

# **Cavity (CAV) Package Reference Manual**

The MELCOR Cavity (CAV) package models the attack on the basemat concrete by hot (often molten) core materials. The effects of heat transfer, concrete ablation, cavity shape change, and gas generation are included, using models taken from the CORCON-Mod3 code. The coding of the models is identical to that in CORCON-Mod3, but interfaces have been modified for integration into the MELCOR framework. This integration couples the Cavity package models to thermal-hydraulic boundary conditions in the Control Volume Hydrodynamics (CVH) package, to sources of core debris from the Core (COR) and/or Fuel Dispersal Interactions (FDI) package, and to the standard MELCOR input, output, plotting, and restart capabilities. The fission-product release models in CORCON-Mod3—originally developed as the separate VANESA code—are included in MELCOR as part of the RadioNuclide (RN) package.

This Reference Manual provides an overview of modeling in the CAV package. User input for running MELGEN and MELCOR with the CAV package activated is described in the CAV Package Users' Guide. The fission-product release models (VANESA) and available input are described in the RN Reference Manual and Users' Guide, respectively.

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## 1. Introduction

The Cavity (CAV) package in MELCOR models the attack on the basemat concrete by hot, often molten, core materials. The effects of heat transfer, concrete ablation, cavity shape change, gas generation, and debris/gas chemistry are included. The package consists of models taken from the CORCON-Mod3 code [1] together with all necessary interfaces to the MELCOR database and to other packages in MELCOR.

Before the initial release version of CORCON-Mod3 [2] was incorporated into MELCOR and into CONTAIN [3], a number of modifications were made to the coding that had no effect on results calculated by the stand-alone code, but allowed the direct use of all routines containing phenomenological models and properties data *without modification* in the systems codes. These changes involved a restructuring of the internal database and of the interfaces to input and output routines (including diagnostics and plotting) and to routines that provide boundary conditions for the CORCON models.

Boundary conditions for temperature and pressure used by the cavity models are obtained from an associated CVH control volume, rather than from user input as in the stand-alone CORCON. Any overlying coolant (water) pool is considered part of the boundary condition rather than part of the cavity model and is modeled by CVH. Heat and evolved gases are delivered as sources to the associated CVH volume.

Debris from the Core (COR) package, the Fuel Dispersal Interactions (FDI) package, or the External Data File (EDF) package is ordinarily deposited into the cavity through the Transfer Process (TP) package. However, initial contents may also be defined in CAV input and arbitrary addition rates may be prescribed by input to the TP package. When debris is deposited, no spreading calculation is performed because it is assumed to spread instantaneously to the maximum area permitted by the cavity geometry.

The CAV packages uses the CORCON-Mod3 properties routines, which are currently independent of the general Materials Properties (MP) package in MELCOR.

The phenomena modeled by the CAV package may be treated in more than one location in a MELCOR calculation. Transfer of material between cavities is allowed based on three tests: axial rupture, radial rupture, or a transfer triggered by a Control Function. Each of the three types of rupture (axial, radial, and triggered) can overflow to a separate cavity, but only "one-way" transfers are allowed. That is, if material can overflow from cavity 1 to cavity 2, it is not permitted to flow from cavity 2 back to cavity 1, either directly or through intermediate cavities. These ruptures can be used to model such phenomena as failure of the pedestal in a BWR Mk I or of the diaphragm slab in a BWR Mk II. Triggered transfers may also simulate (in a qualitative way) the effects of the spreading of debris across a flat floor.

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The VANESA model [4] was integrated into CORCON-Mod3 to calculate the release of fission products and the generation of aerosols from debris in the cavity. The structure of MELCOR requires that radionuclides associated with debris in the cavity be treated by the RadioNuclide (RN) package, which maintains time-dependent inventories for each RN class in each cavity. The relevant subroutines from CORCON-Mod3 were therefore made part of the RN package. They are identical to the routines in the latest stand-alone version of CORCON-Mod3 and in CONTAIN; an interface is provided through a utility entry in the RN package that duplicates the functionality in the stand-alone code. See the RN package Reference Manual for more details.

Several options for direct user input of internal heating of the debris by fission products are allowed, but this heating is ordinarily calculated by the RN and DCH (Decay Heat) packages, based on RN inventories. Therefore, the effects on internal heating of relocation of debris into or between cavities, as well as the effects of RN releases within each cavity, are automatically accounted for.

## 2. Phenomenology

This section gives a qualitative description of the processes modeled in the CAV package in MELCOR, and the physical picture on which the models are based. The information is largely derived from Section 2.1 of the CORCON-Mod3 Manual [1]. Interfaces to other MELCOR packages are noted in the discussion.

The attack of core debris on concrete in a light water reactor is primarily thermal and may be considered quasi-steady for much of the period of a reactor accident. Decay heat and heat from chemical reactions is generated in the debris and is transferred either through its top surface or to the concrete floor. Boundary conditions at the surface, including temperature and the presence or absence of water, are obtained from the associated control volume in CVH. Heat lost from the cavity top surface is treated by CVH as a source into that control volume.

The quasi-steady partition of the heat transfer to the concrete floor and through the debris top surface is determined by the ratio of the corresponding thermal resistances. Thus, debris behavior and concrete ablation are dominated by conservation of energy, with heat transfer relations providing the most important constitutive relations.

Under the conditions visualized by the CORCON developers, the heat flux to the concrete floor is sufficient to decompose it, releasing water vapor (from both adsorbed water and hydroxides) and carbon dioxide (from carbonates) and to melt the residual oxides. The surface of the concrete is typically ablated at several centimeters per hour and molten oxides and molten steel from reinforcing bars in the concrete are added to the debris pool. The decomposition gases are strongly oxidizing at debris temperatures and will be reduced, primarily to hydrogen and carbon monoxide, on contact with metals in the debris. Ultimately, the reacted and unreacted gases enter the atmosphere above the debris pool,

where they may or may not burn immediately. (Modeling of these containment phenomena is not included in CORCON.) These gases (with appropriate enthalpies) are treated as sources in the associated control volume in CVH. The possibility that the combustible gases will burn is considered by the BUR package.

