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PROGRESS IN UNDERSTANDING OF DIRECT CONTAINMENT HEATING PHENOMENA
IN PRESSURIZED LIGHT WATER REACTORS*

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ABSTRACT

Progress is described in development of a mechanistic understanding of direct containment heating phenomena arising during high-pressure melt ejection accidents in pressurized water reactor systems. The experimental data base is discussed which forms the basis for current assessments of containment pressure response using current lumped-parameter containment analysis methods. The deficiencies in available methods and supporting data base required to describe major phenomena occurring in the reactor cavity, intermediate subcompartments and containment dome are highlighted. Code calculation results presented in the literature are cited which demonstrate that the progress in understanding of DCH phenomena has also resulted in current predictions of containment pressure loadings which are significantly lower than are predicted by idealized, thermodynamic equilibrium calculations. Current methods are, nonetheless, still predicting containment-threatening loadings for large participating melt masses under high-pressure ejection conditions. Recommendations for future research are discussed.

I. INTRODUCTION

Direct containment heating (DCH) arises during high-pressure severe accident sequences in light-water reactors (LWRs) which lead to ejection of molten core material from the reactor vessel into the reactor cavity region beneath the vessel and, subsequently, transport of finely-divided melt to regions of containment downstream of the cavity. The molten material would consist, primarily, of uranium and zirconium oxides and unreacted zirconium and iron. The stored energy of the melt consists of its sensible energy, its latent heat energy and the chemical reaction energy of its components. Direct energy transfer from the melt to the containment atmosphere would lead to heating and pressurization of the containment atmosphere.

The objectives of this paper are to review progress that has been made in the development of the

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phenomenological understanding and analytical methods required to predict DCH scenarios in pressurized water reactors (PWRs) and to characterize the research which needs to be performed in order to reduce uncertainties in prediction of DCH containment loads. Section II describes the DCH scenario and the relevant phenomena in various regions of the containment building. Bounding thermodynamic calculations of DCH containment loading are discussed in Section III. A description of our current understanding of DCH phenomena and associated uncertainties is presented in Section IV. A summary and recommendations for future DCH research are described in Section V.

II. THE DCH SCENARIO

A. Background

The Zion Probabilistic Safety Study (ZPSS)¹ recognized the possibility of severe accident conditions whereby melt could accumulate in the lower head of PWR pressure vessels under high-pressure reactor coolant system (RCS) conditions. Failure of the vessel at a location in contact with the melt would then lead to pressure-driven ejection of melt from the vessel into the reactor cavity region, shown in Fig. 1 along with other features of the Zion containment building, beneath the vessel. The study also suggested that the subsequent blowdown of the steam-hydrogen mixture would lead to ejection of a coherent mass of melt from the reactor cavity and deposition of the melt on the water-flooded floor of the containment building. The melt was assumed to eventually quench, producing steam as the containment loading mechanism.

Sandia National Laboratory (SNL) conducted the SPIT and HIPS^{2,3} series of experiments which simulated the process of high-pressure melt ejection. These experiments provided observations of the jet which issued from an orifice in the experimental melt pressure vessel and of the processes of interaction of the blowdown gas with the melt in the 1/20-th and 1/10-th scale concrete models of the Zion reactor cavity. These experiments, using iron-alumina thermite as the core melt simulant, provided evidence that forms the basis of the current understanding of reactor cavity phenomena. The experiments indicated that the blowdown gas very effectively removed the

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melt from the cavity models and that this process of "melt dispersal" from the reactor cavity models was accompanied by fragmentation of the melt into droplets, with a spectrum of diameters ranging from aerosol (microns) to several millimeters. This view of high-pressure reactor cavity dispersal phenomena in the Zion cavity was subsequently verified by Spencer, et al.⁴ and by Turu, et al.⁵ The SNL experimental results also suggested that the high-velocity molten jet from the reactor vessel is fragmented in transit to the base of the cavity under the influence of dissolved gas release and high relative velocity at the edge of the jet.

The earliest calculations of DCH containment loading^{6,7} performed in the context of the USNRC Containment Loads Working Group (CLWG) deliberations,⁸ were based upon a conceptual model which postulated, based upon the experimental results, that droplets of molten core material (corium) were ejected from the reactor cavity into the containment atmosphere. These droplets would interact thermally and chemically with the containment atmosphere. From a computational point of view the entire containment building was represented as a single, adiabatic control volume. Thermodynamic equilibrium⁶ and rate-dependent⁷ calculations were performed, where it was assumed that the metallic constituents of the melt would oxidize by direct reaction with the available oxygen supply in the containment building dome. Interactions between droplets and atmosphere, both chemical and thermal, were computed to be quite efficient because of the large assumed control volume and large possible droplet interaction time. Containment-threatening pressure loadings were predicted when large quantities of melt were assumed.

A further refinement of the view of the DCH accident scenario developed upon recognition that the containment dome region, containing the large quantity of oxygen to drive the chemical reactions, is separated from the reactor cavity by intermediate subcompartments which are densely packed with equipment and various other structures. Melt droplets, driven by the steam/hydrogen blowdown gas from the reactor cavity, would likely encounter structure along their trajectories and could be removed from the flow field prior to reaching the containment dome. This view, initially expressed within the activities of the CLWG and demonstrated in small-scale experiments^{9,10} raises the possibility that the melt droplets could be trapped on structure prior to complete transfer of energy to the containment atmosphere.

The central role of hydrogen generation and combustion in the context of DCH was first postulated by Turu,¹¹ who observed that steam-metal reaction would be initiated in the reactor cavity during the vessel blowdown and melt dispersal process. Hydrogen generation, therefore, would begin in the reactor cavity with reaction rates that are extremely large when calculated assuming, typically, 1-mm diameter zirconium droplets and using accepted rate-limiting mass transfer models.¹² The possibility for copious quantities of hydrogen generated within the reactor cavity

and in its vicinity has been recognized by Bergeron¹³ and discussed recently by Powers.¹⁴ There are as yet, however, no experimental data available to aid in assessment of the extent of hydrogen generation during a DCH scenario. Since no significant quantity of oxygen is available in the reactor cavity, the hydrogen cannot burn until it reaches the oxygen supply available either in the intermediate subcompartments or in the containment dome region. Upon reaching the containment dome the hydrogen may burn, despite large steam concentrations, due to high gas temperature or due to the presence of high-temperature particulate.

