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MODELING DIRECT CONTAINMENT HEATING PHENOMENA WITH CONTAIN 1.12*

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ABSTRACT

CONTAIN is a detailed mechanistic computer code developed at Sandia National Laboratories for the integrated analysis of light water reactor severe accident containment phenomena. The most recent version of the code, CONTAIN 1.12, incorporates models for the phenomena of high pressure melt ejection (HPME) and the subsequent processes collectively known as Direct Containment Heating (DCH). CONTAIN 1.12 was used to model the Limited Flight Path 8A (LFP8A) experiment conducted at the Surtsey test facility at Sandia National Laboratories. In the experiment, 50 kg of molten thermite was injected into a scale model of the Surry cavity and then blown into the Surtsey vessel by high pressure steam. A seven-cell best-estimate CONTAIN model, using only a minimum of measured data, was used to simulate the LFP8A experiment. A comparison of the experimental and calculated results indicated that CONTAIN 1.12 was accurately modeling the physical processes involved in DCH phenomena, but that the method of injecting the molten debris into the cavity in the CONTAIN model was causing the code to over-predict the chemical reaction and heat transfer rates between the molten debris and the system atmosphere. CONTAIN 1.12 predicted the peak vessel pressure to within less than 2% of the experimental value, but missed the timing on the pressure peak by approximately 1.75 s over the course of a 10 s calculation.

NOMENCLATURE

d_o	=	orifice hole size, m
F_{trap}	=	trapping fraction rate, s^{-1}
g	=	gravitational acceleration, m/s^2
Ku	=	Kutateladze number
L	=	fall height, m
L_{tfi}	=	distance to first impact, m
M	=	mass of airborne debris, kg
T	=	temperature, K
T_g	=	bulk gas temperature in a cell, K
t	=	time, s
t_1	=	time of flight to first structure, s
t_2	=	time of flight from first to second structure, s
V_g	=	gas velocity, m/s

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V_{jet}	=	velocity of debris jet, m/s
V_t	=	terminal fall velocity, m/s
w	=	mass flux in cell, kg/m^2-s
w_o	=	mass flux at the entering orifice, kg/m^2-s
w_x	=	mass flux at point of impact x, kg/m^2-s

Greek Symbols

α	=	user input parameter describing the rate of jet expansion
λ_{tr}	=	trapping fraction rate for TOF/KU model
ρ	=	bulk gas density, kg/m^3
ρ_a	=	gas density in cell for trapping, kg/m^3
ρ_d	=	debris droplet density, kg/m^3
ρ_g	=	gas density, kg/m^3
ρ_o	=	density of entering gas, kg/m^3
σ	=	liquid surface tension,

Subscripts

gft	=	gravitational fall time
tfi	=	time of first impact

1. INTRODUCTION

CONTAIN is a detailed mechanistic computer code developed at Sandia National Laboratories for the integrated analysis of light water reactor severe accident containment phenomena (Murata et. al., 1989). The code was developed under the sponsorship of the USNRC, and includes state-of-the-art mechanistic models for a wide variety of physical and chemical processes that occur within the nuclear reactor containment during a severe accident. The most recent version of the code, CONTAIN 1.12, incorporates models for the phenomena of high pressure melt ejection (HPME) and the subsequent processes that contribute to containment loading (Washington and Griffith, 1990). The HPME and the subsequent physical and chemical processes within the containment produce an efficient transfer of energy from the dispersed core debris to the containment atmosphere, resulting in a potential threat to containment integrity (NUREG-1079). Collectively, these phenomena are referred to as direct containment heating (DCH). This paper reports on the modeling of DCH phenomena with CONTAIN 1.12, and discusses the results of a comparison between best-estimate code calculations and a limited flight path test conducted at the Surtsey facility at Sandia National Laboratories.

One of the first major tests of the DCH modeling capabilities in CONTAIN 1.12 is the comparison to experimental results from the limited flight path (LFP) separate effects tests currently being conducted at the Surtsey facility at Sandia National Laboratories. In these experiments, molten corium is ejected into a simulated reactor containment in various configurations. CONTAIN 1.12 has been used to model the Surtsey LFP test configuration to simulate the test results and identify weaknesses in our current understanding of DCH phenomena. Of particular interest is the ability of the new models in CONTAIN to simulate the transport of gases and debris within the Surtsey vessel. Several of the new DCH models present in CONTAIN 1.12 incorporate parametric elements, and the experimental results have been used to give valuable insight into the performance of these correlations.

2. CONTAIN 1.12 DCH MODELS AND CAPABILITIES

The new DCH capabilities in CONTAIN 1.12 include models for the flow of debris and gases, debris de-entrainment on structures, debris chemistry involving Zr, Fe, O_2, and H_2O, and convection and radiation heat transfer between debris and the environment within containment (Washington and Griffith, 1990). Also included are mechanistic models for the initial melt ejection, ablation of the vessel hole by escaping core material, gas blowthrough and mixed gas/core debris ejection, entrainment of debris from the cavity floor, de-entrainment of debris on cavity structures and surfaces, and dispersal of debris into the main containment atmosphere. These mechanistic models were taken from the codes CORDE, a HPME and debris dispersal modeling code developed at Winfrith in the UK, and from GASBLOW2, a HPME modeling code developed at Sandia National Laboratories (Washington and Griffith, 1990). For some of these processes, such as debris entrainment from the cavity floor, a number of correlations developed through experimental and analytical investigations have been incorporated into CONTAIN 1.12.

The CORDE and GASBLOW2 models that were incorporated into CONTAIN 1.12 were tested on a suite of standard test problems. However, all of these test problems were full-scale simulations of nuclear reactor systems. When the CORDE/GASBLOW2 modules were applied to the scaled geometry in the LFP8A experiment, a number of unexpected difficulties were encountered with the models. Preliminary investigations indicate that these difficulties are scale-dependent, in the sense that they were not encountered in large or full-scale simulations. Debugging efforts are currently underway to permit the use of the CORDE/GASBLOW2 models in future simulations of the LFP experiments.