The full concrete response is extremely complicated, with elements of ablation, transient conduction, decomposition of hydroxides and carbonates in advance of the ablation front, and transport of gases and liquid water through the pores of the concrete. Further, the length scale of the temperature profile is often comparable to the size of the coarse aggregate in concrete, making any assumption of homogeneous properties questionable.

In CORCON and in CAV, concrete response is modeled as quasi-steady ablation. The thermal diffusivity of concrete is extremely small, a few times  $10^{-7}$  m<sup>2</sup>/s. Over the time scale of interest in cavity phenomena (hours), the amount of heat which can be transferred into concrete (by transient conduction) under nonablative conditions is usually small compared to the amount of heat which must be removed from core debris through other mechanisms to maintain its temperature below the ablation temperature. Therefore, if the debris temperature is below the ablation temperature, the concrete floor surface is modeled as an adiabatic boundary.

Gas released at the bottom of the debris pool is assumed to rise through it as bubbles. Gas released at the side of the pool may also form bubbles that rise to the surface. At sufficiently high gas release rates, a stable gas film may form at either the bottom or side interfaces. Gas bubbles rising through the debris pool increase its volume. This "level swell" increases the depth of the pool and area of its radial interface with the concrete floor.

The rising bubbles also promote the production of aerosols containing fission products stripped from the fuel debris. The processes involved, reactive vaporization and bubble bursting, are treated by the VANESA model [4] in the RN package in MELCOR. This model calculates the removal and relocation of fission products and the resulting sources of aerosols for the MAEROS aerosol physics model (also part of the RN package). All necessary data concerning the temperature and bulk composition of the debris and the gas generation rates are passed by CAV to a utility entry in RN; the fission product inventories themselves are part of the RN database. The subroutines that implement VANESA in the RN package are identical to those that implement it in CORCON-Mod3.

Experimental evidence (cited in Reference 1) shows that the various oxidic species in the melt are highly miscible, as are the metallic species, but that the two groups are mutually immiscible. Previous versions of CORCON assumed that the core debris would stratify into distinct layers based on the relative densities of the phases. The passage of gas bubbles through the interface between layers can overcome this separation if the gas flux is high or the density difference is small by entraining droplets of the lower (denser) material and mixing them into the upper one. If entrainment occurs, the degree of mixing achieved is determined by a balance between entrainment and reseparation as the denser droplets settle out under the influence of gravity. The debris may therefore be fully stratified,

partially mixed, or fully mixed, and the state may change as the densities and gas fluxes change during a debris-concrete interaction.

There is a possibility that an overlying coolant layer (water) could interact with molten debris so as to break it up and form a coolable debris bed. In the MAAP code [5], this breakup and quenching is assumed to occur; it is not considered in CORCON, nor is it included in the current version of the MELCOR CAV model.

As the core-concrete interaction progresses, the debris pool grows as concrete oxides are added to it; its surface area increases, and internal heating decreases. Therefore, debris temperatures and heat fluxes decrease, and the possibility of refreezing arises. Substantial freezing of the metal phase may occur. However, the large internal heating and small thermal conductivity of the oxidic phase prevent the formation of steady, solid crusts thicker than a few centimeters. Therefore, unless the debris is spread over an extremely large area, the interior of the oxidic phase will remain molten for a long time, probably for weeks.

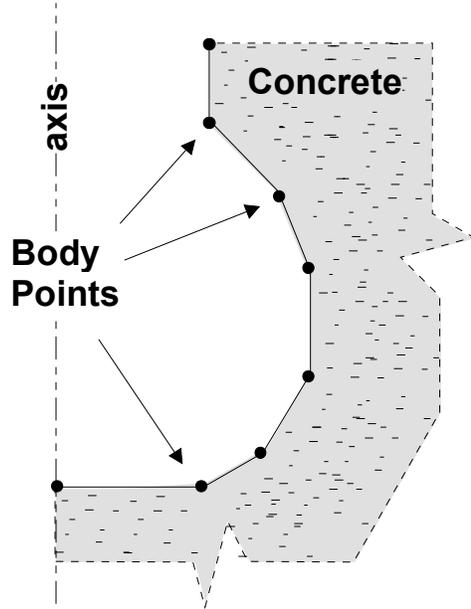
### 3. Models

Documentation of the CORCON-Mod3 [1] remains the primary reference for most of the submodels in the Cavity package. The following subsections briefly summarize the material contained there, while noting modifications made for incorporation into MELCOR.

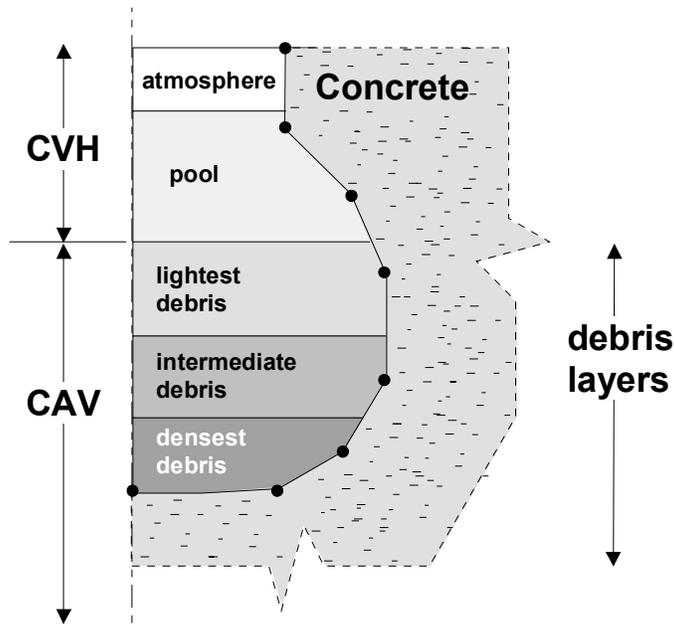
#### 3.1 System Components

The physical system considered by the Cavity package consists of an axisymmetric concrete cavity, a multilayered debris pool, and a set of boundary conditions (provided by CVH) at the top surface of the debris, as illustrated in Figure 3.1.

