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A Preliminary Model for Core/Concrete Interactions

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Walter B. Murfin

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A PRELIMINARY MODEL FOR CORE/CONCRETE INTERACTIONS

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ABSTRACT

A preliminary model is described for computing the rate of penetration of concrete by a molten LWR core. Among the phenomena included are convective stirring of the melt by evolved gases, admixture of concrete decomposition products to the melt, chemical reactions, radiative heat loss, and variation of heat transfer coefficients with local pressure. The model is most applicable to a two-phase melt (metallic plus oxidic) having a fairly high metallic content.

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A Preliminary Model for Core/Concrete Interactions

1. Background

In the highly unlikely event of failure of coolant flow or loss of coolant in a Light Water Reactor (LWR) core followed by failure of certain engineered safety features, it has been hypothesized that the fission product decay heat could melt the reactor core. The molten core could also melt through the reactor pressure vessel and would eventually contact the concrete base.

Carbiener et al.¹ estimated that the molten core could penetrate the concrete base in approximately 18 hours (+10, -5 hours). They assumed that the initial penetration mechanism would be by rapid spalling of the concrete. During decomposition of the concrete, quantities of CO_2 and H_2O were expected to be released, with an attendant increase in containment pressure.

Levine² and Bazant³ have reviewed the available literature on the decomposition of concrete. Levine pointed out that the melt would contain large quantities of steel and that the water vapor and CO_2 released from the concrete could be expected to react with molten iron in the melt, releasing H_2 and CO to the containment atmosphere. These gases, being flammable, have the potential for greater pressure generation than do H_2O and CO_2 .

In order to resolve what gases could be expected and to gain a better understanding of the molten core/concrete interactions, the U.S. Nuclear Regulatory Commission requested Sandia Laboratories to undertake an experimental program which was ultimately initiated July 15, 1975. A complete description of the program is found in Reference 4, and a summary of recent experimental results is found in Reference 5.

The Nuclear Regulatory Commission also requested Sandia Laboratories to formulate a mathematical model of the interaction. This work has been divided into two phases: (1) a preliminary, approximate model to be based on the earliest experimental results, and (2) a more detailed and refined model to be formulated when more data become available.

This report describes the first phase of the modeling project. Because a usable model was desired at the earliest possible time, many important and interesting phenomena could only be approximated. The model is therefore not predictive in the sense that fidelity to an actual core meltdown can be confidently expected. However, it is believed that the model can be used to describe major phenomena qualitatively and to determine the relative importance of many effects.

1.1 Summary of Experimental Data

Dahlgren⁵ has described the experimental progress through March 1976. The phases of the program of most interest to the modeling effort are the deposition of corium type melts onto concrete and the response of concrete to high heat fluxes. The data from an additional study on the kinetics and stoichiometry of the thermal decomposition of concrete had not been reduced at the time of the modeling and have not yet been integrated into the model.

Significant data from the deposition of steel melts onto concrete were:

1. High gas blowing rates were observed,
2. There was an immediate, clear-cut separation of metallic and oxide constituents,
3. Only minor spallation was observed ($\sim 5\text{mm}$),
4. The gases evolved burned readily,
5. The cooling rate of the metal was measured in one test,
6. The cooling rate of the oxide, although less accurately known, was also measured,
7. The oxide slag rapidly crusted, but the gases readily broke through the crust,
8. The final recession of the concrete was measured,
9. An initially flat cavity base became rounded, and
10. The metal did not wet the concrete, whereas the slag layer did.

Experiments on the response of concrete to high heat fluxes showed that:

1. The recession rate varied with the incident flux, and
2. The recession rate was not strongly dependent on composition.

In addition, simulant experiments⁶ showed that pure conduction across a vapor boundary might be a reasonable description of the heat transfer process.

1.2 Insights from Experimental Program

The information obtained from the early phases of the experimental program was necessarily largely qualitative. However, some important insights were gleaned:

1. Gas induced circulation cells are the primary mechanism for convection,
2. Density driven separation of immiscible layers is rapid,
3. Each layer is probably nearly isothermal, except for the boundary,
4. The recession rate is not constant,
5. The gases from decomposing concrete (H_2O and CO_2) have ample time to react with iron,
6. The metal does not wet the concrete, whereas the oxide readily does - hence the heat transfer coefficient for the oxide/concrete interface should be higher than for the metal, and
7. Although the geometry of the cavity is complex, the bottom is generally rounded so that a hemisphere is a reasonable first approximation.

The model has been largely based on these general insights, with the addition of the existing quantitative data.

2. Conceptual Description of Model

A schematic conceptualization of the two layers is shown in Figure 1. Each layer (metal and oxide) is considered to be well mixed and isothermal in its interior as long as the layer is molten. Heat transfer from layer to layer takes place across a boundary layer or film whose thickness varies with the violence of mixing. The two main layers are assumed to be in intimate contact with each other, but there can be a vapor layer at the interface with the decomposing concrete. The thickness of the boundary layer can be different for each main layer; however, in each layer, it is uniform around the periphery of the layer. Heat is radiated to the containment, conducted into the concrete, and interchanged between layers.

A hemispherical segment, possibly intersected by a cylinder, is assumed. Figure 2 shows the possible geometric regimes and also indicates how the geometry can change as the problem advances.

Figure 1. Schematic Conceptualization

Figure 2. Geometry

Flows of material are shown in Figure 3. Material can be interchanged between layers. For example, iron oxides created by reaction of the steam with iron in the metallic part of the melt are assumed to be rapidly incorporated into the oxide layer. Solid or liquid decomposition products are assumed always to go promptly to the appropriate melt layer. However, gaseous products will not pass through the melt if the interface with the concrete is vertical.