A complete description of the DCH models in CONTAIN 1.12 is well beyond the scope of this paper. However, debris chemical reactions and debris trapping are two DCH phenomena that are of particular importance in the LFP8A experiment and are described in more detail. Chemical reactions can occur in the system atmosphere during a DCH event if Zr and/or Fe metal is present and the atmosphere contains oxygen and/or steam. In CONTAIN 1.12, it is assumed that all debris particles in a cell have the same size and temperature. Therefore, debris chemical reactions are only computed once for each cell and the effect is multiplied for the number of droplets in the bulk field for that cell. Another important aspect of the chemistry model is that the constituents in a cell are assumed to be evenly divided among all droplets in the bulk field of that cell.

Models are included for the following chemical reactions:

1) $Zr + O_2 \longrightarrow ZrO_2$

2) $2\ Fe + O_2 \longrightarrow 2\ FeO$

3) $Zr + 2\ H_2O \longrightarrow ZrO_2 + 2\ H_2$

4) $Fe + H_2O \longleftrightarrow FeO + H_2$

These reactions are treated in a hierarchical fashion, where Zr is favored over Fe in any reaction, and where the oxygen reactions are favored over the steam reactions. As a result, the model treats reactions in the order they are listed above. All reactions are assumed to go to completion, except for iron/steam.

The chemical reaction of Zr and Fe metal in the debris field is modeled in CONTAIN using a rate-limiting mechanistic approach. In this approach, the reaction rate is governed by the rate at which oxygen and steam can be transported to the drop (gas-side) and then transported within the drop as it chemically reacts (drop-side). The details of the calculation of the drop and gas-side reaction rate constants, and the relationship between these calculations and the hierarchial chemical reaction scheme, are presented in the CONTAIN 1.12 documentation (Washington and Griffith, 1990).

Trapping is the process of debris removal resulting from interaction with containment structures and/or gravitational fallout. The trapping process is not well-understood, and experiments have shown that particle trapping is subject to scale distortions (Tarbell, 1988). A variety of methods for modeling trapping are available in CONTAIN 1.12. These models are mostly parametric, although there is some degree of mechanism associated with some of the approaches. All models for trapping are based on the assumption that debris is removed according to

$$\frac{dM}{dt} = -F_{trap}\, M \qquad (1)$$

Equation (1) is integrated over time to model the removal of debris from the atmosphere.

Trapped debris is held in a repository and allowed to cool at a user-specified rate. The energy lost during this cooling is, by default, assumed to be deposited in the floor if one is present. The user may distribute this energy to structure surfaces or may specify that it be lost from the problem. CONTAIN input parameters allow the user to control the trapped debris heat loss rate as well as the repository for the energy loss.

The difference between the various trapping models present in CONTAIN 1.12 is the way in which F_{trap} is determined. The following four models are available:

1	USER	User-specified F_{trap} values
2	GFT	Gravitational fall time
3	TFI	Time of first impact
4	TOF/KU	Time of flight/Kutateladze

<u>USER Trapping Model</u> The simplest and most parametric trapping model is the USER model. In this model, the user simply specifies the fractional removal rate for debris trapping for each cell. A constant can be specified or a parameter table can be used to vary the trapping rate as a function of time or particle temperature.

<u>GFT Trapping Model</u> In this model, the trapping rate is taken to be the gravitational fall rate of a sphere in the cell atmosphere.

$$F_{trap} = \frac{V_t}{L_{gft}} \qquad (2)$$

The terminal fall velocity, V_t, is computed by CONTAIN using the properties of the gases in the cell evaluated at T_g. The fall height, L_{gft}, is by default the cell height, although other values may be specified. The GFT trapping rate will also be computed and used in the TOF/KU model if velocities are sufficiently high that the Kutateladze criterion for particle sticking is not met by the second impact.

<u>TFI Trapping Model</u> In the TFI trapping model, debris is trapped at a rate equal to the transport time required for debris to reach the first structure in the cell. The debris jet enters the cell through an orifice of diameter d_0, and travels a distance L_{tfi} before striking a structure in the cell. The velocity upon impact is calculated from the jet expansion law

$$W_x = W_o \cdot \frac{\alpha L_{tfi}}{d_o} \left(\frac{\rho}{\rho_o}\right)^{1/2} \qquad (3)$$

The initial velocity is assumed to be the gas flow velocity from a specific flow path into the cell. The flow path is specified in the CONTAIN input. The trapping fraction rate is calculated by

$$F_{trap} = \frac{V_{jet}}{L_{tfi}} \tag{4}$$

If a flow path is not specified or if the gas flow through the specified path is not into the cell, the GFT model will be used. In addition, the TFI trapping rate is limited so that it will not be slower than the GFT rate. The distance to first impact, L_{tfi}, is by default the cell height. However, the value may also be specified by the user.

TOF/KU Trapping Model The TOF/KU model is a combination of the GFT model, TFI model, and a Kutateladze criterion based model; hence the name "time of flight/Kutateladze" model. In this model, debris is conditionally removed from the cell atmosphere depending on the Kutateladze number of the impact of debris upon the first structure in the cell. The velocity and distance to the first impact are determined in the same way as for the TFI model. If the first impact condition does not result in de-entrainment, then a second impact on another structure is considered, where the velocity of the second impact is assumed to be an average cell gas/debris cloud velocity. If both conditions fail, GFT trapping is used in the cell.

The Kutateladze number for debris entrainment represents the ratio of kinetic energy to surface tension forces and is defined as

$$Ku = \frac{\rho_g V_g^2}{\left(\rho_d g\sigma\right)^{1/2}}, \quad \rho_d >> \rho_g \tag{5}$$

Using the gas entrainment law, the gas density at the point of impact with the first structure may be written as

$$\rho_g\big|_{\text{at structural impact}} = \rho_1 = \frac{\rho_o \rho_a \left(w/w_o\right)}{\rho_a + \left(\frac{w}{w_o} - 1\right)\rho_o} \tag{6}$$

where w/w_o is determined from the TFI model.

The Kutateladze criterion at the point of impact with the first structure in the cell can be written as

$$Ku_1 = \frac{\rho_1 V_1^2}{\left(\rho_d g\sigma\right)^{1/2}} \tag{7}$$

where V_1 is the gas velocity upon impact as calculated by the TFI model.