B. DCH Accident Conceptual Scenario

The ideas described above have led to the emergence of a picture of the DCH accident scenario which has wide acceptance and which forms the basis for integrated modeling of DCH phenomena¹⁵ in PWRs. The Zion plant, shown in Fig. 1, here serves as a representative system. The accident scenario is described below.

Molten corium, consisting of oxides and unreacted zirconium and stainless steel, is assumed to have accumulated within the lower plenum of a PWR pressure vessel, with the reactor coolant system at "high" pressure. The containment building initially contains a mixture of air, steam and hydrogen released from the reactor vessel during the in-vessel core degradation phase of the severe accident. The vessel fails in the region of the molten material and the corium is ejected as a molten jet through a breach in the vessel wall into the reactor cavity. The jet, in transit, is fragmented by expansion of dissolved gases and by stripping at the edge of the jet. The molten corium spreads under its own momentum across the cavity and accumulates there. Steam, which follows the melt from the vessel, flows at high velocity through the reactor cavity, finely subdivides the melt and carries some fraction of the melt as droplets into the subcompartments just above the cavity. Thermal and chemical transfer interactions occur between the steam and droplets within the cavity and the subcompartments. Hydrogen is produced as the steam reacts with the unreacted molten metallics. As the melt flows through the subcompartments, a portion of the suspended droplets will likely be deposited on structures. As the gas flows around the intervening structures to the upper dome region of containment, therefore, only a fraction of the molten material which exits the cavity will be carried with it. This material will then interact with the atmosphere in the dome region. A portion of the hydrogen produced in the subcompartments and the cavity will be transported to the dome region. Combustion of the hydrogen generated in-vessel and the hydrogen generated following vessel failure would occur if conditions in the containment dome permit.

The above scenario would be modified if it is assumed that water is initially present in the reactor cavity or if water droplets are assumed suspended in the containment atmosphere. Because of the paucity

of experimental data and analytical models pertinent to scenarios involving the presence of water in the reactor cavity or in containment atmosphere prior to high-pressure melt ejection, the effects of water will not be reviewed here.

III. THERMODYNAMICS OF DCH CONTAINMENT LOADING

The current detailed, rate-dependent, multi-region phenomenological modeling embodied, for example, in the CONTAIN code¹⁶ was preceded by bounding, simplified, single-cell models.⁶ The DHEAT and CONTAIN codes, for example, were used to perform thermodynamic equilibrium calculations of the DCH containment loading.⁶ The DHEAT model assumed an adiabatic containment, complete chemical reaction of the available iron and zirconium with oxygen and thermal equilibration of the gas atmosphere, reactants and reaction products. Quench of the melt in water pools was also modeled. None of the calculations performed on the time frame of the CLWG included the incremental loading attributable to the combustion of hydrogen generated in-vessel prior to the failure of the reactor vessel. Even without this additional loading mechanism, the bounding calculations led to predictions of extremely large pressure loadings, compared with estimates of containment failure pressure, when large quantities of melt were assumed.

Thermodynamic equilibrium calculations such as those described above provide an upper limit to the DCH containment pressure loading and serve as a basis for comparison with more mechanistic, rate-dependent calculations. Because of its importance as a reference point, a thermodynamic equilibration model "EBAL" was written at BNL to compute an upper limit on containment loading which includes the burn of in-vessel hydrogen. The EBAL model assumes, as does DHEAT, a single-cell containment atmosphere consisting of nitrogen, oxygen, steam and hydrogen. The melt constituents are iron, iron oxide, zirconium, zirconium oxide and uranium dioxide. The metallics can react with steam to produce hydrogen; the hydrogen can then burn in oxygen. In the absence of oxygen the steam-metal reactions will occur. Water can also be assumed present in the atmosphere and participate in the thermal equilibration process. All of the metal is assumed to react as long as oxidant is available. All species' specific heats are treated as temperature-dependent quantities.

Calculations were performed with EBAL using Zion and Surry as prototypes of "large-dry" and "subatmospheric" PWR containments, respectively. It was assumed that all melt which exits the reactor vessel participates in DCH. Table 1 presents the DCH initial conditions for the two sets of calculations. The effects of melt inventory and hydrogen burn parameters were investigated. The calculation results for containment pressure rise are shown in Fig. 2 along with estimated containment failure conditions. The results indicate that if all the available hydrogen were to burn, then the computed upper limit containment pressure rises are containment-threatening over a broad range of participating melt mass. If it

is assumed that the metallic melt constituents react with steam, but that the resulting hydrogen does not burn, then the computed pressure rises are considerably lower. Containment-threatening loads are predicted only for the largest of core melt inventories if hydrogen burns are postulated not to occur.

The above pressure rise estimates result from assumptions which are clearly conservative. It is shown in Section V that when the EBAL single-cell, adiabatic thermodynamic equilibrium model is replaced with the CONTAIN code's multi-cell, rate-limited physics approach which incorporates assumptions based upon available experimental data, the computed containment pressure rise estimates (for the Surry plant) are considerably lower than those shown in Fig. 2.

IV. REVIEW OF DCH PHENOMENOLOGY

A. General Methodology Requirements for DCH Analysis

Based upon the DCH scenario outlined in Section II, a containment response methodology is required which describes and integrates the phenomenology occurring in three regions of containment: (i) the reactor cavity, (ii) the "intermediate subcompartments" and (iii) the containment dome. There are large differences in geometry of each region among the many U.S. PWR containment systems. Methods must be developed for the phenomena occurring in each region of containment which can accommodate the differences in plant containment design. The motion of the melt through the various regions of containment must be followed, while computing the integrated release of energy from the melt to the containment atmosphere, the quantity of hydrogen produced and burned and the energy transfer to water in containment. Models for these various rate dependent exchange processes must be integrated into a methodology for prediction of the pressure and temperature response of the containment building.

