ from Case 1 only in the initial values of the gas temperature and pressure. At 2000 K, which is typical of DCH conditions, reaction is almost 95% complete within 1 second, and is almost 75% complete even at a gas temperature of 1200 K.

As discussed in the main text, there do exist scenarios (water quench, rapid primary system blowdown) in which the temperatures would be low enough to slow or stop reaction once the debris and the atmosphere thermally equilibrate. Furthermore, reaction with steam of metallic drops consisting largely of iron will not generate nearly as much energy as do the zirconium drops considered here, and will therefore tend to cool more rapidly once any zirconium present is consumed. Under these conditions, the interplay between debris temperature, reaction rate, energy generation, and heat transfer will be important in governing the actual extent of reaction. The present model is insufficiently detailed to give accurate results as to the extent of reaction in such cases. The remaining cases in Table A.2 were defined to illustrate some of the difficulties.

In Case 7, the debris is assumed to consist of 33.3% Zr and 66.7% Fe, and parameters are otherwise as in Case 5. The reaction of Zr is almost complete in this case, which means that the large majority of the potentially-available chemical energy will be realized even though only 30% of the iron reacts. Case 8 is similar to Case 7 except that temperatures of debris and gas, and the gas-particle velocity v_d , are adjusted to values more typical of some encountered in the actual containment calculations of the main text (e.g., those with moderate amounts of co-dispersed water and the rapid-blowdown scenarios). The extent of reaction is increased somewhat, but results are still qualitatively similar: almost all the potential reaction energy is released, while hydrogen generation is about 60% of the maximum possible.

In Case 9, the debris is assumed to have the same composition as that assumed in the Surry calculations. The Zr/Fe ratio is still 0.5, but the corium is almost 80% oxides by mass. The calculation was run assuming intermixed metals which are segregated from the oxides ($f_{Zr}^0 = 0.333$, $f_{Fe}^0 = 0.667$). From the point of view of the reacting debris, this scenario is identical to that in Case 8, i.e., the inert oxides should have no effect and the extent of reaction should be the same. The results show, however, that the calculated Zr reaction falls to 60%, and only 10% of the iron reacts. These decreases are artifacts of the single-field debris model: the reaction energy is forced to heat the entire bulk debris field, and heat transfer is calculated using the entire bulk debris surface area. In reality, only the masses and surface areas of the reacting drops should be included in assessing their energy balance, given the assumption of segregated metals and oxides.

The impact of the single-field debris model's limitations becomes much more severe when debris injection is spread over a five second interval as in the actual DCH analyses discussed in Sections 3-5 of this report. Time constants for gas-debris thermal equilibration are of the order of 0.1 s in this scenario; hence, after a few tenths of a second, the bulk debris field is calculated to be cooled substantially below the injection temperature. Freshly-injected debris is instantly equilibrated with the cooler bulk debris field in the calculation, and the fresh debris never has a chance to undergo even a transient period of rapid reaction during cool-down. Case 10 gives the results: zirconium reaction is now calculated to be minor, and iron reaction is negligible. Thus, the model with the single-field limitations calculates that only ~12% of the total reaction energy would be liberated and even less of the potential hydrogen generation is calculated to occur, yet Case 8 shows that, if the spurious single-field effects could somehow be eliminated, the same basic model would otherwise yield 60% of the potential hydrogen generation and almost all of the potential energy release.

The impact of the single-field limitations is almost entirely through the strong temperature-dependence of the drop-side reaction rate limit. Cases 11-13 give results for calculations analogous to Cases 8-10 except that a value of D_d equal to $10^{-8} \text{ m}^2/\text{s}$ is now assumed, independent of temperature. Comparison of Case 11 with Case 12 shows that the addition of inert oxide now makes virtually no difference. Precise comparisons with the case involving the 5-second injection time (Case 13) are not straightforward to make, because there is now no reaction cutoff, but it is evident from the results that the extended injection and the accumulated inert oxide debris are not interfering with efficient reaction in this calculation.

These results show that use of the single-field model with a temperature dependence such as that of Eq. 14 runs serious risks of grossly underpredicting the extent of reaction in actual DCH containment analyses. Hence, a constant diffusivity, chosen as discussed in Section A.2.2, was adopted for most of the calculations, with the use of the temperature-dependent form being limited to a few sensitivity studies. One conclusion does seem clear: if a calculation with the present model using expressions such as Eq. 14 indicates that there is little sensitivity to this variation (as in the Surry base case), then it is safe to assume that the true sensitivity actually is small indeed.

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