If $Ku_1 \leq Ku_{T1}$, where Ku_{T1} = threshold value for first impact, then t_{tr} from the TFI model is used. The kinetic energy of the incoming jet was not able to overcome the surface tension forces of the debris, and the debris remained de-entrained upon the first structure. However, if $Ku_1 > Ku_{T1}$, then TFI de-entrainment will not occur and an impact with the second structure in the cell is considered.

For impact with the second structure, the Kutateladze criterion is written as

$$Ku_2 = \frac{\rho_a V_2^2}{(\rho_d g\sigma)^{1/2}} \tag{8}$$

where V_2 = average cell gas/debris cloud velocity.

If $Ku_2 < Ku_{T2}$, where Ku_{T2} = threshold value for second impact, and $Ku_1 > Ku_{T1}$, then the trapping rate is governed by the time it takes to make the second impact:

$$\lambda_{tr} = (t_1 + t_2)^{-1} \tag{9}$$

However, λ_{tr} is limited by the value calculated from the GFT model. The GFT model is also used if $Ku_2 > Ku_{T2}$. The TOF/KU model is the most mechanistic of the CONTAIN trapping models.

3. DESCRIPTION OF EXPERIMENTAL SETUP AND PHENOMENA

Physical Description The LFP experimental facility consisted of a 1:10 scale model of the Surry reactor cavity connected to the bottom of the Surtsey pressure vessel. Simulated core debris was liquified in a melt generator attached to the cavity and then forced into the cavity by a high-pressure steam source. After the molten debris was ejected into the cavity, it was swept up into the Surtsey vessel by high pressure steam passing through the cavity and out into the main containment atmosphere. The experimental setup is shown in Figure 1. A complete report on the LFP test series is currently being prepared (Allen and Pilch, 1990).

In the LFP8A experiment, a generic structure was placed within the Surtsey vessel at a nominal height of 8 m above the floor of the vessel. The structure was a 5.16 cm thick concrete slab that measured 2.44 m by 2.44 m and was placed perpendicular to the vertical axis of the vessel. In addition, a 30 cm steel overhang was attached to each side of the concrete slab. The overhang was used to limit the amount of debris that was swept up above the slab in the vessel. The slab was intended to simulate a subcompartment structure in the Surry Plant, where debris exiting the cavity would strike the Residual Heat Removal Platform and either be trapped on the concrete ceiling, deflected back to the floor, or be re-entrained in the gas flow and travel above the structure.

The initial conditions for the LFP8A experiment were measured just prior to the initiation of the test. The initial temperature and pressure in the cavity and vessel were 293 K and 0.16 MPa, respectively. The atmospheric composition was 99.5 mol.% Ar, 0.38 mol.% N_2 , and 0.08 mol.% O_2. The molten thermite was at a temperature of approximately 2500 K. It consisted of 20.0 kg of Al_2O_3 , 24.6 kg of Fe, and 5.4 kg of Cr, for a total thermite mass of 50 kg. The steam accumulator contained approximately 4.17 kg of superheated steam at a temperature of 570 K and a pressure of 2.8 MPa. The hole connecting the melt generator to the cavity body had a diameter of 3.5 cm, which remained constant for the duration of the experiment (Allen and Pilch, 1990).

Observed Phenomena As the debris in the melt generator reached the molten state, a brass plug separating the thermite from the cavity vaporized almost instantaneously. This event marked time t=0 for the recorded phenomena. The molten debris was ejected into the cavity by pressurized steam contained in the accumulator. All of the thermite in the melt generator was ejected into the cavity within approximately 0.4 s after the vaporization of the brass plug. Very little mixing of the thermite and the driving gas was observed during the initial ejection, although the molten material was mixed violently within the cavity after the initial ejection was complete. The driving gas entered the cavity at approximately 0.4 s, following the ejected thermite (Allen, 1990). The molten debris was entrained by the steam passing through the cavity and swept up into the Surtsey vessel. The debris jet then struck the concrete platform suspended within the Surtsey vessel, where debris particles either stuck to the surface or rebounded and fell to the bottom of the vessel. A small amount of the debris was re-entrained and swept above the concrete structure towards the upper head of the containment volume. In the LFP8A experiment, approximately 60% of the initial debris remained trapped in the cavity region, and was not ejected into the Surtsey vessel.

4. CONTAIN MODEL

Discretization The CONTAIN 1.12 model of the LFP8A experiment consisted of seven computational cells. A diagram of the model is presented in Figure 2. The cavity and steam supply system were subdivided into four CONTAIN cells: the melt generator/steam accumulator, the horizontal body of the cavity, the cofferdam connecting the cavity body to the chute, and the chute connecting the cavity to the Surtsey vessel. The Surtsey vessel was divided into three CONTAIN cells: one for the region below the concrete slab, and two cells for the region above the slab. The slab was placed 7.7 m above the floor of the Surtsey vessel, with equal flow areas around each side.

The cell descriptions are as follows:

Cell 1: horizontal body of the cavity
Cell 2: cofferdam connecting cavity body and cavity chute
Cell 3: chute connecting cavity body to the Surtsey vessel
Cell 4: Surtsey vessel beneath the suspended concrete slab
Cell 5: Surtsey vessel above the suspended concrete slab
Cell 6: Surtsey vessel above the suspended concrete slab
Cell 7: melt generator/steam accumulator

Modeling Assumptions and Approximations A number of critical assumptions and approximations were made in modeling the LFP8A experiment with CONTAIN 1.12. However, it should be noted that only two pieces of experimental data were used in constructing the CONTAIN model of the LFP8A experiment; the timing of the ejection of thermite into the cavity, and the fraction of debris that was dispersed from the cavity. Experimental observations indicated that all of the thermite was injected into the cavity by 0.4 s into the test, a fact that was used to construct the debris source mechanism described below. Only 39.2% of the debris actually entered the Surtsey vessel, so the mass of dispersed debris was adjusted to reflect this result. With these two exceptions, the CONTAIN 1.12 model of the LFP8A experiment was essentially a best-estimate blind post-test analysis.