Several "lumped-parameter," multi-cell containment analysis codes have been modified for DCH analysis. The CONTAIN code, with its Interim Direct Heating Model,¹⁶ has been modified to permit integrated, parametric calculations of DCH loading. The MAAP code is also being used to predict DCH phenomena, although the details of the modeling principles are unpublished.¹⁷ The HMC code has been modified to incorporate models of DCH phenomena.¹⁸

DCH initial conditions are determined by the in-vessel melt progression. Large uncertainties exist in prediction of the rate of accumulation of melt on the lower vessel head, in the mode, timing, and location of vessel failure and on the composition of the melt discharging from the vessel. The initial breach area is uncertain, as is the rate of growth of the breach area as melt flows out of the vessel. Initial breach of the vessel via failure of instrument tube penetrations has been proposed, followed by ablation of the resulting hole to a diameter of approximately

0.5 meter.¹⁹ It is noted, however, that massive circumferential failure of the lower vessel head has also been suggested. These issues are being addressed as part of the USNRC MELPROG development program²⁰ and will not be discussed further here.

Issues related to reactor cavity, intermediate subcompartment and containment dome are addressed below.

B. Reactor Cavity Phenomena

1. General Remarks

The thermal, chemical and hydrodynamic interactions which take place within the reactor cavity are thought to strongly influence the subsequent rate of transfer of corium stored energy to the containment atmosphere. The major reactor cavity quantities which must be characterized in order to predict DCH energy transfers are the droplet size distribution and mass flux of gas constituents (especially hydrogen) and melt exiting the cavity. The mechanisms which govern these quantities involve complex multi-phase interactions between molten corium and high-speed, three-dimensional, chemically reacting, compressible gas flows. The current understanding of reactor cavity phenomena under accident conditions is based upon a combination of experimental observations from small scale experiments using both high-temperature and low-temperature molten fluid simulants, simplified calculations and conjecture. Integral experiments involving all features of reactor cavity phenomena have not yet been carried out.

The discussion which follows is presented in two parts. The first part presents a discussion of the major relevant phenomena as we understand them. Because of the dominance of the "reactor cavity dispersal" DCH issue, this is addressed separately in its own section.

2. Reactor Cavity Thermal Hydraulic Phenomena

It is useful for the discussion which follows to choose a specific reactor cavity configuration and a set of "typical" DCH accident initial conditions. Figure 1 shows a view of the Zion reactor cavity. Table 1 presents the definition of a set of initial conditions for a postulated accident in the Zion plant occurring at a primary system pressure of approximately 7 MPa. The vessel breach diameter, after ablation, is assumed to be 0.55 m.

The DCH scenario is postulated to begin with development of a breach of the reactor vessel and ejection of melt into the reactor cavity. Observations made in the SNL SPIT experiments³ led to the conclusion that nitrogen had been dissolved in the iron-alumina melt which, upon release from the pressurized melt chamber, was released from solution and rapidly expanded. This provided the mechanism for the observed breakup of the jet. A model has been proposed to characterize the process.¹⁹ It has been

proposed that hydrogen would be dissolved in molten corium under accident conditions and that, similarly, the molten jet would break up in the process of flow to the cavity floor. This breakup process would result in a production of droplets with some size distribution. This scenario has not yet been verified in experiments with prototypic fluids. The resulting drop size distribution has not been characterized.

Ejection of liquid melt from the vessel would continue until the depth of the molten pool is sufficiently shallow to allow entrainment of gas into the melt, at which point "gas blowthrough" would occur.¹⁹ It is expected that at this point a period of two-phase melt ejection would begin under conditions of two-phase flow at the vessel breach. The two-phase period is believed characterized by a process of atomization of the discharging melt at the breach. Pilch summarized correlations to predict the droplet sizes produced during atomization processes.¹⁹ They have not, however, been verified under prototypic DCH accident conditions. Upon exhaustion of the melt supply from the vessel the blowdown of steam and hydrogen from the vessel would continue until the gas supply is exhausted.

Droplets produced from the jet breakup and two-phase atomization processes would be directed from the vessel to the cavity floor. At this point, current analytical methods do not permit us to follow their trajectories. It is quite possible that these droplets would lose their identities and would be absorbed into the bulk of melt which would exist at this time in the cavity. Aerosol-size droplets would more likely stay suspended in the cavity, perhaps to be swept out by the steam upon gas blowthrough. More detailed mechanistic understanding of these droplet production mechanisms must be accompanied by improved methods which will enable us to track the droplets formed from these mechanisms through the reactor cavity.

Figure 3 presents "typical" computed mass flow rates of melt and primary system steam exiting the pressure vessel, based upon the Zion parameters of Table 1. The gas blowdown is computed assuming isentropic expansion through an orifice. Calculations indicate that the period of single phase melt ejection would last about 4 seconds, during which approximately 75% of the melt would be discharged from the vessel. Melt jet velocities of typically 30 m/s are computed. The two-phase period, characterized by the process of atomization of the discharging melt at the breach, would last about 4 seconds. Based upon the conditions of Table 1, the single phase gas blowdown is expected to last about 15 seconds.

Tutu, et al.⁵ have provided high-speed photographic observations of the behavior of the melt within the reactor cavity in small-scale experiments involving low-temperature melt simulant materials under conditions which are prototypic of high-pressure accident conditions. The experiments involved no dissolved gases in the melt and the walls of the cavity do not release gas upon contact with melt, as

would concrete. These experiments, discussed in more detail below, indicate that the melt simulant enters the reactor cavity, splashes and spreads in all directions and covers all the surfaces of the cavity prior to "gas blowthrough." Gas, which then follows the melt into the cavity, appears to strip the melt from films along the walls, entraining the liquid into the gas stream. The gas carries the droplets out of the cavity exit. The flow patterns within the reactor cavity, deduced from the movies, suggest the existence of a complex, recirculating, three-dimensional flow field within the cavity. The applicability of these observations to prototypic accident conditions, of course, may be influenced by the experimental simulation limitations, described briefly above.