The shape of the concrete cavity is described by a series of so-called *body points* lying in a vertical cross-section of the concrete surface. The initial shape is defined by user input. The concrete itself is described by specifying an average chemical composition; its thermochemical properties are then obtained from an internal database of properties for the component species. A number of standard compositions are available by name as built-in defaults, or the user may define composition and melting temperatures through input.



(a) Cavity Geometry



(b) Cavity Contents and Boundary Conditions

Figure 3.1 Cavity System Components

The modeling assumes that all oxidic species in the debris are mutually miscible, as are all metallic species, but that oxides are not miscible with metals. If the densities of the phases are different, the debris will tend to separate into distinct oxidic and metallic phases under the influence of gravity, but this stratification may be partially or completely overcome by the stirring effect of gas bubbles. If the density difference is sufficiently small and the gas bubbles sufficiently large, droplets of a lower (denser) layer can be entrained across the interface to mix with a lighter layer above it.

The debris pool is modeled as a number of layers filling some part of the concrete cavity. Pure-phase and mixed-phase layers may be included, and the ordering of the layers is assumed to be determined by their densities, with the densest on the bottom and the lightest on top. Many configurations are possible, as discussed in Section 3.2. Layer volumes, including the swelling effects of gas bubbles, determine the elevations of layer interfaces and of the debris surface.

### **3.2 Debris Layering and Mixing**

Five possible types of debris layers are considered in CORCON; each has a conventional three-letter designation in the associated documentation. In order of increasing density they are:

- LOX: Pure oxide, less dense than the metallic phase;
- LMX: Mixed phases, less dense than the metallic phase;
- MET: Pure metal;
- HMX: Mixed phases, more dense than the metallic phase; and
- HOX: Pure oxide, more dense than the metallic phase.

If only oxides are present, the debris is called LOX by convention. The possibility of creating mixed-phase layers was introduced as part of the enhanced modeling in CORCON-Mod3. The major assumptions concerning these mixed layers is very specific:

The LMX layer is formed by entrainment of metal from MET or HMX into a previously existing LOX layer, and consists of a suspension of discrete droplets of metal in a less-dense continuous oxidic phase. The mixing is assumed to be complete so that the LOX layer is converted to an LMX layer in the process; LMX and LOX cannot exist simultaneously. The entrainment competes with settling of the denser metal droplets from LMX back into the lower layer (or to form a new MET layer if there is no lower metal-containing layer present).

The HMX layer is formed by entrainment of oxides from HOX into a previously existing MET layer, and consists of a suspension of discrete droplets of oxide in a less-dense continuous metallic phase. The mixing is assumed to be complete so that the MET layer is converted to an HMX layer in the process; HMX and MET cannot exist simultaneously. The entrainment competes with settling of the denser

oxide droplets from HMX back into HOX (or to form a new HOX layer if there is none present).

Under these assumptions, there are 15 possible configurations of the debris. These can be summarized as follows:

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
LOX				X	X	X					X				X
LMX							X	X	X	X		X	X		
MET	X			X			X				X	X		X	
HMX		X	X		X	X			X	X					
HOX	X	X		X	X		X	X	X						

where "X" denotes the presence of the layer.

Three options are available for the treatment of layering and mixing of debris in CORCON. They are (1) enforcement of complete mixing, (2) enforcement of complete stratification, and (3) mechanistic modeling of the entrainment and separation processes. The first of these (complete mixing) is the default in the CAV package in MELCOR, but the user may specify any of the options by input of MIXING on the CAVnnak record.

### 3.2.1 Enforced Mixing

This is the simplest of the options, with the debris always considered to form a single layer. If both metals and oxides are present, the layer will be HMX or LMX (configuration 3 or 13), depending on the relative densities of the phases. If there is only a single phase, it will be either MET or LOX (configuration 14 or 15). As noted previously, this is the default treatment in MELCOR.

### 3.2.2 Enforced Stratification

This was the only option available in CORCON in versions prior to Mod3, in which the possible creation of heterogeneous mixtures of metals and oxides was not considered. It was therefore the only option available in versions of MELCOR prior to 1.8.3.

When this option is specified, the possibility of two oxidic layers, physically separated by a metallic layer, is allowed for. If the initial oxide phase is sufficiently rich in UO<sub>2</sub> (fuel) to be more dense than the initial metallic phase, it is assumed to form an oxidic layer beneath the one containing the metals. An oxide slag, rich in concrete and steel oxides and less dense than the metals will then accumulate on top of the metal layer. Thus, the most

general structure of the debris pool is a light oxide layer (LOX), over a metallic layer (MET), over a heavy oxide layer (HOX).

This three-layer configuration (configuration 4) can persist until dilution by less dense concrete oxides renders the HOX layer less dense than the MET layer. The configuration is then (instantaneously) converted to one containing only MET and LOX (configuration 11), with the latter layer combining the previous contents of HOX and LOX. Addition of UO<sub>2</sub>-rich debris to a debris pool in the LOX-over-MET configuration can result in an oxide mixture that is denser than the contents of MET. When this occurs, the LOX is eliminated and the configuration is (instantaneously) converted to one of MET over HOX (configuration 1). These changes in configuration are effected by checking the relative densities of adjacent layers at every step of the calculation, and relocating and/or combining the layers as appropriate.

### 3.2.3 Mechanistic Mixing

The most general option uses mechanistic models for entrainment and separation developed by Green [6, 7, 8] to predict the occurrence and extent of mixing. One consequence of this modeling is to eliminate the instantaneous change in debris configuration (often referred to as "layer flip") resulting from an insignificant change in the relative densities of the debris phases. Instead, the phases will become increasingly strongly mixed whenever their densities approach equality (unless there is no gas flow to drive the mixing).