The first modeling assumption was that the molten thermite was injected into the cavity at a constant rate over the first 0.4 s of the calculation. The top of the melt generator was connected to a steam accumulator. When the brass plug separating the molten debris and the cavity was vaporized, the connection between the steam accumulator and melt generator opened, and the pressurized gas ejected the thermite into the cavity. The volume of the steam accumulator was much greater than the volume of the melt generator, leading to an almost constant pressure on the thermite as it was forced into the cavity. In addition, little or no mixing of the driving steam and thermite was observed in the LFP8A experiment; the material was essentially ejected as a homogeneous "plug" of molten debris. The assumption neglects friction and acceleration effects, but is consistent with experimentally observed behavior.

As a second modeling assumption, the ejected molten debris was treated as a debris source term in the cavity. The CONTAIN model of the LFP8A experiment initially used the debris entrainment and dispersal models from CORDE/GASBLOW2 to simulate the ejection of the molten debris from the cavity, but unexpected difficulties with these code modules prevented their use. Debugging efforts are currently underway to allow the use of CORDE/GASBLOW2 in future simulations of the LFP experiments. However, based on experimental observations the violence of the ejection process dispersed the material quickly in the cavity. This dispersal created a situation similar to that which was assumed by the use of the debris source model in CONTAIN. A debris particle size of 0.8 mm was chosen for the injected debris, based on the measured particle sizes from previous Surtsey HPME experiments (Allen, 1990).

Next, the melt generator and steam accumulator volumes were added together to form a single CONTAIN cell. The volume was then treated as a single pressurized cell containing the initial mass of steam at the experimentally measured initial temperature and pressure. A flow path between this cell and the cavity was opened at t=0.4 s, after all of the molten debris had been injected into the cavity cell. Experimental observations show that virtually all of the thermite is ejected from the melt generator ahead of the driving gas, so permitting the driving steam to be injected into the cavity simultaneously with the molten debris would not accurately reflect the experimentally observed behavior. In a HPME accident in a nuclear plant, it is hypothesized that the corium would first be deposited on the cavity floor and then swept out of the cavity by the blowdown gas.

A final modeling approximation involved the substitution of Zr for the Cr present in the melt. CONTAIN 1.12 does not have Cr chemistry models, but the thermite used in the LFP experiments contained a significant amount of Cr. Because the anticipated Cr reactions are highly exothermic, neglecting these chemical reactions could introduce significant and non-conservative errors into the calculation. Since CONTAIN 1.12 has the ability to model Zr chemistry, the Cr present in the melt was replaced by Zr. The mass of Zr substituted for the Cr was selected to produce roughly the same amount of energy that would be released by the Cr in the chemical reactions. The approximation is not ideal, but the Zr chemistry model at least calculates the correct gross exothermic energy release expected from the Cr. The approximation was certainly preferable to neglecting the presence of Cr entirely.

The behavior of debris ejected into the Surtsey vessel atmosphere represented an extremely important aspect of the simulation. Of particular importance was the length of time the debris particles remained airborne in the Surtsey vessel, since this time period directly influenced the amount of heat transfer and chemical reactions that took place between the debris and the containment atmosphere. As described in Section 2, CONTAIN 1.12 has a number of models available for simulating the trapping process, with the most mechanistic being the TOF/KU (time-of-flight/Kutateladze) model. The TOF/KU model was selected for use in the LFP8A model because it was the most mechanistic trapping model available in CONTAIN 1.12 and was the best suited for modeling the expected trapping behavior. The debris was assumed to enter cell 4 in the Surtsey vessel and impact the horizontal portion of the suspended concrete slab. The steel overhang attached to the edges of the slab was then specified as the second structure in the cell for the TOF/KU trapping model.

5. DISCUSSION OF RESULTS

Figure 3 presents the calculated pressure in the Surtsey vessel vs. the results of the LFP8A experiment. Only a single curve is presented for the CONTAIN results, since the pressures in cells 4, 5, and 6 were essentially identical. The CONTAIN model predicted a small and almost linear pressure increase over the first 0.4 s of the calculation, while the debris was being injected into the cavity cell. When the high pressure steam began entering the cavity at 0.4 s, the calculated pressure increased sharply and reached a peak value of approximately 0.336 MPa at about 2 s into the test. The calculated pressure in the vessel then gradually decreased to approximately 0.292 MPa after 10 s. The experimental results behaved in a similar manner, with the pressure quickly rising to a peak value of 0.330 MPa, and then gradually decreasing to about 0.292 MPa at a time of 10 s. However, the peak pressure value measured in the LFP8A experiment appeared at about 3.75 s into the test, which was approximately 1.75 s after CONTAIN predicted a peak pressure.

The calculated and experimental pressure curves in the vessel were quite similar in magnitude and shape, but appeared to be somewhat out of phase. CONTAIN predicted the correct magnitude and general behavior of the DCH pressurization, but did a poor job of modeling the timing of the phenomena. It was theorized that the method of injecting the molten debris into the cavity was responsible for the discrepancy between the calculated and experimental results. In the calculation, the steam injected into the cavity at 0.4 s encountered almost the full inventory of molten debris in dispersed form. As a result, chemical reactions between the debris and steam occurred quite rapidly, and the debris was quickly ejected into the Surtsey vessel atmosphere.

In the experiment, a sizable portion of the molten debris was deposited on the floor, walls, and ceiling of the cavity region prior to the entrance of the driving steam. Although the molten debris that escaped being trapped in the cavity was quickly entrained and ejected into the vessel atmosphere, heat transfer and chemical reactions between the steam and debris were certainly less efficient and rapid than the CONTAIN model predictions. CONTAIN 1.12 postulated a perfectly dispersed debris field in the cavity as the steam entered. As a result, the debris ejected from the cavity in the experiment took longer to interact with the injected steam and reach the Surtsey vessel atmosphere than was predicted by CONTAIN. Although no time-resolved debris ejection information was gathered from the experiment, this theory conforms to physical expectations and explains the timing discrepancy between the calculated and experimental results.