Figure 3. Flow of Material

Gas induced circulation cells are shown in Figure 4. In a normal cell, more gas passes through the outside of the melt and circulation follows the top drawing. However, if the lower layer is hotter than the upper layer, more gas flows through the center and the circulation direction can be reversed. Even if one layer is frozen, as shown in the lower sketches, a circulation cell would be expected in the other molten layer. As a general rule, it is to be expected that a circulation cell will be set up if (1) the material is molten and (2) there is appreciable gas flow. The intensity of the circulation (and hence the thickness of the boundary layer) will depend on the rate of gas flow. Other factors influencing the boundary layer thickness include melt viscosity and gas flow path; these factors are not dealt with in this simple model.

Figure 4. Gas Induced Circulation Cells

3. Detailed Description of Model

3.1 Temperature History

The temperature in the i -th layer is described by

$$\frac{d}{dt} (M_i C_{pi} T_i) = \frac{d}{dt} Q_i \quad (1)$$

where

$i = 1, 2$ (metal or oxide)

M_i = mass of i -th layer

C_{pi} = specific heat of i -th layer

T_i = temperature of i -th layer

$\frac{d}{dt} Q_i$ = net rate of heat added to i -th layer

t = time

This is approximated by the finite difference equation

$$\frac{M_i^{n+1} C_{pi}^{n+1} T_i^{n+1} - M_i^n C_{pi}^n T_i^n}{\Delta t} = \dot{q}_i^{n+1/2}$$

where the superscripts n , $n+1/2$, and $n+1$ refer to the beginning, middle, and end of the time step. It has been found that the specific heats and heat rates are slowly varying quantities; and it is possible, with reasonably small error, to use these at the beginning of the time step only. With these simplifications, we have:

$$T_i^{n+1} \sim \frac{T_i^n M_i^n}{M_i^{n+1}} + \frac{\dot{q}_i^n \Delta t}{M_i^{n+1} C_{pi}^n} \quad (2)$$

The small error introduced is believed to be clearly justified by the much greater ease of programming and speed of solution.

The rate of heat addition is the sum of internal decay heating, enthalpy of entering materials, internal reactions, and heat conducted from the other layer. This is reduced by radiation losses, enthalpy of material leaving, heat conducted to the concrete, heat lost to the other layer, and heat required to dissociate any concrete products not dissociated at the melt/concrete interface. The net rate of heat gain in the i -th layer is

$$\dot{q}_i^i = \dot{q}_{int}^i + \dot{q}_{ent}^i + \dot{q}_{react}^i + \dot{q}_{cond}^{ji} - \dot{q}_{leav}^i - \dot{q}_{rad}^i - \dot{q}_{conc}^i - \dot{q}_{cond}^{ij} - \dot{q}_D^i$$

where

$\dot{q}_i^i$ is the net rate of heat gain in layer i

$\dot{q}_{int}^i$ is the internal (decay) heating in layer i

$\dot{q}_{ent}^i$ is the enthalpy rate of entering material

$\dot{q}_{react}^i$ is the net reaction heat rate

$\dot{q}_{cond}^{ji}$ is the rate of heat conduction from layer j (zero if $T_i > T_j$)

$\dot{q}_{leav}^i$ is the enthalpy rate of material leaving

$\dot{q}_{\text{rad}}^i$ is the radiation loss rate

$\dot{q}_{\text{conc}}^i$ is the rate of heat lost to the concrete

$\dot{q}_{\text{cond}}^{ij}$ is the rate of heat conduction to layer j (zero if $T_j > T_i$)

$\dot{q}_D^i$ is the rate of heat of dissociation of concrete products not dissociated at the melt/concrete interface

The enthalpy rate for material entering is

$$\dot{q}_{\text{ent}}^i = \sum_{j=1}^{nm} \dot{m}_j^i h_j(T_{\text{ent}})$$

where

nm = number of materials entering

$\dot{m}_j$ = rate of mass addition of material j

$h_j(T_j)$ = enthalpy of material j at temperature T_{ent} (see 3.6)

The enthalpy rate for material leaving is

$$\dot{q}_{\text{leav}} = \sum_{j=1}^{nm} \dot{m}_j h_j(T_{\text{leav}})$$

where

$\dot{m}_j$ = rate of mass loss of material j

T_{leav} = the temperature at which materials leave the layer, and other symbols are as previously defined

For all solid or liquid materials, T_{leav} is the temperature of the isothermal central region of the layer. However, it is possible for gases to transit the material so rapidly that they do not come into thermal equilibrium with the layer. An "equilibrium thickness" is assumed. The exit temperature is

$$T_{\text{leav}} = T^i - \exp(-x^i/x_r^i)(T^i - T_{\text{ent}})$$

where

T_{leav} = the exit temperature for gases

x^i = thickness of layer i

x_r^i = reference thickness for layer i (this is one of the parameters used to enforce agreement with experimental results)

T^i = central temperature of layer i

T_{ent} = temperature of entering gases

3.2 Materials Properties

The properties of layer i (conductivity, specific heat) are averaged according to the formula

$$\bar{x}_i = \sum_{j=1}^n f_j x_j(T_i) \quad (3)$$

where

$\bar{x}_i$ is the average property for the i-th layer

n is the number of species present in the i-th layer

x_j is the property of species j at temperature T_i

f_j is the weight fraction of species j

Density is averaged by the formula

$$\frac{1}{\bar{\rho}_i} = \sum_{j=1}^n \frac{f_j}{\rho_j}(T_i) \quad (4)$$

where

$\bar{\rho}_i$ is average density for the layer

ρ_j is the density of species j at temperature T_j

and all other symbols are the same as in Eq. (3).