The entrainment model assumes that bubbles passing through the interface between two layers may carry material from the lower layer into the upper one if they are large enough. The critical diameter depends on density ratios and on the surface tension of the liquid-liquid interface; above the threshold, a correlation is used to determine the volume of condensed-phase material entrained by each gas bubble. The separation model is based on the terminal velocity of falling droplets of a size corresponding to the critical Weber number for the onset of droplet oscillations.

Competition between these processes defines the net rate of mixing or separation at the various layer interfaces. The model considers entrainment of oxides from HOX into HMX or LMX, or into MET to form HMX, and of metal from MET or HMX into LMX or into LOX to form LMX. It also considers the possibility that a mixed layer is unstable and will separate to produce a new HOX layer below HMX or a new MET layer below LMX.

After release of the initial version of CORCON-Mod3 [2], the numerical implementation of the models into MELCOR was modified to provide numerical stability with reasonable timesteps. The entrainment rate depends primarily on the gas flux; therefore, over a finite timestep,

$$\dot{m}_e(t) \approx \dot{m}_e(0) \quad (3.1)$$

However, the separation rate is proportional to the mass of the discontinuous phase in the mixed layer, and has the form

$$\dot{m}_s(t) = \frac{M_D(t) v_{\text{settle}}}{L_M} \quad (3.2)$$

where  $v_{\text{settle}}$  is the settling velocity,  $M_D$  is the mass of droplets suspended in the mixed layer, and  $L_M$  is thickness of that layer.

The mass of suspended droplets therefore satisfies

$$\frac{dM_D}{dt} = \dot{m}_e(t) - \dot{m}_s(t) \approx \dot{m}_e(0) - \frac{M_D(t)}{\tau_s} \quad (3.3)$$

where

$$\tau_s \equiv \frac{L_M}{v_{\text{settle}}} \quad (3.4)$$

is the time constant for separation. Equation (3.3) has the analytic solution.

$$M_D(t) = M_D(0) + [\dot{m}_e(0)\tau_s - M_D(0)](1 - e^{-t/\tau_s}) \quad (3.5)$$

Equation (3.5) expresses the fact that entrainment and separation approach a balance where the mass of suspended droplets  $M_D^{ss}$  is

$$M_D^{ss} = \dot{m}_e \tau_s \quad (3.6)$$

with a characteristic time  $\tau_s$ . Independent treatment of the competing processes will be numerically unstable unless the timestep,  $\Delta t$ , is less than  $\tau_s$ , and the results will be dependent on timestep unless  $\Delta t$  is *much* less than  $\tau_s$ . Because the time constant may be relatively short compared to the rates at which conditions are changing, the revised

version of CORCON-Mod3 applies the analytic solution given by Equation (3.5) over a timestep. This requires moving a net mass

$$\Delta M_e^{net} = (\dot{m}_e^0 \tau_s - M_D^0) (1 - e^{-\Delta t / \tau_s}) \quad (3.7)$$

from the lower layer to the upper layer during the timestep, where superscript 0 denotes evaluation at the start of the step. If the net move is positive, it must be limited to the contents of the lower layer. If it is negative, it cannot—by its very form—exceed the mass of droplets initially suspended in the upper layer. This change in numerical implementation has eliminated almost all of the instabilities observed in layer mixing in the initially released version of CORCON-Mod3.

### 3.3 Energy Generation and Heat Transfer

The fuel/concrete interaction is driven primarily by decay heat power generated within the debris pool, with heat from oxidation reactions also contributing. In stand-alone CORCON, the decay heating is calculated by an internal model based on an initial fission product inventory and fits to the decay powers for each of the 27 elements in CORCON. In MELCOR, this heating is calculated by the RN and DCH packages; the model is conceptually very similar to that in CORCON (see the RadioNuclide (RN) and Decay Heat (DCH) Package Reference Manuals and Reference 1), but the CAV database contains no information on the location—or relocation—of the fission products. (The exact model used in stand-alone CORCON is therefore not available, even as an option, in MELCOR.) Heat sources based on control functions and/or tabular functions are also permitted, primarily for simulation of experiments.

For the calculation of energy conservation, each debris layer is treated as a lumped mass with a single (average) temperature. The heat flux between the interior of each layer and each of its interfaces (with another layer, with concrete, or with the pool or the atmosphere in the bounding control volume) is treated separately. Continuity of the heat flux determines the temperature of each interface.

The possible heat transfer regimes within each debris layer are conduction and natural convection, based on conventional correlations, and bubble-enhanced convection based on Kutateladze [9] and surface renewal [10] models. The correlations are implemented in such a way that they reproduce correlations for convective heat transfer in internally heated fluid layers (in the absence of gas flows) developed by Kulacki and co-workers [11, 12, 13] with a maximum error of 30 percent and an average error closer to 10 percent. An enhancement factor developed by Farmer [14] is applied at the top surface of the debris (adjacent to the coolant or the atmosphere) to account for the greater surface area of the unstable surface.

The modeling includes the possibility that the interior of a layer may be fluid, with heat transfer by convection, while one or more of its axial and radial surfaces is covered by a solid crust, with heat transfer by conduction [15]. In all cases, only one-dimensional effects are considered, and the situation is assumed to be quasi-steady.

Losses from the surface are calculated, based either on radiation and convection in the absence of overlying water or on a complete pool boiling curve in its presence. The representation of the boiling curve is the one used in CORCON [1], and includes convection, nucleate boiling, transition boiling, and film boiling regimes. In the film boiling regime, the effects of coolant subcooling and of gas barbotage (injection of noncondensable gas at the coolant interface), both of which can greatly increase both the film boiling heat flux and the temperature at which the film collapses (the Leidenfrost point), are also included.