The calculated and experimental values for the cavity pressure further supported the theory that the method of injecting the debris into the cavity in the CONTAIN model was responsible for the timing discrepancy in the results. The pressures in the cavity region vs. time are presented in Figure 4. As the debris began entering the cavity, both the calculated and experimental results exhibited a short spike in the cavity pressure. CONTAIN then calculated a large pressure spike immediately after the high pressure steam began entering the cavity cell. The pressure in the cell reached approximately 0.81 MPa and then quickly dropped back as the gas and debris exited the cavity. However, the experimental results did not indicate any sudden spike as the steam began entering the cavity. These results support the theory that the dispersed debris in the CONTAIN model reacted rapidly and efficiently with the incoming steam, while in the experiment the steam/debris interaction was much slower.

Figure 5 presents the temperatures in the vessel vs. time. The calculated temperatures increased only slightly over the first 0.4 s, then increased rapidly after steam began to enter the cavity and peaked at about 2.0 s. The temperature below the concrete slab peaked at about 676 K, while the temperature above the slab reached around 400 K. The experimentally recorded temperatures matched the calculated results quite poorly; the peak experimental temperature below the slab was about 513 K, and occurred at about 5 s into the test. No temperature readings were taken above the slab. The difference in the calculated and experimental temperature magnitudes probably resulted from the fact that CONTAIN calculated a cell average temperature, while the experimental values were taken from discrete points along the wall of the Surtsey vessel. The temperatures along the center of the vessel were probably much higher than the experimental results indicated, since in the experiment the vessel atmosphere was not perfectly mixed (Allen, 1990). The discrepancy in the timing of the temperature peak was attributed to the difference in the debris interaction rates described above.

The mass of airborne debris vs. time in the model is presented in Figure 6. As can be seen in Figure 6a, the total mass of airborne debris increased approximately linearly during the first 0.4 s of the calculation, peaking at approximately 18 kg. The linear behavior reflected the CONTAIN debris source model in cell 1 in the cavity. During the initial source period, a small amount of airborne debris appeared in cell 4 in the Surtsey vessel As the debris was injected into the cavity, heat transfer from the hot particles caused the cavity gas to heat and expand into the vessel. Since CONTAIN uses a no-slip assumption for the gas/particle mixture, a portion of the debris in the cavity moved out into the vessel with the cavity gas prior to the injection of the driving steam. At 0.4 s, the driving steam entered the cavity and quickly forced the debris out into the Surtsey vessel. As expected, most of the debris remained in cell 4 below the concrete slab. However, as shown in Figure 6b, a small amount of debris appeared to have been airborne in cells 5 and 6, above the slab, between 0.5 s and 1.7 s.

The airborne debris was removed from the vessel atmosphere by the trapping process. In the first 0.4 s of the calculation, a small amount of debris was trapped in cell 4. This represented the gravitational fallout of the debris that was moved into the vessel as the cavity gas expanded. After the high pressure steam entered the cavity at 0.4 s, debris that entered the Surtsey vessel was rapidly trapped in the cell below the concrete slab. Virtually all of the debris entering the vessel rebounded from the slab and drifted to the lower floor of cell 4. A small amount of debris was transported above the slab, and then trapped on the dome and upper slab surface. Post-experiment analysis of the test apparatus revealed that approximately 9% of the debris was trapped on the underside of the slab, 2% of the debris was trapped above the slab, and the remaining 89% of the debris fell to the lower head of the Surtsey vessel (Allen and Pilch, 1990). The CONTAIN results using TOF/KU trapping model default values predicted that no debris was trapped on the underside of the slab, 4% of the debris was trapped above the slab, and the remaining 96% of the debris fell to the lower head of the Surtsey vessel.

A significant amount of hydrogen was generated in the cavity during the early stages of the test. For the first 0.4 s of the calculation, no hydrogen was present in the system. Immediately after the high pressure steam began entering the cavity, the hydrogen concentration in the three cavity cells increased to approximately 75.0 mol.%. However, as the entering steam swept the debris out through the cavity and into the vessel, the hydrogen concentration rapidly dropped, virtually disappearing by 0.75 seconds into the calculation. An analysis of gas grab bottles opened in the cavity between 0.5 s and 2.5 s revealed a peak hydrogen concentration of 54.1 mol.%. However, this value may have actually been higher, since the grab sample apparently leaked (Allen and Pilch, 1990).

6. CONCLUSIONS

The severe reactor accident containment modeling code CONTAIN 1.12 was used to model a HPME experiment performed at the Surtsey test facility at Sandia National Laboratories. The experiment, LFP8A, consisted of the injection of 50 kg of molten thermite into a 1:10 scale model of the Surry cavity connected to the Surtsey containment vessel. A seven-cell best-estimate CONTAIN model, developed using only a few pieces of experimental data, was used to simulate the experiment. In addition to the new debris chemistry models, the CONTAIN simulation employed the TOF/KU trapping model to simulate the splashing of debris off of a concrete slab suspended in the Surtsey vessel to simulate a generic containment structure.

The magnitude of the pressure response calculated by CONTAIN for the Surtsey vessel agreed extremely well with the experimentally determined values, differing by less than 2%. In addition, the TOF/KU trapping model correctly predicted that the majority of the debris injected into the Surtsey vessel would rebound from the concrete slab and drift to the bottom of the vessel. However, the calculated and experimental results for the transient vessel pressure behavior differed significantly. CONTAIN predicted a much more rapid pressurization of the Surtsey vessel than was indicated by the experimental measurements. This was probably due to the fact that CONTAIN predicted a much more rapid interaction of molten debris with the injected steam and the vessel atmosphere than occurred in the experiment.

Because of problems with the mechanistic debris entrainment and dispersal modules from CORDE/GASBLOW2, the CONTAIN model was forced to simulate the injected molten debris with a particle source in the cavity cell. Based on the experimentally observed behavior of the system, debris was injected in the form of dispersed particles into the cavity cell at a constant rate over the first 0.4 s of the test. In the physical situation, the debris is partly de-entrained on various cavity surfaces and must be re-entrained by the high velocity steam moving through the cavity before significant chemical and heat transfer processes can take place. By injecting the debris in the form of airborne particles, CONTAIN over-predicted the rate at which chemical interactions and heat transfer would take place between the debris and the surrounding gas during the first seconds of the test. The result was the observed phase shift between the pressurization curves for the experimental and calculated results.