Density, conductivity, and specific heat are used in the model as functions of temperature. When a step change of properties occurs (at phase changes), the change is considered to take place over a few degrees interval, and the step is averaged over the interval.

The species considered are UO_2 , ZrO_2 , FeO , CaO , SiO_2 , Cr_2O_3 , NiO , and Al_2O_3 in the oxide layer and Fe, Zr, Cr, and Ni in the metal layer. Material properties have been taken from References 7-10.

3.3 Temperature Profiles and Circulation Cells

The assumed temperature profile is shown in Figure 5. The interior of layer 1 is at a uniform temperature T_1 , and the interior of layer 2 is at a uniform temperature T_2 . There is a uniform gradient from T_1 to the surface temperature T_s and to the interface temperature T_{12} across the boundary of thickness δ_1 . There is a uniform gradient from T_2 to the interface temperature T_{12} and to the temperature T_{2c} , on the melt side of the concrete interface. The boundary gradients are not necessarily equal.

Figure 5. Temperature Profiles in Circulating Material

3.3.1 Boundary Temperature

The surface temperature, T_s , is found by equating flows of heat to and from the surface, by a solution of the equation

$$\frac{k_1}{\delta_1} (T_1 - T_s) = \sigma \epsilon (T_s^4 - T_w^4) \quad (5)$$

where

k_1 = thermal conductivity

δ_1 = boundary layer thickness

T_1 = temperature of interior of layer

T_s = surface temperature

σ = Stefan-Boltzmann constant

ϵ = effective emissivity

T_w = temperature to which the surface is radiating

For the original sump area, T_w is an average temperature of the material above the sump (arbitrarily taken to be 500°C). However, if the cavity is larger than the original sump, the outer region "sees" material at the temperature of decomposing concrete - taken to be 1100°C.

The emissivity can vary with time and temperature and is not well known. Any desired refinements in the radiative heat loss can be accommodated by changing the emissivity.

The temperature at the interface between layers is

$$T_{12} = \frac{k_1 \delta_2 T_1 + k_2 \delta_1 T_2}{k_1 \delta_2 + k_2 \delta_1} \quad (6)$$

the temperature at the concrete interface is discussed in Section 3.4.

3.3.2 Boundary Layer Thickness

The thickness of the boundary layer is assumed to grow at a rate*

$$\frac{d\delta_i}{dt} = \frac{0.72\alpha_i}{\delta_i} \quad (7)$$

where α_i is the thermal diffusivity. This allows the boundary layer to grow at a reasonable rate when the material is frozen. However, when the layer is molten, various constraints always govern, so that the thickness is more appropriate for a gas driven circulation cell.

A limiting volumetric gas flow per unit area of interface is chosen such that for higher gas flows an intense circulation cell is formed. In intense circulation cells, the boundary layer can become as thick as 0.5 percent of the total depth of the layer and is never allowed to be less than 5 mm.

At gas rates below the limiting rate, if both layers are molten, the boundary layer is allowed to grow to 2.5 percent of the total layer thickness but is again constrained to be at least 5 mm thick - this is called a moderate circulation cell. If one layer is frozen, a weak circulation cell is formed in the other layer and the boundary layer can grow up to 5 percent of the layer depth. There is no constraint on the growth of the boundary layer in a frozen material.

These constraints on the boundary layer thicknesses give temperature differences between metal and oxide layers similar to those observed in experiments, viz, a few hundred degrees.

* Note that this equation is valid only for solid materials. It is used, for want of a better relationship for molten material as well. However, other constraints invariably operate in molten layers.

The equations used to determine the constraints are given below (see Figure 5).

I. Both layers molten

$$\begin{aligned}
 & \left. \begin{aligned}
 x_{1I} &\geq .99x_1 \\
 \text{Subject to the constraint} \\
 \text{that } \delta_1 &\geq 0.5 \text{ cm} \\
 x_{2I} &\geq .99x_2 \\
 \text{Subject to the constraint} \\
 \text{that } \delta_2 &\geq 0.5 \text{ cm}
 \end{aligned} \right\} \dot{G} \geq \dot{G}_{MX} \\
 & \left. \begin{aligned}
 x_{1I} &\geq .95x_1 \\
 \text{Subject to the constraint} \\
 \text{that } \delta_1 &\geq 0.5 \text{ cm} \\
 x_{2I} &\geq .99x_2 \\
 \text{Subject to the constraint} \\
 \text{that } \delta_2 &\geq 0.5 \text{ cm}
 \end{aligned} \right\} \dot{G} < \dot{G}_{MX}
 \end{aligned} \tag{8}$$

where

x_1 = thickness of upper layer, cm

x_{1I} = thickness of isothermal region of upper layer, cm

x_2 = thickness of lower layer, cm

x_{2I} = thickness of isothermal region of lower layer, cm

$\dot{G}$ = volumetric gas flow rate per unit area of interface, cm/s

$\dot{G}_{MX}$ = limiting gas flow rate (see Section 4.2)

Note that $\delta_1 = (x_1 - x_{1I})/2$

$\delta_2 = (x_2 - x_{2I})/2$

II. One layer frozen

No constraint in frozen layer, and $x_1 \geq .9x$ for molten layer where x is the thickness of the molten layer.