The concrete surface is treated using a quasi-steady ablation model. If concrete is ablating, it presents a constant temperature boundary condition defined by the ablation temperature,  $T_a$ . This temperature is obtained either from internal data or user input. Under quasi-steady conditions, changes in the sensible heat content of the preheated region in advance of the ablation front may be neglected. (As mentioned in Section 2, the thermal diffusivity of concrete is extremely small. The *total* heat content of this region is therefore small, and is neglected.) The rate of ablation (in  $\text{kg/m}^2\text{-s}$ ) is then proportional to the heat flux ( $\text{W/m}^2$ ) from the debris to the concrete surface. Their constant of proportionality is simply the inverse of the heat of ablation  $h_a$ .

If the heat flux to a concrete surface at an assumed temperature of  $T_a$  would be negative, no ablation can be taking place, and heat transfer can affect only the thermal boundary layer in the concrete. Under these conditions, change in the heat content of this boundary layer is neglected and the concrete surface is treated as an adiabatic boundary. Further decomposition of concrete in advance of ablation is also neglected.

An additional thermal resistance is included between the debris and the concrete. CORCON-Mod3 allows this resistance to be calculated using either a gas film or a slag film model. In each case, separate models are provided for the bottom and side surfaces of the debris.

The gas film models are based on the assumption of a gas film between the debris and the concrete. An analog of Taylor-instability-bubbling film boiling is used on nearly horizontal surfaces [16], and an analog of attached-flow film boiling is used on strongly inclined surfaces. A transition from bubbling to flow is made over a range of inclination angles. Details of the model are presented in Reference 1.

A detailed slag film model was developed by Bradley [17], based on a picture of transient growth and removal. He found that when the resulting thermal resistance of the slag film was combined with the resistance within the debris layer, the net heat transfer coefficient between the interior of the debris and the concrete surface could be adequately

represented as a constant multiple (0.29) of the latter coefficient over a wide range of conditions. The heat transfer coefficient for the slag film model is therefore calculated in CORCON as 0.41 times the heat transfer coefficient between the interior of the debris and its surface, for either the bottom and side surfaces of the debris, so that the net heat transfer coefficient is  $1.0 \cdot 0.41 / (1.0 + 0.41) = 0.29$  times the internal heat transfer coefficient.

The model to be used may be selected independently for the bottom and side surfaces of the debris. The default in MELCOR 1.8.3 and later versions is to use the gas film model in both places, consistent with previous versions of MELCOR. The user may specify which model is to be used on the bottom and/or side surfaces by input of GFILMBOTT or GFILMSIDE on the CAVnnak record, as described in the CAV Package Users' Guide. (There is no default for the choice of models in stand-alone CORCON-Mod3, and the Manual [1] provides no recommendation.)

### **3.4 Concrete Ablation and Cavity Shape Change**

In steady-state ablation, the incident heat flux and the ablation rate are directly proportional; the ratio is simply the volumetric ablation enthalpy. Therefore, the heat flux to the concrete at each body point in the cavity profile is used to calculate the local ablation rate. A new position of the body point is then calculated, displaced along the local normal to the surface. To maintain calculational stability, the cavity profile is then rezoned, and the body points are interpolated back onto a series of guiding lines called rays, as illustrated in Figure 3.2. The effect of the rezone is that the body points must follow the rays, and their spacing along the cavity profile is constrained. As shown in the figure, all but one of the rays pass through a user-defined origin. The final ray lies parallel to the axis, through the outermost point on the flat bottom of the cavity, and serves to ensure that this flat bottom remains flat. The scheme evolved from the CASCET model [18] written by ACUREX/Aerotherm Corporation under contract to Sandia.

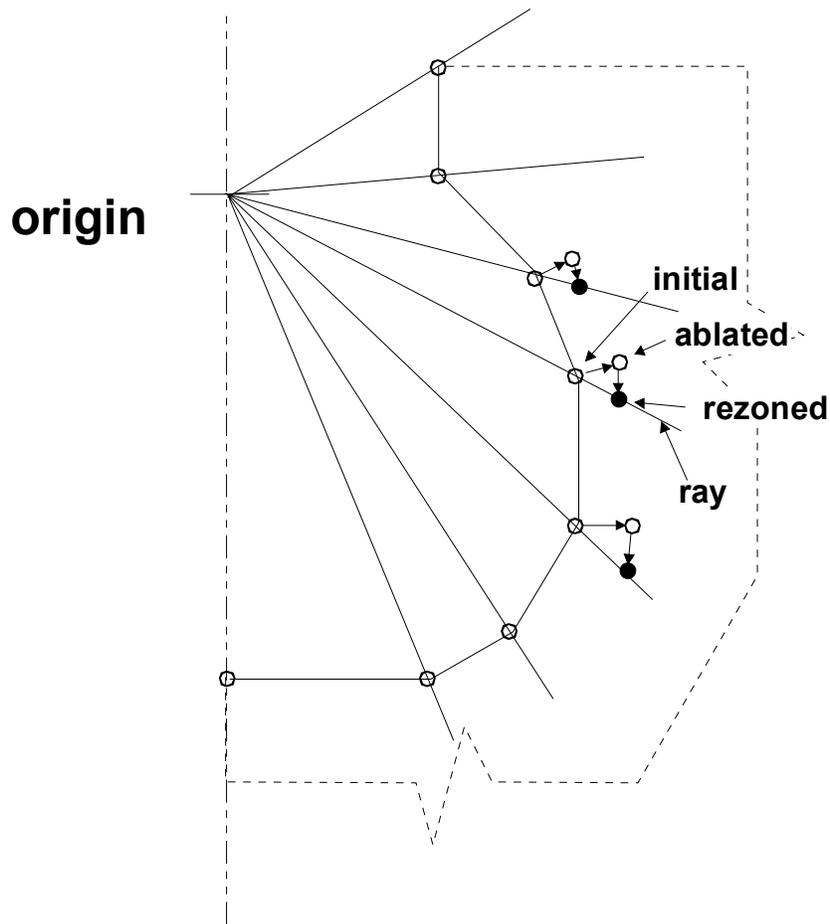


Figure 3.2 Position and Motion of Body Points

### 3.5 Chemistry

The chemistry considered in the Cavity package of MELCOR involves interactions between concrete decomposition products and metallic species in the debris pool. Equilibrium chemistry is assumed, without consideration of rate limiting effects. The calculational method is very general and is based on minimization of the total Gibbs function for a metallic phase, a gaseous phase, and an oxidic phase. Each of the three phases is treated as an ideal solution; that is, the entropy of mixing is considered, but any heat-of-solution effects are ignored.