Detailed verification of the above observations is lacking in high-temperature simulant experiments. Experimental techniques have not been developed to probe the interior of the reactor cavity for detailed flow regime and flow field observations in such experiments. The evidence pertaining to the nature of melt-gas cavity interactions in the available high-temperature simulation experiments are (i) high-speed x-ray movies taken at the exit of the model cavities and (ii) the structure of the resolidified debris recovered after the experiments.^{4, 21} The data from dry-cavity (no pre-existing water) experiments suggest that the melt simulants are ejected from the cavity as dispersed droplets. Droplet size distributions have been deduced from post-test samples of solidified debris collected in several experiments.^{3, 21, 22} The particles collected in the various experiments were found external to the cavity models and, while still molten, had very likely experienced at least one interaction with structure prior to deposition on the structure. The nature of the interaction of high-velocity, high surface tension droplets with structures is not understood. It has been assumed that the resulting particle size distributions are characteristic of the melt at the discharge of the reactor cavity during the experiments. It is noted, however, that the situation is somewhat more complex and that the assumption is subject to question.

The available particle size data from experiments which were designed to simulate high-pressure DCH conditions indicate that the mass-mean particle diameters were in the range of approximately 0.5-1.0 μ m.^{3, 21, 22} Measured particle diameters ranged from aerosol-size (microns) to several millimeters. These data represent distributions resulting from samples of post-test collection of a sampling of debris which were ejected from the cavity during the transient melt ejection process. The droplets were created from the melt by a combination of mechanisms, none of which are completely understood. They result from breakup of the melt jet by the action of dissolved gases, atomization at the vessel breach, splash, entrainment processes from liquid films and secondary droplet breakup (Weber breakup). The droplets were presumably swept from the cavity by the flowing gas, followed trajectories to the nearest

structure, bounced, perhaps shattered, and continued to their final destination where, eventually, they were sampled.

Since the mechanisms of droplet formation are not known, application of the available droplet size data base to full-scale, prototypic accident conditions is fraught with difficulty. While models of reactor cavity phenomena are being developed,^{23, 24} including descriptions of droplet behavior, much development, evaluation and assessment remains to be done. At present, in DCH analyses that are being performed,^{15, 25} it is assumed that the particle size data discussed above is applicable to "high-pressure" accident conditions. As such, the characteristic mass-mean droplet diameter applicable to accidents with initial vessel pressure of approximately 7 MPa is assumed to be in the range 0.5-1.0 μ m. There is at present no verified method of computing the diameter of droplets for accidents with higher or lower initial vessel pressure.

Measurements of local thermal and hydrodynamic conditions within the experimental reactor cavities have not been performed. As a result, conditions under accident circumstances can only be surmised based upon the above experimental observations and simplified models of the phenomena. It is assumed that a dispersed melt droplet flow regime exists within the reactor cavity, perhaps with intermittent liquid films existing on the walls. As a result, it is expected that efficient heat transfer between the melt and the blowdown gas will take place and, with its low heat capacity, it is expected that the gas will heat to temperatures approaching the melt temperature during its transit through the cavity. Calculations based on a one-dimensional reactor cavity model suggest that this was the case in the SNL Surtsey DCH-1 test.²³ A consequence of the gas heating is acceleration of the gas. Calculations based upon the Zion cavity with initial conditions as listed in Table 1 indicate that the peak cross-sectionally averaged gas velocity just under the vessel, where the gas temperature is 500K would be about 188 m/s. At the same time, the gas velocity at the cavity exit, where the gas temperature could be in the range 1500K-2500K, would be in the range 565-940 m/s. With the above assumptions, therefore, gas velocities within the reactor cavity can be several hundred m/s with gas temperatures approaching the melt temperature.

3. Reactor Cavity Metal-Steam Reaction and Hydrogen Production

No DCH experiments have been performed using molten corium simulants together with high-pressure steam as the blowdown fluid. Plans are being made at SNL to perform such experiments in the Surtsey facility.²⁶ Our current understanding of metal-steam chemical reaction phenomenology within the reactor cavity, therefore, is largely based upon an experimental data base related to zirconium-steam and iron-steam chemical reactions.^{27, 28} This information is supplemented by the thermal-hydraulic observations described above, theoretical considerations and conjecture.

The available, one-dimensional models of reactor cavity interactions^{23,24} have not been used to predict cavity chemical reaction phenomena. Published calculations of the extent of metal-steam reaction in the reactor cavity have been performed using single-droplet heat and mass transfer models and bounding thermodynamic equilibrium models.

Single-droplet models and calculations have been reported by several authors.^{11,12,14} They assume a dispersed melt droplet flow regime in the reactor cavity, that zirconium or iron droplets are suspended in a steam flow and that the steam supply is effectively unlimited. The reaction rates are governed by either steam diffusion through a steam-hydrogen layer external to the droplets or by steam diffusion through the molten liquid. The relative velocity of steam and droplet is either specified by assumption or through solution of a momentum equation for a droplet in a specified gas flow field. A single-droplet model, developed at BNL for scoping calculation purposes, assumes that a droplet is released into the cavity gas flow and is accelerated by drag forces. The droplet, released under the reactor vessel, is assumed to travel along the cavity axis. The gas velocity along the cavity is assumed to vary due to the heatup of the gas, described above. A gas temperature distribution is assumed based upon judgment and the velocity distribution is computed based upon an assumed steam discharge flow rate and the ideal gas law. Transient single droplet momentum and energy equations are solved while accounting for metal-steam reaction and hydrogen production. Either liquid-phase or gas-phase diffusion is assumed to govern the reaction rate.

Typical calculation results are shown in Fig. 4, which presents the extent of chemical reaction of zirconium in steam as a function of droplet path length (cavity lengths are typically 15 m) for several droplet diameters with an initial droplet temperature of 2500K. For these conditions the chemical reaction is gas-phase diffusion limited.²⁹ These calculation results support earlier conclusions,^{11,14} that, based upon single-droplet models, the metal-steam reaction would be nearly complete for droplets with diameters less than 1 mm and very extensive for diameters up to several millimeters. The potential for extensive hydrogen generation within the reactor cavity, therefore, is great.