3.4 Heat Transfer to Concrete

The melt/concrete interface is schematically depicted in Figure 6.

Figure 6. Interface Between Melt and Concrete

An initial estimate of the temperature on the concrete side of the interface is given by

$$T_{ic}^T = \frac{k_m \delta_c h_i T_m / R_c^2 + (k_c \delta_m h_i / R_m^2 + k_c k_m / R_i^2) T_c}{k_m \delta_c h_i / R_c^2 + k_c \delta_m h_i / R_m^2 + k_c k_m / R_i^2}$$

The trial temperature, T_{ic}^T , is compared with the decomposition temperature of Ca(OH)_2 , T_{DC} , and the temperature for vaporizing free water, T_w . The actual temperature is set as follows:

$$T_{ic} = T_{ic}^T, \quad (T_{ic}^T < T_w)$$

$$T_{ic} = T_w, \quad (T_w < T_{ic}^T < T_{DC})$$

$$T_{ic} = T_{DC}, \quad (T_{DC} < T_{ic}^T)$$

The temperature T_{im} on the melt side of the decomposing interface is calculated by

$$T_{im} = \frac{R_m^2 k_m T_m + R_i^2 h_i \delta_m T_{ic}}{R_m^2 k_m + R_i^2 h_i \delta_m} \quad (9)$$

where

k_m = thermal conductivity of melt

T_m = temperature of melt

h_i = interface heat transfer coefficient

δ_m = thickness of thermal boundary layer in melt

R_m , R_i , and R_c are radii; R_m to the midpoint of δ_m ; R_i to the decomposing interface, and R_c to the midpoint of δ_c .

The rate of recession, $\dot{x}$, is

$$\dot{x} = \frac{R_i^2 \delta_c h_i (T_{im} - T_{ic}) - R_c^2 k_c (T_{ic} - T_c)}{q_{CD} \rho_c R_i^2 \delta_c} \quad (10)$$

where

δ_c = "thermal penetration distance" in the concrete (see Section 3.4.1)

T_c = initial temperature of the concrete

q_{CD} = heat of decomposition of the concrete (see Section 3.5)

ρ_c = density of concrete, and other symbols are explained in Equation (8)

If $T_{ic} = T_{DC}$, the recession rate represents the rate at which the decomposition front moves into the concrete. If $T_{ic} = T_w$, decomposition is not taking place, and $\dot{x}$ is the velocity with which the water vaporization front is moving into the concrete. If $T_{ic} < T_w$, there is no surface recession or water evaporation and this computation is bypassed.

The heat of decomposition, q_{CD} , is described more completely in Section 3.5.

3.4.1 Depth of Thermal Penetration in Concrete

Figure 7 represents schematically a thermal front and an ablation front both travelling into the concrete. The velocity of advance of the thermal front is

$$\dot{x}_t = \frac{0.72\alpha_c}{\delta_c} * \quad (11)$$

where

α_c = thermal diffusivity of the concrete

δ_c = thickness of thermal layer

* This equation has been taken, by analogy, from the advance of the thermal front into a slab of material, one face of which is maintained at a fixed temperature. It is not strictly applicable to spherical or cylindrical geometry; however, the radii R_m , R_i , and R_c are all very nearly the same, so that error is small.

Figure 7. Thermal and Ablation Fronts

The velocity of the ablation front, $\dot{x}_a$, was computed in the preceding section. The thickness of the thermal layer is

$$\delta_c = \int_0^t (\dot{x}_t - \dot{x}_a) dt .$$

3.4.2 Variation of Concrete Properties

Thermophysical properties of concrete are dependent on moisture content.¹¹ Concrete at high temperatures would be expected to be drier than the unaffected material. The experimental program^{4,5} has shown that water (in addition to that evaporated) is driven outward from the heat-affected zone.

The properties of oven-dry and saturated concrete are computed in the model, using the method of Loudon and Stacy.¹² Material is considered to be completely dry at temperatures above the boiling point of water and fully saturated below that temperature.

The property, x , (conductivity, specific heat, density) is then averaged over the heated zone by the formula

$$\bar{x} = f_{\text{DRY}} x_{\text{DRY}} + f_{\text{WET}} x_{\text{WET}}$$

where

f_{DRY} = fraction of heated zone assumed dry

x_{DRY} = property x, oven dry

f_{WET} = fraction of heated zone assumed wet

x_{WET} = property x, at 10% moisture.

Note that $f_{\text{WET}} = [(T_w - T_c)/(T_{ic} - T_c)]$, and $f_{\text{DRY}} = 1. - f_{\text{WET}}$. Where T_w , T_c , and T_{ic} have been previously defined.

3.5 Concrete Decomposition

At the time of formulation of the model, experimentally based decomposition data were not available. A theoretical model due to Levine¹³ has been used.

Straight line fits to the data of Reference 13 have been used for the heat of dissociation and dissociation temperature of Ca(OH)_2 , CaCO_3 , and the vaporization of free water. The equations used in the model are

$$\begin{aligned}T_{\text{Ca(OH)}_2} &= 796. + 17.3(P-1.) \\ \Delta H_{\text{Ca(OH)}_2} &= 1342 - 6.37(P-1.) \\ T_{\text{CaCO}_3} &= 1160. + 37.4(P-1.) \\ \Delta H_{\text{CaCO}_3} &= 1653. - 10.9(P-1.) \\ T_{\text{H}_2\text{O}} &= 373. + 12.31(P-1.) \\ \Delta H_{\text{H}_2\text{O}} &= 2263. - 37.67(P-1.)\end{aligned}\tag{12}$$

where

$T_{\text{Ca(OH)}_2}$ = dissociation temperature of Ca(OH)_2 , K

$\Delta H_{\text{Ca(OH)}_2}$ = heat of dissociation of Ca(OH)_2 , J/gm

T_{CaCO_3} = dissociation temperature of CaCO_3 , etc.