The fact that CONTAIN correctly predicted the magnitude of the vessel pressurization indicated that the code was accurately modeling heat transfer and chemical reactions with the molten debris. In addition, because the CONTAIN calculation used a best-estimate model primarily with default parameters in the various chemistry, heat transfer, and trapping models, the close agreement between the experimental and calculated results gives some confidence in CONTAIN 1.12's ability to model a HPME event. The verification of the TOF/KU trapping model for the simple LFP8A geometry was an important result, since the model had not been previously tested against experimental results. Although the discrepancy in the timing of the pressurization curves indicated the importance of a more mechanistic approach in providing debris sources in CONTAIN, the overall agreement between the calculated and experimental results showed that CONTAIN 1.12 is a useful tool for the analysis of containment response during DCH scenarios.

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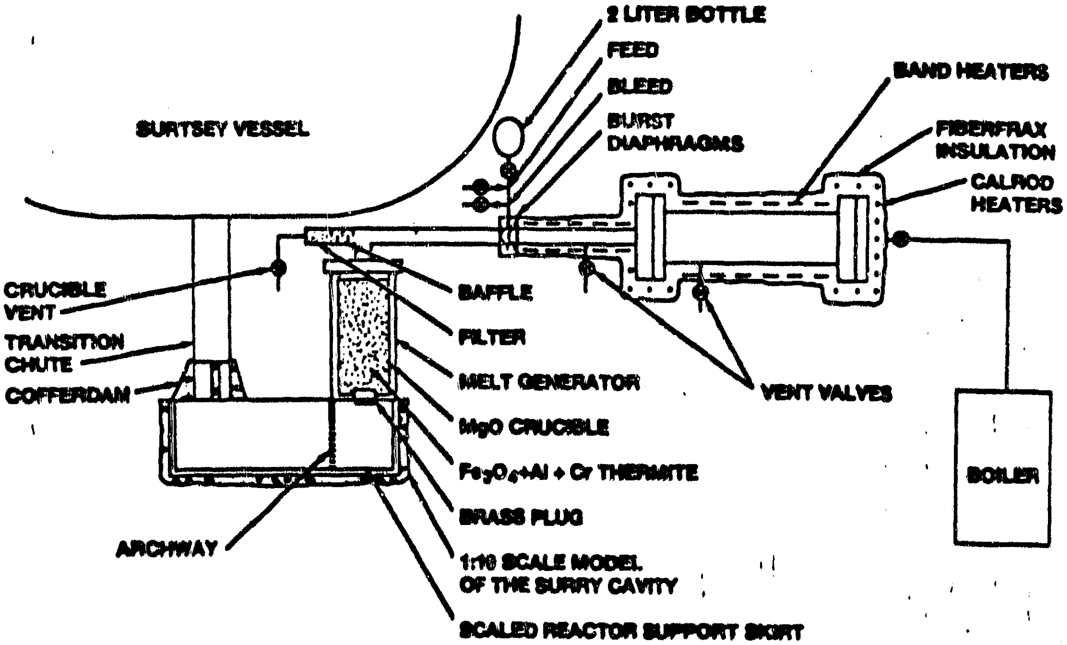

Figure 1. Experimental apparatus for the LFP experiments.

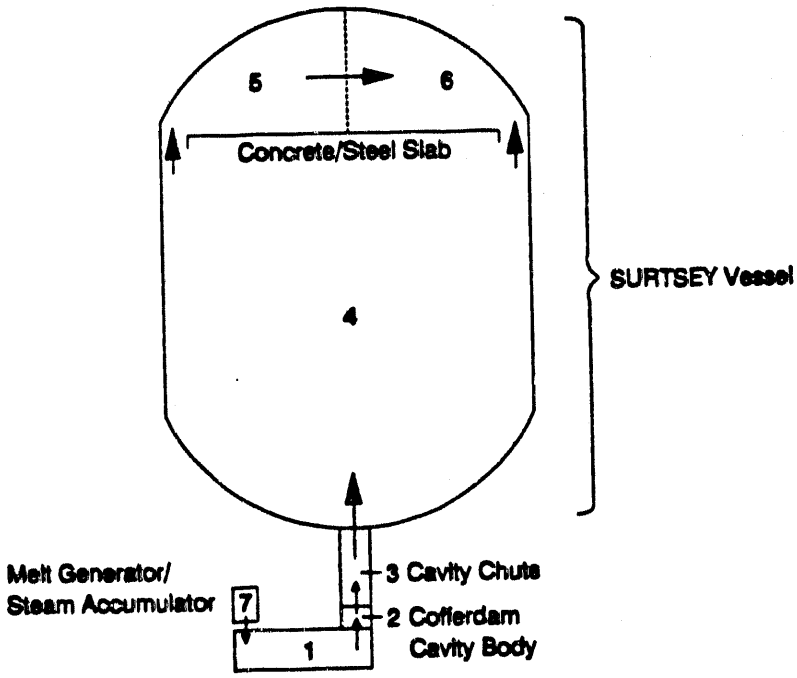

Figure 2. CONTAIN 1.12 model of the LFP8A experiment.