The above calculations indicate that, in the presence of adequate steam, metal-steam reaction rates are large enough to ensure extensive, if not complete, chemical reaction of the metallic melt constituents and hydrogen production within the reactor cavity. Tutu³⁰ has considered the effect of steam inventory on the maximum amount of hydrogen that could be generated in the Zion reactor cavity as a function of the primary system inventory, expressed in terms of the pressure at the instant of vessel failure. The model assumed complete mixing of all the core melt and the entire steam inventory in the primary system. The thermodynamic equilibrium state was computed. The results for the Zion melt

inventory shown in Table 1 indicate that at 7 MPa (1000 psia) sufficient steam is available to react about 50% of the metallic, while at 15 MPa (2200 psia) in excess of 80% of the metallic can be reacted. On a well-mixed assumption basis, therefore, it is clear that hydrogen generation within the reactor cavity can be extensive.

Simplified models such as those described above may overestimate the extent of metal-steam reaction. Several potentially-important effects are not considered. Mass transport rates may be affected by the presence of neighboring droplets. If the local concentration of droplets in the cavity is large, then local steam depletion could occur, thereby either turning off or reducing the rate of reaction. Finally, the presence of diluent oxides should have some effect on the reaction rates. These effects must eventually be accounted for in detailed models of the cavity interaction scenario.

In order to model these effects a much-improved understanding will have to be developed of the high-temperature, high-velocity, multi-phase flow regime within the cavity. Models for droplet entrainment rate, deposition rate and droplet breakup will have to be developed. The Surtsey experiments with steam driver gas will aid in model development. However, separate-effects experiments with instrumentation adequate to probe the multi-phase flow structure within the cavity under very high gas velocity conditions will also be necessary in order to provide the detailed data necessary for model development.

4. Reactor Cavity Melt Dispersal

Of the melt mass delivered to the reactor cavity, the fraction which is swept out of the cavity into the downstream regions of containment is expected to strongly influence the extent of containment pressurization. It is expected that melt can be ejected from a reactor cavity through either the exit of the cavity through which the instrument tubes pass, or through the annulus between the reactor vessel and biological shield if this region is not blocked. Prediction of the melt flow rates through these regions depends upon the ability to model the complex, transient thermal-hydraulic phenomena involving multi-phase interactions between melt and blowdown gas flow discussed above. At the present time no verified models are available with which one can predict the "extent of melt dispersal" during high-pressure melt ejection from a reactor cavity of arbitrary design. One-dimensional cavity models are under development,^{23,24} but the constitutive relations, including entrainment rate, deposition rate, droplet breakup, etc., for the multi-phase interactions must be developed in future research.

In the absence of validated models to predict the fraction of melt dispersed from cavities of arbitrary design, small-scale simulation experiments have been conducted to provide measurements of the dispersal fractions under conditions thought to simulate high-pressure melt ejection conditions. Experiments

have been performed to date using models of the Zion, Surry and Watts Bar cavities in the US,^{3,4,5,9,21,22,23,31} the Sizewell plant in the UK³⁵ and the Ringhals plants in Sweden.³⁶ The experiments related to the US cavities were designed to simulate "high-pressure" melt ejection conditions. The BNL experimental conditions⁵ were chosen to simulate accident conditions where the vessel pressure is initially about 7 MPa and the vessel breach diameter about 0.4 m. Experiments related to the Zion cavity have been performed at SNL, ANL and at BNL. These experiments range from 1/10-th to 1/42-nd in linear scale. In all but one (DCH-1) of the HIPS and Surtsey experiments performed to date, in excess of 90% of the melt was dispersed from the Zion concrete cavities. In the ANL CWTI-5 and -6 tests^{2c} smaller fractions (61% and 30%, respectively) of melt were dispersed. This was attributed to freezing of the melt on steel cavity surfaces. In the case of CWTI-6 a malfunction occurred in the blowdown gas delivery system which may have also influenced the extent of sweepout. In the BNL experiments,⁵ water was used as the melt simulant for the Zion work. The results showed complete sweepout (~100%) of the water. BNL believes that these results using water overestimate sweepout and will perform verifying experiments with Wood's metal as the melt simulant in the future. The BNL Surry and Watts Bar experiment showed nearly complete dispersal of the Wood's metal melt simulant.

A feature common to all of the dispersal experiments is that the small-scale results must be scaled up to full-scale accident conditions. Tutu, et al.⁵ have performed a scaling analysis based upon a one-dimensional, dispersed, annular flow regime analysis of flow in the reactor cavity. A set of dimensionless parameters have been derived with which the data from small-scale experiments are extrapolated to prototypic conditions. The experimental data and the scaling analysis suggest that the Zion, Watts Bar and Surry reactor cavities would retain little melt under conditions of high-pressure melt ejection. Nearly all the melt would be dispersed into the downstream regions of containment. The UK Sizewell and Swedish Ringhals experiments were conducted under low vessel pressure conditions. A facility to study high-pressure conditions is under development in the U.K.

The experimental results cited above showing limited melt retention capability within the cavity models studied and their interpretation do not necessarily apply to cavity systems not yet studied. The results do suggest, however, that if a particular cavity is suspected of containing features which would appear to favor melt cavity retention, then a prudent measure would be to perform experiments to evaluate the specific design features.