P = pressure, atm

The vaporization of free water does not indicate decomposition of the concrete. However, it is assumed that dissociation of the calcium hydroxide will crumble the matrix. Even if the remaining constituents do not melt or dissociate, they will be absorbed into the melt. The dissociation temperature of calcium hydroxide is lower than the dissociation temperature of calcite or the melting point of silica; therefore, it is only necessary to determine whether the calcium hydroxide will dissociate to determine whether decomposition occurs. If the temperature T_{CaCO_3} is less than T_{im} (Section 3.4), calcite will also be decomposed in the interface. If the melting point of silica is less than T_{im} , silica will be melted in the interface. It is assumed that alumina can be released but not melted before incorporation into the melt.

In reality, the oxidic constituents of concrete decomposition are mutually soluble. It would be more realistic to consider a liquid solution leaving the interface. Unfortunately, the problem of determining the melt temperature and properties introduces excessive complication.

3.6 Enthalpy of Products Entering or Leaving Melt

Polynomial approximations are used for the heat content of species entering or leaving the melt. The approximations (generally taken from Reference 9 or fits to the data of Reference 10) are:

$$\text{CO}_2 ; h = .733T + 2.524 \times 10^{-4}T^2 - 2.63 \times 10^{-8}T^3$$

$$\text{CaO} ; h = .748T + 1.81 \times 10^{-4}T^2$$

$$\text{SiO}_2 ; h = 1.39T$$

$$\text{Al}_2\text{O}_3 ; h = 1.36T$$

$$\text{ZrO}_2 ; h = .605T$$

$$\text{H}_2 ; h = 13.87T + 8.5 \times 10^{-4}T^2$$

$$\text{FeO} ; h = .846T$$

$$\text{H}_2\text{O} ; h = 2263. - 37.67(P-1.) + 4.19T' + 2.09 (T-T')$$

$$(T' = 373 + 12.31(P-1.))$$

where

h = enthalpy, J/gm

T = temperature, K

P = pressure, atm.

In addition, any concrete products not dissociated or melted at the melt/concrete interface must have their heats of dissociation removed from the melt if they are later dissociated within the melt. The only products to which this could apply are calcite and silica. A test is made for dissociation; and, if $T_{im} < T_D$, $T_o > T_D$, the heat of dissociation is removed from the oxide layer. Here T_{im} is the temperature on the melt side of the melt/concrete interface, T_D is the dissociation or melting temperature, and T_o is the temperature of the oxide layer.

3.7 Flow of Material

Because of the probable complexity of material flow paths, some simplifications have been required. The following arbitrary rules are applied:

- a. All oxides are promptly transmitted directly to the oxide layer,
- b. All metals are promptly transmitted directly to the metal layer,
- c. Gases entering a layer leave the layer in the same time step,
- d. Gases released at a vertical interface flow directly to the atmosphere, without transitting the melt,
- e. Gases released at a nonvertical interface flow through the molten melt layers,
- f. Gases bypass frozen layers,* and
- g. Gases bypass any layer if at least 5 cm of the layer boundary is below the freezing temperature of the layer.**

* Note, however, that experiments have shown that a freezing layer becomes "honey-combed" with small gas passages. The rationale for imposing this rule is that it is believed that gases passing through holes in a solid metal layer would cease to interact with the layer as soon as a heavy oxide surface was built up. This may not have been observed in experiments because of the short time scale of the experiments.

** In experiments, it has been observed that thin crusts are easily broken. However, it is believed that there must be some crust thickness for which gases cannot break the crust. For lack of better information, 5 cm has been chosen as the limiting crust thickness.

At early times, the oxide is heavier than the metal and would be on the bottom. Some part of the oxides from reactions in the metal layer and from decomposition of concrete would probably float on top of the metal, resulting in a three-layered melt. This possibility has been ignored in the model. It is believed that the major part of the concrete decomposition products will be incorporated into the oxide layer. The principal effect of a thin layer of oxide floating on the metal will be to raise the emissivity of the metal, cooling it faster and increasing its density. (The change in density is small, but could conceivably be important in determining the time at which the metal layer becomes more dense than the oxide.)

A continuous check is made on the relative average densities of the metal and oxide layers, and the denser layer is always considered to be underneath.

3.8 Melting Points

The oxide melting point is extremely complex; in fact, it is naive to speak of clear cut melting or freezing points. Some species will be precipitated from the melt as the temperature drops, perhaps remaining as solid inclusions in a viscous, semi-liquid matrix. Owing to the continuous precipitation, the oxide layer will become more and more viscous as the temperature decreases. Experiments reported in Reference 5 have shown, however, that the gases readily penetrate even a very viscous slag.

Approximate fits have been made to the binary phase diagrams of each oxide species with all other oxide species. Each phase diagram has been considered to be that of an isomorphous system, although in reality eutectic systems are more commonly formed. The solidus temperature of the melt is assumed to be the lowest solidus temperature of any pair for which both constituents of the pair represent at least 2.5% of the melt. The liquidus temperature is assumed to be the highest liquidus of any such pair.