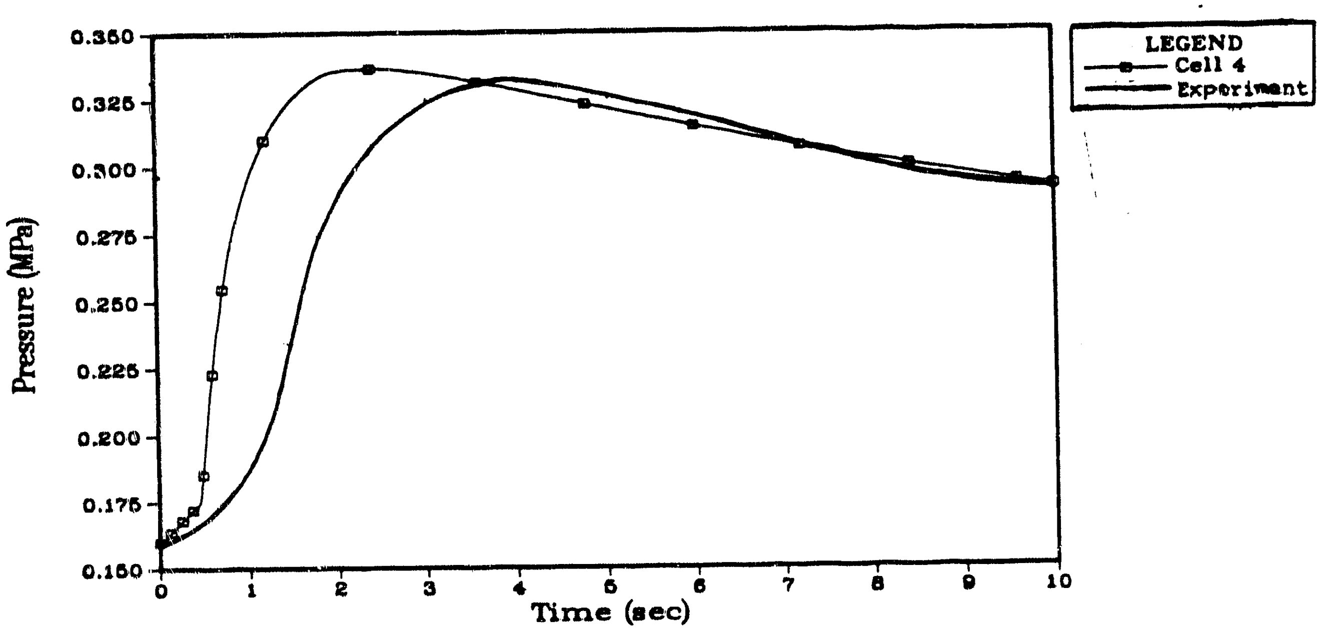

Figure 3. Pressure vs. time in the Surtsey vessel.

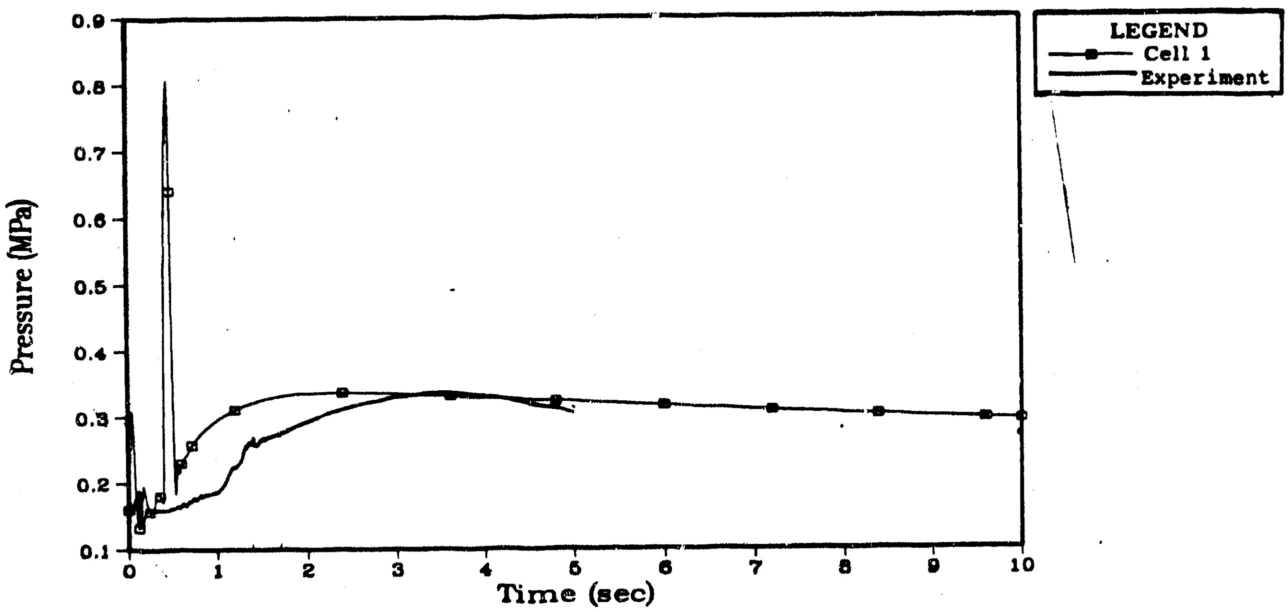

Figure 4. Pressure vs. time in the cavity.