C. Intermediate Subcompartments and Containment Dome

Observations of specific plant geometries suggest that upon exiting the reactor cavity, the dispersed melt flow would strike a wall or other surface upon exiting either vertically or somewhat obliquely

from the cavity. Figure 1 shows the Zion seal table enclosure boundary as the first structure within the steam generator room which the melt would encounter downstream of the cavity exit. In the case of Surry the first surface would be the floor of the residual heat removal (RHR) space. Typically the first structure surface would be 5-10 meters above the exit of the cavity. Scoping calculations such as described above suggest that the gas velocities entering this region would be several hundred m/s and droplet velocities perhaps half as much. BNL experiments performed using models of the Zion containment suggest that the structures exert a strong influence on the flow which issues from the cavity, redirecting the flow and, very likely, changing its droplet size characteristics. Recent Surtsey experiments strongly suggest that the size distribution of melt droplets which impinge on a surface would very likely be modified by the interaction with structure.³¹

The nature of the melt-structure interaction, e.g., bounce, sticking, shattering, film formation, etc., would determine the subsequent surface-to-volume ratio of the melt and, hence, the effectiveness of the melt in transferring its energy to the containment atmosphere. The ability to predict the melt-structure interactions depends on the ability to follow the motion of droplets to the surface, to predict the resulting changes in droplet size and flow regime resulting from the interactions and to predict the gas flow field around complex obstacles to the flow. Efforts to apply the KIVA code³² to this problem are under way in addition to efforts to understand the droplet-structures interaction process.³³ At present, however, there is no useful methodology available with which to compute the consequence of melt-structure interactions. We are, therefore, at present unable to accurately model the flow and melt atmosphere interactions beyond the first structure which presents itself to the flow exiting the reactor cavity.

The available lumped-parameter containment analysis methodologies used to predict DCH loading compute the thermal and chemical interactions between melt and atmosphere within the intermediate subcompartments assuming a given droplet size and effective droplet lifetime, related to the "trapping fraction" in CONTAIN,¹⁶ within a given subcompartment. Because of the current uncertainties described above, both quantities must be treated parametrically by analysts, using judgment based upon experiment and observation of plant design features and dimensions.

A generally-useful methodology to predict the fraction of melt transported from the intermediate subcompartments to the containment dome is not available. Data from small-scale experiments suggest that between 1 and 15% of the melt would be transported to the dome in the Zion containment system, depending on the presence or absence of water in the cavity.⁹ The remainder would be trapped on structure, in water or on the floor of the lower subcompartments. Methods for extrapolation of such estimates from small-scale experiments to prototypic conditions are not

available. The estimates, moreover, are expected to be highly plant-specific and experiments must be performed for each plant under consideration. At the present time the DCH analyst must make judgments regarding the expected extent of melt transport to the containment dome region and implement these judgments using the available computer code parameters. Parametric treatment of melt transport in containment is necessary to cover the uncertainties. Further BNL experiments are planned to study melt transport in the Zion and Surry containment systems. It is believed that a multi-dimensional, gas-liquid fluid dynamics methodology will be required in order to predict the transport of melt through the various subcompartments of containments. In the absence of such a methodology, observations from scale-model experiments will be required for each containment under consideration in order to provide guidance for the judgments required in implementing available lumped-parameter containment analysis codes.

It is believed that the steam-hydrogen mixture exiting the cavity would flush some fraction of the oxygen initially present out of the subcompartment above the reactor cavity into the upper region of containment. Hydrogen generation would continue in the subcompartment region as long as droplets are suspended and steam is available. The hydrogen in this region, however, would have little oxygen available for extensive reaction to occur. The steam exiting the cavity would, together with the action of buoyancy, force the hydrogen into the upper dome where the hydrogen would encounter oxygen and burn if conditions permit. There are no experimental data available to verify these conjectures. They are based upon conceptual analysis of the DCH scenario. These features are observed in recent CONTAIN DCH calculations.¹⁵ A result which is predicted by CONTAIN suggests that some hydrogen could remain "trapped" in the lower subcompartment after depletion of vessel blowdown steam. This hydrogen would not be transported by buoyancy to the containment dome region on a time frame which would permit contribution to the DCH containment pressure rise through the combustion process. The efficiency of hydrogen transport to the containment dome from the lower subcompartments should be considered in future work. At the present time the credence of this effect must be carefully considered by the analyst.

Calculations suggest¹⁵ that the steam-hydrogen mixture temperature in the intermediate subcompartments can be as high as 2000K and that jets or plumes of such mixtures would be transported to the containment dome. The dome region at this point would contain a mixture of steam, air and hydrogen (produced in-vessel prior to vessel failure) under conditions which, at prevailing pre-DCH low containment temperature, would be steam inerted with respect to hydrogen burn capability. Experimental data for the flammability limits of hydrogen under the above conditions are not available. Interpretation of the available data base, however, suggests that if the mixture temperature entering the dome is higher than 1000K, then conditions are effectively hypergolic, i.e., the

hydrogen would burn upon contact with available oxygen.³⁴ The pre-existing hydrogen in the containment dome would also burn as the dome temperature increases due to the various exothermic reactions occurring in the region. Melt droplets entering the containment dome region could act as local sites for hydrogen combustion. The efficiency of these various hydrogen combustion processes is uncertain at this time. Experiments under prototypic accident conditions are necessary to develop the appropriate models. It is noted, however, that the high temperatures and extensive hydrogen generation that are being predicted^{13,15} for the lower subcompartments using current methods are strongly influencing judgments concerning the extent of hydrogen combustion. Experiments are needed, not only concerning hydrogen combustion limits, but also to verify the ability to predict the conditions in the lower subcompartments.

The above discussion presents the view that the division of containment into several discrete regions, i.e., cavity, subcompartments, dome, plays an important role in the course of DCH interactions between melt and atmosphere. Important effects involve melt transport and hydrogen generation, transport and combustion. This observation strongly suggests that experiments with high-temperature reacting melts, driven by steam, should eventually be performed in a facility which can simulate the compartmentalized geometry of containment systems. These experiments would be designed to substantiate the results of lumped-parameter code modeling of multi-compartment phenomenology.

V. SUMMARY

The present understanding of the direct containment heating scenario in PWRs and relevant phenomenology has developed over a period of several years. There continue to exist large uncertainties in DCH initial conditions and in the description of the controlling DCH phenomenology. There appears, however, to have developed a technical consensus on the DCH scenario, as described in Section II.