As the temperature of the melt is reduced, some species precipitate, releasing their heat of fusion to the melt and effectively raising the specific heat. The effective specific heat is calculated by

$$C_p' = C_p + \sum_{i=1}^n f_{wi} h_{fi} \sum_{\substack{j=1 \\ j \neq i}}^n (1 - \delta_{ij}) a_{ij} f_{wj} / (T_{lij} - T_{\delta ij})$$

where

C_p' = effective specific heat

C_p = specific heat of oxide layer

f_{wi} = weight fraction of species i

h_{fi} = heat of fusion of species i

δ_{ij} = Kronecker delta, $\delta_{ij} = 1, i = j$; $\delta_{ij} = 0, i \neq j$

$a_{ij} = 1, T_{\delta ij} < T_o < T_{lij}$

$a_{ij} = 0$, otherwise

T_{lij} = liquidus temperature for pair i, j

$T_{\delta ij}$ = solidus temperature for pair i, j

This procedure ignores such effects as heat of solution. While not strictly correct, it does have the desired effect of distributing the increase of the effective specific heat of the range of temperatures at which precipitation should be occurring. The heats of fusion employed are given in Table I.

TABLE I
Heats of Fusion

<u>Species</u>	<u>H_f (J/gm)</u>
UO ₂	274
ZrO ₂	708.
FeO	436
CaO	1346
SiO ₂	193.6
Al ₂ O ₃	1068
Cr ₂ O ₃	688.
NiO	677.
Fe	289.
Zr	225.
Cr	281.
Ni	300.

The melting point of the metal layer is more easily addressed, because the metals rapidly approach an alloy of Fe and Ni. A 20°C temperature difference between liquidus and solidus is assumed for the metals.

3.9 Reactions

The reactions considered in the core melt are

The first three and last two reactions are assumed to be limited by the mass of gases available, i.e., that all of the CO_2 and H_2O are reacted. This assumption is based on the experimentally observed fact that when concrete is attacked by a few centimeters of molten steel, the gases appear to react completely. It is assumed that the reactions can be rate limited if the mass rate of flow is large or if the residence time is short. The quantity used for testing for rate limiting is

$$G = \frac{(\dot{M}_{\text{CO}_2} + \dot{M}_{\text{H}_2\text{O}})}{x_m A} \quad (14)$$

where

$\dot{M}_{\text{CO}_2}$ = mass rate of CO_2 , gm/s

$\dot{M}_{\text{H}_2\text{O}}$ = mass rate of H_2O , gm/s

x_m = thickness of metal, cm

A = area of metal/oxide interface, cm^2

When the quantity, G, is 10 times greater than in the experiments, it is assumed that only 1/10 of the gases can be reacted. When the weight fraction of the metallic element is less than 20 percent, it is assumed that the reactions are limited by the available mass of metal.

$$f = f_1(G)f_2(f_m) \quad (15)$$

where

f = fraction of gas available for reaction

$f_1(G)$ = fraction available, dependent on quantity G

$$f_1 = 1, G \leq 7.5 \times 10^{-4} \quad (16)$$

$$f_1 = .1, G > 7.5 \times 10^{-3}$$

$$f_1 = 1. - 133.333(G - 7.5 \times 10^{-4}), 7.5 \times 10^{-4} < G \leq 7.5 \times 10^{-3}$$

$f_2(f_m)$ = fraction available dependent on weight fraction of other reactant

$$f_2 = 1, f_w(R) \geq 0.2 \quad (17)$$

$$f_2 = \frac{f_w(R)}{0.2}, f_w(R) < 0.2$$

where $f_w(R)$ is the weight fraction of Fe or Zr in the melt.

The mass rate of gases available for reaction are:

$$\dot{m}_r = f\dot{m}_g$$

$$\dot{m}_g = \text{total mass rate.}$$

The fourth reaction listed should be very rapid, provided that both reactants (FeO and Zr) are in intimate contact. However, the reaction will be limited by the rate at which circulation brings the reactants together at the metal/oxide interface. The rate of this reaction could have been made a function of gas flow, because the gases are the primary mechanism for circulation in the melt. However, this is believed to be an unnecessary complication; the effect desired is simply that the metallic zirconium be rapidly depleted. As a compromise, it is assumed that this reaction would proceed with a time constant of 300 seconds.

Zirconium is always preferentially oxidized, relative to iron, provided that the weight ratio of Zr to Fe exceeds 1:1000. At lower ratios, the oxidation shifts toward iron.

The net effect of the two reactions involving Zr is that essentially all metallic zirconium is depleted in a few minutes.

The last two reactions have been considered identical to the steam oxidation of zirconium and iron, respectively.

Straight line fits have been used for the heats of reaction. Endothermic reactions are considered positive.

$$\begin{aligned}\Delta H &= -7760 - 1.15(T-2000) \text{ (H}_2\text{O with Zr)} \\ \Delta H &= -22.29 + 2.24 \times 10^{-5}(T-2000) \text{ (H}_2\text{O with Fe)} \\ \Delta H &= 377. - .0271(T-2000) \text{ (CO}_2 \text{ with Fe)} \\ \Delta H &= -6708. + .16(T-1800) \text{ (FeO with Zr)}\end{aligned}\tag{18}$$

where ΔH is the heat of reaction, J/gm metal.

3.10 Cavity Growth

The geometry of the problem was briefly treated in Section 2. The geometric regimes are a hemispherical segment, a hemispherical segment intersected by a cylinder, and a near cylinder.

3.10.1 Hemispherical Segment

The growth is computed at the midpoints of each layer and at the center of the bottom layer. A circle is passed through the new midpoints and translated vertically until it passes through the new bottom point. The radius of the top of the segment is not permitted to exceed the maximum cylindrical radius. The process is shown in Figure 8.