Two separate reactions are considered. The first involves reactions in the interior of the debris. For a pure metal layer, it is modeled as mutual equilibrium among the metal layer and the gas bubbles and concrete decomposition oxides passing through it. For a mixed-phase layer, the oxidic constituents of the layer are included as reactants. The primary effect is the oxidation of metals by the  $H_2O$  and  $CO_2$  in the bubbles. However, if the metallic phase contains significant amounts of Zr, it can also reduce the concrete oxides

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to produce metallic Al, Ca, and Si. The user may specify that these reactions be ignored (as in older versions of CORCON) through input of CTOXYREA on record CAVnnak; in this case, only the products of metal oxidation are included in the oxide phase.

The second reaction involves mutual equilibrium among the metal layer, the gas film at its radial boundary, and the products of metal oxidation. Concrete decomposition (and other) oxides are not included in this reaction.

The gaseous reactants are H<sub>2</sub>O and CO<sub>2</sub>, and the principal gaseous products are H<sub>2</sub> and CO. The full equilibrium calculation in CORCON predicts the formation of small amounts of additional gaseous species including hydrocarbons and various dissociation products such as atomic hydrogen. Most, if not all, of these species are predicted to occur in quantities insufficient to warrant their inclusion in the control volume inventories. To ignore them would violate mass conservation, and there is insufficient information to unambiguously convert them to "equivalent" amounts of significant species. The problem can be avoided by imposing constraints in minimization of the Gibbs function to eliminate consideration of any gaseous species other than H<sub>2</sub>O, CO<sub>2</sub>, H<sub>2</sub>, and CO. This option was added to stand-alone CORCON-Mod 3 after its initial release, and is used in MELCOR. The results conserve mass and represent a restricted equilibrium state consistent with the modeling of atmosphere chemistry in MELCOR. We believe this to be a reasonable approach. If it were desired to include additional gases such as methane, only a trivial change to coding would be required. This is because the Gibbs function to be minimized has not been changed, but only the domain over which it is minimized.

The equilibrium calculation sometimes predicts the "coking" reaction in which CO<sub>2</sub> is fully reduced to condensed carbon (rather than simply to CO), primarily in the presence of metallic Zr. Because simulant experiments have not provided overwhelming evidence either for or against the occurrence of coking, the user is permitted to specify whether this reaction will be permitted in CORCON. The default in MELCOR is to suppress the production of condensed carbon, but the user may enable this production by input of the COKE parameter on the CAVnnak record.

In stand-alone CORCON, the chemistry includes an extremely simplified consideration of fission products; in MELCOR, this calculation is entirely replaced by the VANESA model [4] in the RN package.

### **3.6 Mass Transfer and Associated Heat Effects**

The processes involved include the injection of concrete decomposition products (condensed and gaseous) into the debris pool, the addition of core and structural materials from other packages through the use of TP, the addition of debris from rupture or overflow of another cavity, and the production of condensed-phase materials from chemical reactions. Also involved is the transport of all these materials to their proper locations, whether within a debris layer in CAV or in a CVH volume. These processes modify both

the mass inventories and the energy contents of the various debris layers and determine the mass source delivered to CVH and its associated enthalpy.

The masses and enthalpies of all debris layers are updated for mass transfer and associated heat transfer in two passes. These passes follow the paths of gaseous and condensed-phase concrete decomposition products, and of the products of chemical reactions involving these materials. The updating procedure is designed to account for successive interactions of transported materials, from the location where they are born to the location where they reside at the conclusion of the advancement procedure.

The first pass, upward through the debris pool, follows the rising gases and rising condensed-phase materials from concrete decomposition or melt/gas reactions. (The direction of motion of condensed-phase materials is determined by its density relative to the density of the local layer material.) The materials are thermally equilibrated with any layers they pass through, and their mass and energy are ultimately added to the layer where they end up (condensed phases) or to the associated CVH volume (gases). For condensed-phase materials, this final layer is assumed to be the first layer encountered that already contains that phase: HMX, MET, or LMX for metals, and any layer *but* MET for oxides. A new LOX layer may be formed to accommodate rising oxides from concrete ablation or metal oxidation or none already exists. Similarly, a new MET layer may be created to accommodate steel from melting reinforcing bars in concrete if the pool contains only a dense oxide layer.

Melt/gas chemical reactions are evaluated during this upward pass, following rising bubbles and flowing films. The composition of the layer involved is modified to reflect the effects of the reaction and, if the reaction takes place in the pure metal layer (MET), the condensed phase oxidic products are added to the rising inventory. The gas composition is modified appropriately, and the heat of reaction is assumed to remain with the layer in which the reactions occurs.

The second pass, downward through the debris pool, is similar; it follows any material entering from above (from another cavity or from a TP), and any sinking reaction and/or concrete ablation products. If the mechanistic mixing model is used, mixing calculations are done during the downward pass. This differs from the initially released version of CORCON-Mod3 [2]. The change was made because separation of a mixed layer can create a new pure-phase layer *below* it, and the revised order of calculations greatly simplifies the logic in treating this possibility.