While the possible range of DCH initial conditions is extremely broad, consideration of the phenomenology has focused around a rather narrow range of parameters. Experimental and analytical modeling have been carried out based upon a scenario involving high-pressure ejection of melts involving large fractions of core inventory, typically 75%, including oxides and metallics. The initial vessel pressure has been considered around 7 MPa (~1000 psia) and vessel failure has been assumed to occur as failure of an instrument tube penetration. The penetration is typically assumed to increase by ablation to about 0.5 m when the steam flow from the vessel is initiated. Melt temperature is typically assumed to be 2500K. The description of DCH phenomenology is incomplete and uncertainties are great, even with this selected initial condition. The uncertainties are even greater when initial conditions are postulated to deviate from this set of conditions. In the absence of experiments which incorporate all relevant

features of DCH scenarios, the present understanding of DCH phenomenology derives from experiments using both high- and low-temperature simulant materials, calculations based upon simplified models, integrated computer code calculation and conjecture based upon best engineering judgment.

For the conditions described above it is believed that the steam flow in the reactor cavity (those studied to date) would completely eject the melt from the reactor cavity and would also finely divide the melt into droplets whose diameters are characteristically a millimeter or less in diameter. Conditions within the cavity are in a thermophysical regime which lie well outside the limits of current understanding of multi-phase flows and which will require time and resources to unravel. It is believed, however, that melt droplets will be suspended in the steam/hydrogen gas flow for several tenths of a second within the cavity and for at least a similar time outside the cavity. Based upon simplified calculations of metallic droplet reaction rates, the droplets may be suspended for sufficient time to extensively react, producing copious quantities of hydrogen. While mechanisms can be identified which could limit the extent of hydrogen production, the methods to perform more realistic calculations do not exist at present.

Extremely high gas and liquid flow velocities, complex boundary conditions, material properties, turbulence, flow regime changes, etc., combine to characterize a thermophysical regime within the intermediate subcompartments which is beyond the predictive capability of existing multi-phase methodologies. It is believed, however, that continued hydrogen generation will take place in this region of containment. Significant quantities of melt will be deposited on structure, leading to removal of this melt with its stored thermal and chemical energy from subsequent interaction processes. Simplified calculations, however, suggest that a significant fraction of the melt energy can be transferred to the gas prior to deposition on structure. Furthermore, if the melt is assumed to settle in water, the quench would supply steam for additional pressurization of containment.

Hydrogen generated in the lower regions of containment will be transported at assumed high temperature to the containment dome which would contain the bulk of the oxygen supply for combustion. Some fraction of the melt droplet inventory, will also be carried to the upper dome where the unreacted metal would oxidize. While a data base to support hydrogen flammability calculations is lacking for containment dome conditions in which the steam inventory is large, computed high temperatures suggest the possibility of extensive combustion of available hydrogen in the upper dome.

The CONTAIN code, with its Interim Direct Heating Model,¹⁶ has been developed to the point where it can be used for parametric calculations of DCH accident scenarios. While many uncertainties exist and highly simplified models are currently implemented,

the modeling contains sufficient flexibility so that a user can implement a wide variety of assumptions to reflect his perceptions of the DCH phenomenology. An extensive study of DCH in the Surry plant has been published.¹⁵ The details of this study cannot be repeated here. Figure 5 presents selected results of several Surry DCH calculations which were configured with assumptions which reflect the scenario discussed above. They reflect complete cavity dispersal, sub-millimeter droplet diameters, reaction rates computed as described above, melt trapping in intermediate subcompartments, efficient (unconditional) hydrogen burn and heat losses to structures. Also shown for comparison are calculations using EBAL, which assumes complete chemical reaction and adiabatic equilibrium, and an estimate of the Surry containment failure pressure. The figure indicates that CONTAIN predicts substantial containment loadings over a broad range of participating melt inventory. It is important to note, however, that the loadings predicted with CONTAIN are of significantly lower magnitude than the adiabatic equilibrium calculation results. It is clear that mitigating effects are being accounted for by CONTAIN and that considerable uncertainty remains in prediction of DCH containment loads. Also shown is a CONTAIN result assuming no hydrogen combustion, a case which would apply if, for example, the containment were inerted. Significant containment loads are also computed for other PWR plants. The reader is referred to Ref. 15 for details of the cited calculations.

Our current understanding of DCH phenomena, together with our ability to model them, leads to prediction of containment loads which are significant when compared to estimates of failure pressure. There are plausible physical grounds to suggest that current methods and perceptions of physical phenomena are leading to containment loading predictions which are conservative. Experiments are planned in the SNL Surtsey facility with high-temperature melts and with steam as driver gas and at BNL with simulant fluids, which will help to assess current DCH lumped-parameter methodology. It is believed, however that much-improved methods will have to be developed, supported by detailed experimental studies of uncharted thermophysical regimes, in order to provide the basis for more realistic modeling and predictions.

Three-dimensional, droplet-gas, distributed-parameter methods will have to be developed, capable of dealing with flows with complex boundary conditions. A start with KIVA has been made,³² but more work will be required for special-purpose calculations to supplement CONTAIN lumped-parameter methods. Experiments will need to be performed in multi-compartment containment models in order to assess effects which are thought to be dependent upon containment compartmentalization. More detailed reactor cavity experiments are needed in order to provide the basis for development of models for droplet size and mass flows of melt and gas constituents ejected from the cavity. High-temperature, large steam fraction, hydrogen flammability limit data needs to be developed to provide a firm basis for DCH hydrogen burn

assumptions. The CONTAIN treatment of hydrogen transport from the intermediate subcompartments to the containment dome must be assessed experimentally and better models developed if appropriate.

The data base currently available to assess DCH accidents will need to be expanded to cover a broader range of potential accident initial conditions. Experiments which model vessel pressures lower and higher than 7 MPa and vessel breach diameters larger than and, perhaps, smaller than 0.5 m will need to be considered. Phenomenological models will have to apply to broader ranges of these variables in order to represent the range of possible accident initial conditions of interest to safety evaluations. The effects of water in the cavity and containment spray water in the atmosphere must be studied in future investigations. More careful attention will have to be given to modeling the various radiation heat transfer processes occurring in containment during DCH scenarios.