Figure 8. Changing Shape of Cavity (Hemispherical Segment)

3.10.2 Hemispherical Segment Intersected by a Cylinder

The radius of the cylinder is initially the sump radius. Whenever purely radial growth occurs, the new cylindrical radius is used for the sump. If the radius of the top of the hemispherical segment becomes as great as the sump radius, additional material is placed in the cylindrical section, i.e., the radius of the top of the hemispherical segment cannot exceed the radius of the cylinder.

If the interface between the metal and the oxide lies within the hemispherical segment, the new hemispherical radius is determined as in 3.10.1. However, the points of growth are the midpoint of the lower layer and a point midway between the interface and the circle of intersection with the upper cylinder (Figure 9).

Figure 9. Changing Shape of Cavity (Hemisphere/Cylinder)

If the interface lies within the cylindrical section, the hemispherical radius grows uniformly and the growth of the cylindrical section is the area-weighted average of the growth of the upper and lower layers.

An approximation to a cylinder is made if the hemispherical radius is much greater than the cylindrical radius.

3.11 Contact with Free Water

Contact with free water is allowed either initially, when the molten core first drops onto the concrete, or whenever the radial growth exceeds a predetermined amount.

It was the opinion of one intimately familiar with experimental work on steam explosions¹⁴ that the melt would have a high probability of granulating on initial contact with water, with rapid heat transfer to the water. It is assumed that initial water is instantly vaporized. The sensible heat of the melt is reduced, and new initial temperatures are computed:

$$T'_m = T'_o = \frac{(M_m C_{pm} T_m + M_o C_{po} T_o - h_w M_w)}{M_m C_{pm} T_m + M_o C_{po} T_o}$$

where

T'_m, T'_o are the new temperatures of metal and oxide (assumed equal)

M_m, M_o are the masses of metal and oxide

C_{pm}, C_{po} are the specific heats of metal and oxide

h_w is the heat of vaporization of water

M_w is the mass of water.

Note that this computation implies that the water initially existed as saturated liquid.

Water contacting the melt later is assumed to boil off quiescently. A numerical approximation is made to the boiling heat transfer coefficient

$$h_B = 1.066 \Delta T^{-0.672} (\Delta T \leq 3.89)$$

$$h_B = 0.11697 \Delta T^{0.955} (3.89 < \Delta T \leq 35.94)$$

$$h_B = 248559. \Delta T^{-3.1126} (35.94 < \Delta T \leq 136.1)$$

$$h_B = .06715 \Delta T^{-1.672} (\Delta T > 136.1)$$

where

h_B = boiling heat transfer coefficient, $J/cm^2/K$

$\Delta T = T_s - T_w$

T_s = surface temperature

T_w = temperature of saturated water

Note that h_B is the heat transfer coefficient, not the heat flux. The form thus appears different from the conventional representation, e.g., Reference 15.

The surface temperature, T_s , is determined by a solution to the equation

$$\frac{K_m (T_M - T_s)}{\delta_m} = h_B (T_s - T_w)$$

where

K_m = melt conductivity (upper layer)

T_m = melt temperature

δ_m = melt boundary thickness,

The heat lost from the melt to the water is:

$$\dot{q}_{mw} = \pi r_o^2 h_B (T_s - T_w)$$

where r_o is the radius of the top surface.

It is implicitly assumed here that the water completely covers the surface of the melt. This could grossly overstate the heat lost to the water if, for example, only a thin stream impinges on the melt.

4. Experimentally Derived Constants

The interface heat transfer coefficients have been chosen to match, as nearly as possible, the metal and oxide cooling curves and total recession in test LSL-1 (Reference 4). The boundary layer thicknesses have been chosen to allow oxide and metal temperatures to differ by a few hundred degrees when both materials are molten, as has been experimentally observed.

4.1 Choice of Interface Coefficients

The interface coefficients have been chosen so that, in a computer simulation of test LSL-1,

1. Metal temperatures drop to the freezing point in 220 sec or less,
2. Slag temperature drops to 1300°C in 160 sec, and
3. Recession is approximately 1.5 cm.

An additional consideration is that the heat transfer coefficient for the oxide should be several times that for the metal, because the oxide is in intimate contact with the concrete.

Figure 10 shows metal temperatures as a function of time for several values of the metal interface coefficient. The oxide coefficient was 0.05 for all trials. Clearly, a value of $0.006 \text{ W/cm}^2/\text{K}$ matches the experiment well. At this pair of values (0.006, 0.05), the oxide temperature at 160 sec was 1350°C , the metal was frozen at 210 sec, and the total recession was 1.3 cm at 10 minutes. After 10 minutes, the heat transfer to the concrete is so low that ablation essentially ceases.

Figure 10. Simulation of Test - LSL-1

4.1.1 Variation of Interface Coefficient with Pressure

Posttest sections have shown a layer of partially decomposed concrete approximately 0.1 inch in thickness. If it is assumed that the conductivity of partially decomposed concrete is similar to that of virgin concrete, the approximate thermal conductance of this layer is $0.1 \text{ W/cm}^2/\text{K/cm}$. The associated vapor layer represents another conductance in series. The overall conductance is

$$h_i = \left(\frac{1}{h_{DC}} + \frac{1}{h_v} \right)^{-1}$$

The thickness of the vapor layer is dependent on local pressure (atmospheric plus static head). By substitution in the previous equation, the overall conductance is

$$h_i = \frac{h_{in} P}{10 h_{in} (P - 1.) + 1}$$

where

h_{in} = nominal interface coefficient at one atmosphere

P = local pressure

4.2 Thickness of Thermal Boundary Layers

Descriptions of the circulation cells have been given in Sections 2 and 3.3. There are two possible methods for changing the thermal boundary thickness: by changing the model of Section 3.3.2 or by changing the limiting gas flow. The latter is far simpler and is the method used.