### 3.7 Debris Spreading

In general, CORCON assumes that debris will spread uniformly and instantaneously across the full width of any cavity into which it is deposited. CORCON-Mod3 added an optional parametric capability to simulate the finite rate of debris spreading by prescribing a maximum radius of the axially symmetric debris pool as a function of time. This can be

used to confine the debris as a slowly spreading or non-spreading glob on the floor for some period of time and/or to delay its contact with the side walls of the cavity for as long as may be desired. One effect will be to reduce the surface area of the debris, thus reducing the rate at which it can lose heat. This modeling may affect the timing of the debris-concrete interaction in cases where the initial debris is largely solidified, and is incapable of ablating concrete at a significant rate until it has become more fluid as a result of continued heating by internal decay heat.

In stand-alone CORCON, the maximum radius must be specified as a function of time by an input table. In MELCOR, it may be specified by a tabular function, a control function, or a channel in an external data file. In most MELCOR calculations, debris will not appear in the cavity until after the reactor vessel fails, and the time of this event will not be known in advance. The control function option allows the radius to be defined as a function of time *relative to debris deposition*. It could also be used to consider the debris temperature (as an indicator of its viscosity) in estimating the spreading rate.

In the initially released version of CORCON-Mod3, the radial surface of spreading debris was subjected to the same thermal boundary condition as the top surface. A subsequent revision allows optional treatment of this boundary as adiabatic. This capability is available in MELCOR.

### 3.8 Energy Conservation

CORCON uses a formulation for the energy equation for debris in the cavity in which temperature-driven heat transfers between layers are treated semi-implicitly, as described in Reference 1. Numerical difficulties associated with addition of new debris were observed during incorporation into MELCOR. The implementation of the equation was substantially modified to improve stability by including modifications made to previous versions of CORCON in the CAV package of MELCOR 1.8.2. The revised numerical treatment is now included in the stand-alone code as well as in MELCOR.

### 3.9 Material Properties

The material properties in the CAV package are those of the stand-alone CORCON code. They include internally consistent specific heats, enthalpies, and chemical potentials for a large number of condensed and gaseous species, based on fits to JANAF [19] and other data. All enthalpies are based on the JANAF thermochemical reference point. All heats of reaction are therefore implicitly contained in the enthalpy data. Also included are data on thermal expansivity and density, thermal conductivity, viscosity, and surface tension.

The list of materials for which properties are defined is contained in Appendix A. These data are independent of the MELCOR data contained in the Water (H<sub>2</sub>O), NonCondensable Gas (NCG), and Material Properties (MP) packages. They are retained both for

consistency with the stand-alone CORCON code and to facilitate incorporating future upgrades to CORCON modeling into MELCOR. Appropriate adjustments to enthalpies are made whenever materials are passed into or out of the Cavity package.

Additional models are included for evaluating the properties of mixtures. Details of the material properties models, and further references, are contained in Reference 1. Most are quite conventional, but two deserve further discussion in this Reference Manual.

In determining the enthalpy of a mixture as a function of temperature, a submodel is used to determine its melting range as defined by solidus and liquidus temperatures. Below the solidus temperature of the mixture, properties for the solid phase of each species—extrapolated, if necessary—are used. Similarly, liquid phase properties (possibly extrapolated) are used above the liquidus temperature. Between solidus and liquidus, the enthalpy is interpolated as a linear function of temperature (corresponding to a constant specific heat).

The melting range for the metallic phase is determined from a fit to the ternary phase diagram for Cr-Fe-Ni; other elements (Zr, C) are simply ignored. If the metal phase contains no Cr, Fe, or Ni, however, the melting point of Zr will be used. The melt range for an oxidic phase is determined by reference to a pseudo-binary phase diagram based on an ideal solution model for the liquid and solid phases. One component is high melting and is assumed to consist of fuel ( $\text{UO}_2$  and  $\text{ZrO}_2$ ); the second component is low melting and includes everything else. The corresponding melting temperatures and effective latent heats are taken from internal data for fuel for the first component and from the properties of the concrete oxides for the second.

Also modeled is the effect of  $\text{SiO}_2$  content on the viscosity of oxidic mixtures, based on a modification of a correlation derived by Shaw [20]. The original correlation was fit to a database containing geologic data for materials with relatively high silica contents; no consideration was given to application of the correlation outside of the range of compositions included in the original database. As implemented in CORCON and in MELCOR, the original correlation has been modified to avoid nonphysical extrapolation characteristics. It is coupled to a conventional Kendall-Monroe [21] mixture model in such a way that the viscosity is a continuous function of composition over an unrestricted range of compositions. Details are given in Reference 22.

#### **4. Comparison to Stand-Alone CORCON**

The Cavity (CAV) package in MELCOR consists primarily of the CORCON-Mod3 code [1]. The calculational routines are identical to those in the stand-alone code, but input, output, and interfaces to boundary conditions are different. In addition, the MELCOR implementation includes several sensitivity coefficients to allow user control of submodels in CORCON. The sensitivity coefficients currently available are:

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1. an additive modification to the concrete ablation enthalpy, and
2. coefficients in many heat transfer relations.

In future versions, we expect to expand this list to allow access to more of the so-called “user flexibility” options available in CORCON-Mod3.

Additional similarities and differences with respect to CORCON-Mod 3 are summarized in Table 4.1.