The progress which has been made in understanding high-pressure DCH phenomenology has led to development of models which are more realistic than the early idealized single-cell, adiabatic equilibrium models. While significant uncertainties remain, current methods are predicting containment pressure loads which are considerably lower than predictions made with the early methods. The pressure loads currently predicted, however, remain containment-threatening over a broad range of participating melt mass. It is believed that more realistic modeling of DCH phenomenology is possible and that additional research may lead to lower predicted containment pressure loads. The experimental and analytical research recommended here are believed necessary in order to provide a basis for development of more accurate and realistic modeling of DCH phenomena.

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Table 1

Zion and Surry Initial Conditions for Calculations

	Zion	Surry
Mass (kg)		
UO ₂ /ZrO ₂	90,000/14,870	79,810/11,140
Zr/Fe	11,000/22,000	8,250/16,500
Mass H ₂ Generated In-Vessel (kg)	484	362
Initial Containment Pressure (MPa)	0.31	0.19
Temperature (K)	406	375
Primary System		
Steam Mass (kg)	9,135	28,680
Temperature (K)	557	619
Pressure (MPa)	7	16
Containment Volume (m ³)	7.7x10 ⁴	5.1x10 ⁴

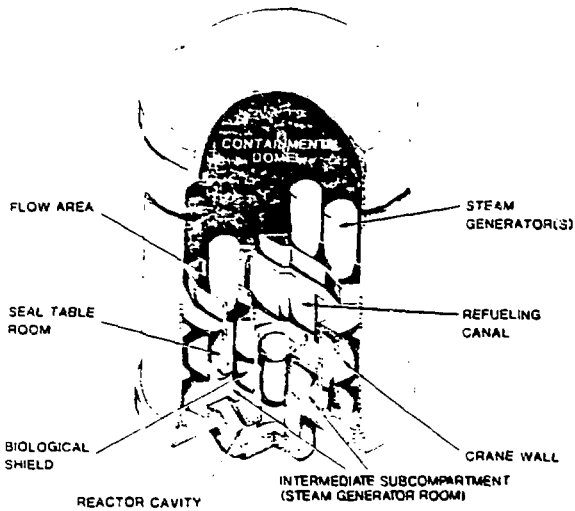


Fig. 1 Schematic Cutaway of Zion Containment

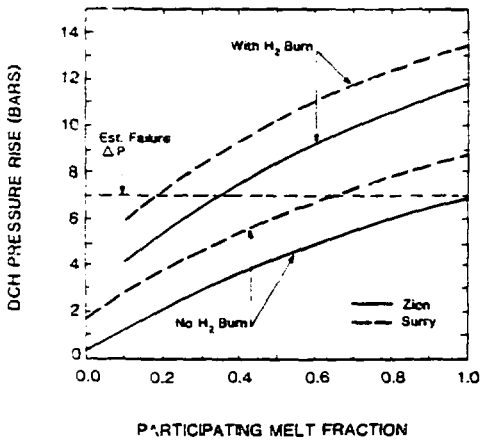


Fig. 2 Results of Thermodynamic Adiabatic Equilibrium Calculations for Zion and Surry

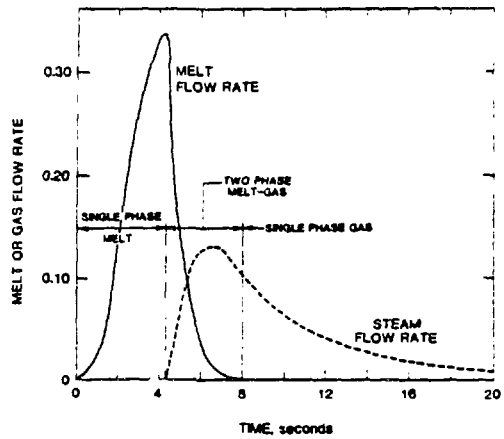


Fig. 3 "Typical" Normalized Discharge Rates of Gas and Liquid from Reactor Vessel During High-Pressure (7 MPa) Melt Ejection

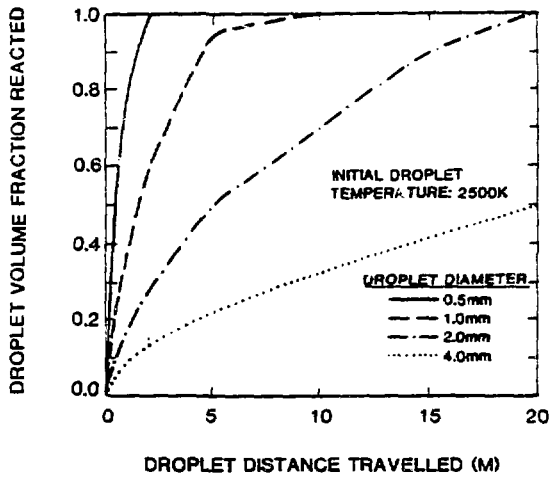


Fig. 4 "Typical" Results of Single-Droplet Model Calculations for Heat Transfer and Chemical Reaction

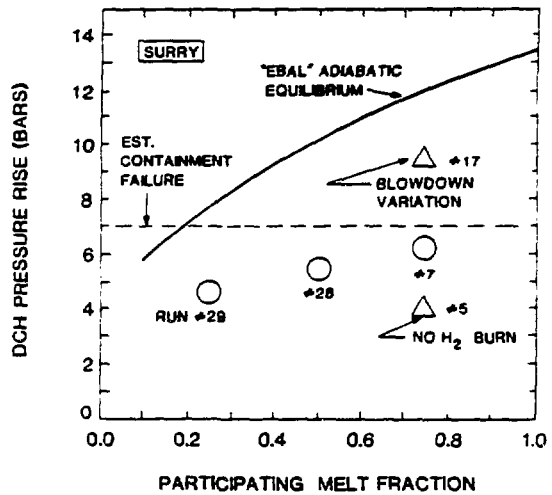


Fig. 5 Comparison of CONTAIN and Thermodynamic Equilibrium Calculations (see Ref. 15 for Description of CONTAIN Runs Cited)