The boundary layer thickness should be chosen so that metal and oxide temperatures can differ by a few hundred degrees; this difference has been experimentally observed. The limiting gas flow was taken in turn to be equal to the early gas flow in test LSL-1, one tenth of that flow, and 10 times that flow.

If the limiting gas flow is very large, the limit is never reached and the thermal boundary is quite thick. If the limiting gas flow is very small, it is always exceeded, and the boundary layer is quite thin. A hypothetical PWR core has been analyzed under all three conditions. The very high limiting flow allows temperature differences between metal and oxide to exceed 1000 K, which is not believed reasonable. The very low limiting flow gives reasonable temperature differences for the PWR core problem, but the steel pour test could not be simulated well. Accordingly, a limiting flow equal to the early flow in test LSL-1 has been chosen as the most reasonable.

5. Sample Problem Results

The results for a hypothetical PWR core on basalt concrete are shown in Figures 11, 12, and 13. For this problem, it was assumed that the core contacted the concrete one hour after accident initiation, at which time 60 percent of the fission product decay power had been volatilized and lost from the core.* The remaining decay power was distributed 30 percent in the oxide and 10 percent in the metal.

* The decay power remaining, and all other parameters of this problem, are intended to be illustrative only and are not intended to represent supposed conditions for any specific core-meltdown accident.

Figure 11. Metal and Oxide Temperatures, Basalt Concrete

Figure 12. Vertical and Radial Penetration, Basalt Concrete

Figure 13: Gases Added to Atmosphere, Basalt Concrete

Figure 11 shows metal and oxide temperatures. Figure 12 shows vertical and radial recession. Figure 13 shows gases added to the containment atmosphere. Figures 14, 15, and 16 show the corresponding results for a limestone concrete. The containment atmosphere could vary from the gas ratios shown, because of later reactions.

Figure 14. Metal and Oxide Temperatures, Limestone Concrete

Figure 15. Vertical and Radial Penetration, Limestone Concrete

Figure 16. Gases Added to Atmosphere, Limestone Concrete

6. General Discussion

The model presented is to some extent based on conjecture. It is the author's opinion that the assumptions are reasonable, but certainly there is no proof of completeness or accuracy. It is also believed that little can be done to improve these conditions until more experimental evidence is received. It is heartening to note, however, that the most realistic experiments can be reasonably well simulated.

Because of the number of assumptions and estimates, it should not be supposed that the model can "predict" such critical variables as the time of containment melt through. The model can best be utilized to determine the general effect of changing parameters on the outcome of the meltdown process. For example, the effect of changing concrete composition on the gases evolved can be estimated, but one should not suppose that the model will accurately predict the time of containment overpressure failure for any specific set of circumstances. The model could be a useful tool in a sensitivity study to explore the importance of various parameters.

7. Variation of Coefficients

The most important experimentally derived parameters are the interface heat transfer coefficients, h_{im} and h_{io} . Factors affecting the accuracy of these coefficients are:

1. the accuracy of experimental measurement,
2. the approximate nature of the model,
3. the accuracy with which physical properties are known,
4. scaling of the small experiments, with times measured in minutes, to a very large core melt, with times measured in hours, and
5. different materials in experiment and core melt.

The net result of these factors is that the interface heat transfer coefficients cannot be known with any accuracy. Based on intuition and engineering judgement, it is believed that 50% higher interface coefficients are as credible as the nominal values.

8. Accuracy of Computations

The possible accuracy of the computations may be observed by reference to Figure 17, which shows a heat balance for a typical problem at a time when the melt temperature is approximately the freezing temperature of the metallic layer.

Net Rate of Decrease of Sensible Heat = 4.04 MW

Figure 17. Schematic Heat Balance

It will be noted that relatively minor changes in the radiation component, in the conduction into the concrete, in the concrete decomposition energy, or in the decay heat could significantly affect the rate of change of the sensible heat of the melt. For example, a 10% change in decay heat would make a 36% change in the sensible heat rate. In fact, changes in decay heat, radiation, heat transfer to the concrete, and conduction into the concrete, which are well within the precision with which these quantities can be known, could change the melt from decreasing to increasing temperature. It has been experimentally observed that penetration almost ceases after solidification; this is also shown in the calculations. In the problem shown in Figure 17, the melt is cooling and will shortly freeze, at which time penetration will be radically slowed. However, the possible parameter changes mentioned above would forestall freezing and even increase the temperature of the melt, thus accelerating the penetration.

It is obvious that computed temperature histories and penetration rates should not be considered indicative of any specific case. The model can, however, be utilized to display a spectrum of possible results.

9. Applicability of the Model

The experiments on which the model is based have been conducted with melts having high metallic content. In these experiments the principal attack on concrete was from the metallic phase. Because the metal layer did not wet the concrete, the attack must be entirely thermal. This is not necessarily the case with the oxide layer. The concrete is wet by the oxide, and the attack could be chemical, diffusive, or simple solution of the concrete by the molten oxide.

Until the method of attack has been more thoroughly explored, the model should be considered of unknown applicability for melts consisting principally of oxides. This may even be so for melts that initially have a reasonable metallic fraction, because the metals are normally burned out by the evolved gases.

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