Table 4.1 Comparison of Stand-Alone CORCON-Mod3 [1] and MELCOR Cavity Package

Feature	CORCON-Mod3	MELCOR
Concrete Cavity, Layered Debris, Debris/Concrete Heat Transfer, Concrete Ablation	Treatment identical	
Ablation Delay	Not permitted	Optional control function
Overlying Water	Simple equilibration of rising gases	Part of CVH SPARC bubble model
Atmosphere and Surroundings	User-input tabular boundary conditions	Boundary conditions from CVH Package
Debris/Water or Debris/Atmosphere Interface	Models and correlations identical; numerics of solution modified for MELCOR	
Fission Product (F.P.) Inventories	Six “pseudo-species” (coarse grouping) included in CORCON; separate detailed inventory for VANESA	Treated in detail by RN package (not part of CAV package inventory)
Internal Heating	Internal model based on F.P. inventories or input table	From DCH package, based on fission product inventories or input table
Fission Product Release	Models and correlations identical; numerics of solution modified by location of model in RN package in MELCOR	

Table 4.1 Comparison of Stand-Alone CORCON-Mod3 [1] and MELCOR Cavity Package

Feature	CORCON-Mod3	MELCOR
Debris/Gas Chemistry	General equilibrium gases, metals, oxides	Same model, minor gas species suppressed
Cavity Rupture/ Debris Overflow	Not modeled	Mechanistic melt-through or "triggered" failure; overflow to lower cavity
Debris Addition	User-input table	Through TP package, from other MELCOR package or table input, or from other cavity overflow or rupture
Debris Spreading	Parametric model; requires user-input table vs. time	Same model, but allows calculation using control functions
Associated F.P. Addition	Based on added UO <sub>2</sub> , or user-input table	Calculated by RN for package providing debris source, or table input
User Control of Modeling	Provided through "user flexibility" options [2]	Provided by user input and sensitivity coefficients; not all "user flexibility" options are enabled
Restart/Fallback Capability	Not available	Provided as part of MELCOR structure
User Input	Fixed format	MELCOR free-field format
Printed Output	Controlled by CORCON input	Essentially identical; controlled by MELCOR input
Plotted Output	Latest version allows use of HISPLTM	Plots available in normal MELCOR manner

The differences between the MELCOR Cavity package and stand-alone CORCON-Mod3 listed in Table 4.1 fall into three distinct groups:

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### 1. Coupling of Phenomena

These differences include the use of calculated boundary conditions such as temperature, pressure, and debris addition rates rather than user-supplied tabular data which must be generated from some independent source, and the provision to allow debris to be relocated between two or more locations when cavity boundaries fail. CAV allows the use of tabular boundary conditions by defining time-specified volumes in CVH and/or tabular debris addition rates through TP and EDF. Both CORCON-Mod3 and MELCOR can calculate internal decay heating based on fission product inventories, with these inventories based on fission product release rates calculated using VANESA. In MELCOR, the decay heat is based directly on the detailed inventories calculated by VANESA; in CORCON-Mod3, these inventories must be approximately mapped back into the coarse group inventories used by the CORCON decay heat model.

### 2. User Control

MELCOR is intended for use as a PRA code while versions of CORCON prior to Mod3 were developed as best-estimate codes. Therefore, MELCOR 1.8.2 allowed more user control of modeling options than did the then-existing versions of CORCON. User flexibility options were made available in CORCON-Mod3. Although there was some overlap in capabilities, several of the sensitivity coefficients in the MELCOR 1.8.2 CAV package have not been reconnected to CORCON-Mod3, and many of the user flexibility options in that code have not yet been made accessible from MELCOR input. This situation will be corrected in later versions of MELCOR.

### 3. User Interface, User Convenience

These differences include revised input formats, restart and fallback capabilities, and plot capabilities, which have no effect on modeling of physical phenomena.

Although the CAV package in MELCOR and the stand-alone CORCON-Mod3 code contain identical versions of all subroutines incorporating phenomenological models and materials properties, they should be viewed as distinct entities because of the differences in treatment of interfaces and calculation of boundary conditions. However, because the basic modeling is identical, it is possible to run equivalent calculations with the two codes under appropriate choices of options and restrictions on boundary conditions.

**APPENDIX A: Species List for CORCON in MELCOR CAV Package**

The following lists the species considered by CORCON and available for use in MELCOR, either as initial contents in the melt or as constituents of concrete:

OXIDES	METALS
SiO <sub>2</sub>	Fe
TiO <sub>2</sub>	Cr
FeO	Ni
MnO	Zr
MgO	Mn
CaO	C(C)
SrO	Na
BaO	Al
Li <sub>2</sub> O	U
Na <sub>2</sub> O	Si
K <sub>2</sub> O	UAl <sub>3</sub>
Fe <sub>2</sub> O <sub>3</sub>	UAl <sub>2</sub>
Al <sub>2</sub> SO <sub>3</sub>	Ca
UO <sub>2</sub>	
ZrO <sub>2</sub>	
Cr <sub>2</sub> O <sub>3</sub>	
NiO	
Fe <sub>3</sub> O <sub>4</sub>	
Mn <sub>3</sub> O <sub>4</sub>	
PuO <sub>2</sub>	
UO <sub>3</sub>	
U <sub>3</sub> O <sub>8</sub>	

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The observant reader may note that several additional species are included in the corresponding list, Table 2.1, in [1]. These include the aluminates, fission products, and element "X", which are (or were) used in internal models in stand-alone versions of CORCON and are not relevant to the implementation in MELCOR.

There are five additional species which may be used in specification of concrete compositions:

CONCRETE CONSTITUENTS
CO <sub>2</sub>
H <sub>2</sub> O <sub>CHEM</sub> (chemically bound water)
H <sub>2</sub> O <sub>EVAP</sub> (evaporative water)
CaCO <sub>3</sub>
Ca(OH) <sub>2</sub>

These are used only in specification of the concrete composition; in particular, CaCO<sub>3</sub> and Ca(OH)<sub>2</sub> are decomposed during initialization into CaO plus CO<sub>2</sub> and into CaO plus H<sub>2</sub>O<sub>CHEM</sub> respectively. The difference between H<sub>2</sub>O<sub>CHEM</sub> and H<sub>2</sub>O<sub>EVAP</sub> is the binding energy which must be overcome to release the chemically-bound water from the concrete.

The list of gases in Table 2.1 of Reference 1 is not relevant to MELCOR input, as the composition of the control volume above the debris pool is determined by the CVH package. In addition, production of all trace gaseous species has been suppressed in the chemical reaction routines so that the only gases considered by CORCON in MELCOR are H<sub>2</sub>, H<sub>2</sub>O, CO, and CO<sub>2</sub>.

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