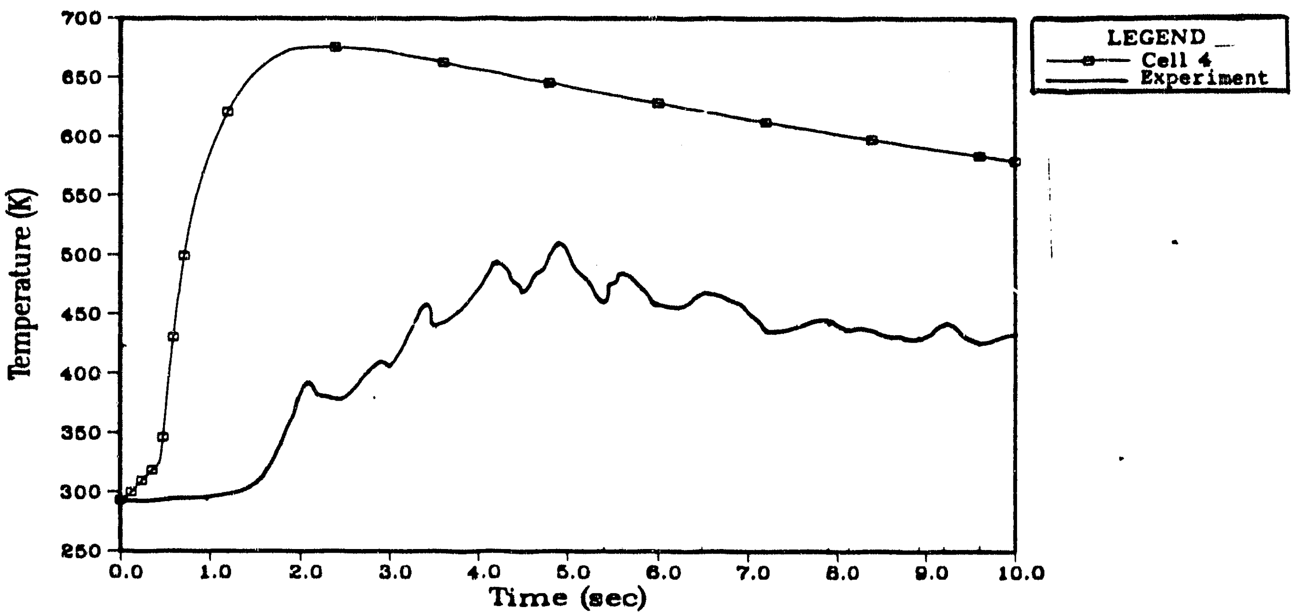

Figure 5. Gas temperature vs. time.

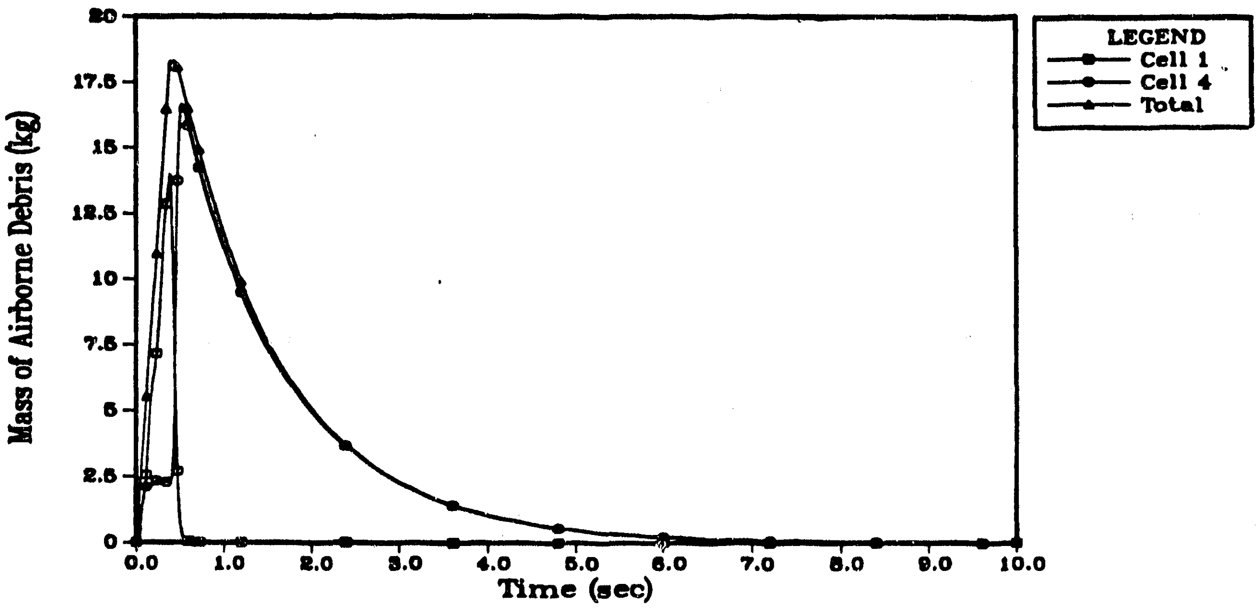

Figure 6a. Mass of airborne debris vs. time.

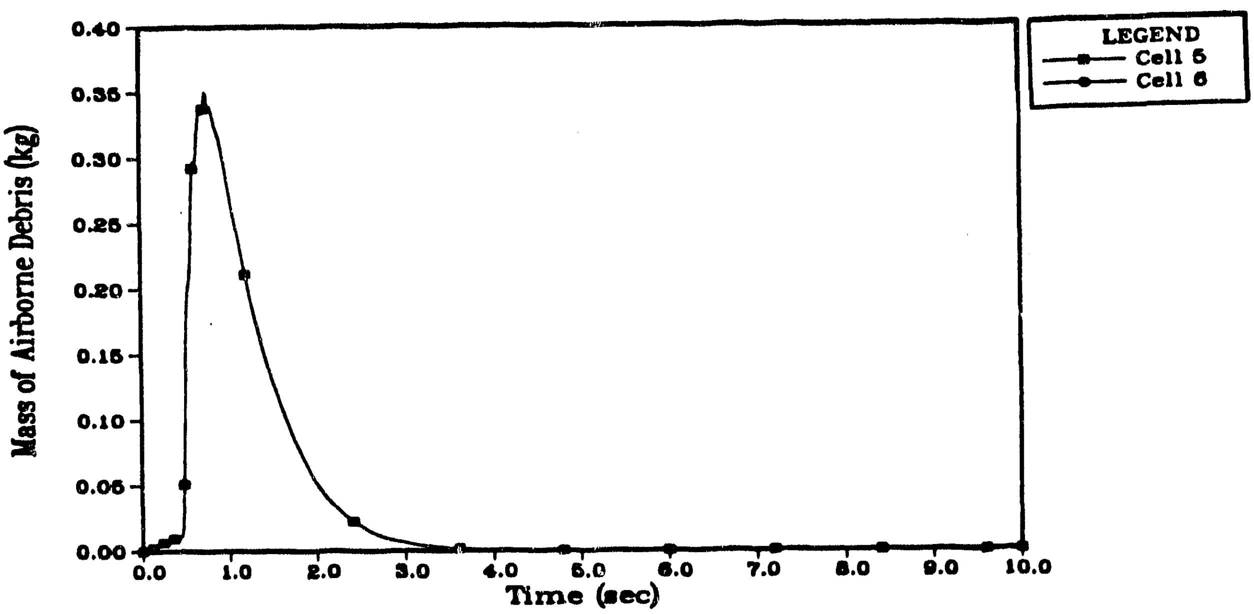

Figure 6b. Mass of airborne debris vs. time in cells 5 and 6.

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