

Fuel Dispersal Interactions (FDI) Package Reference Manual

This document describes in detail the various models incorporated in the Fuel Dispersal Interactions (FDI) package in MELCOR. New in MELCOR 1.8.5 is a FDI sensitivity coefficient used to control the numerical order in which oxygen or steam is used to oxidize DCH metals. This parameter affects the amount of hydrogen that results from burning DCH materials in steam/oxygen atmospheres.

Details on input to the FDI Package can be found in the FDI Users' Guide.

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1. Introduction

The Fuel Dispersal Interactions (FDI) Package in MELCOR calculates the behavior of debris in containment unless or until it is deposited in a cavity modeled by the MELCOR Cavity (CAV) package. Debris enters the package in basically two ways:

- (1) if the Core (COR) package is active, debris enters the FDI package via the Transfer Process (TP) package after the failure of the reactor vessel, or
- (2) in the stand-alone high-pressure melt ejection (HPME) model, debris enters the FDI package through a user interface, which may be either tabular function input or input from an external data file (EDF) via the TP package.

Two types of phenomena are treated in the FDI package:

- (1) low-pressure molten fuel ejection (LPME) from the reactor vessel and
- (2) high-pressure molten fuel ejection from the reactor vessel (direct containment heating). There is currently no plan to model steam explosions within or outside the FDI package in MELCOR.

There is no fission product modeling associated with the FDI package, with one minor exception. In particular, there is no release of fission products from fuel debris modeled in the FDI package. In general, the only function performed by the FDI package with respect to radionuclide modeling is inventory transport. That is, if the FDI package transports fuel debris from one location to another, it calls the RadioNuclide (RN) package and instructs it to transport the fission products associated with the fuel debris in exactly the same way.

The one exception to the foregoing concerns decay heat associated with debris deposited on heat structures by the HPME model. The decay heat associated with deposited debris is treated in essentially the same way as the decay heat associated with fission product aerosols and vapors that settle/deposit on heat structures in the RN package modeling. The RadioNuclide Package Reference Manual discusses this modeling in detail. The decay heat associated with airborne debris in the HPME model and all debris during its short residence in the low-pressure melt ejection (LPME) model is ignored; the energy error associated with its omission should be quite small.

2. Detailed Models

2.1 General Information

The FDI package becomes active whenever debris material enters the package. Debris material typically enters the FDI package in one of three ways. In a reactor plant accident calculation, debris enters the FDI package via the TP package interface from the core (COR) package after failure of the reactor pressure vessel has been calculated. In a stand-alone direct containment heating (DCH) calculation, debris material is sourced into the FDI package either directly from tabular function user input or via the TP package interface to a user-provided external data file (EDF) containing the source. The Transfer Process Package Users' Guide and External Data File Package Users' Guide, along with the FDI Package Users' Guide, provide example input to illustrate the interfaces.

After the introduction of debris material, the FDI package classifies the ejection event as either a low- or a high-pressure melt ejection event on the basis of the ejection velocity passed through the TP package or a flag set by the user for stand-alone DCH calculations.

2.2 Low-Pressure Melt Ejection (LPME) Modeling

The heart of the LPME model that has been incorporated into MELCOR was developed by Corradini et al. [1] at the University of Wisconsin. In this model, heat is transferred from the molten debris to the water pool (if present in the associated control volume) as it breaks up and falls to the cavity floor. The heat transfer is normally dominated by radiation, but a lower bound determined by conduction through a vapor film (the Bromley model for film boiling) is also considered. All of the energy transfer from the molten debris is used to boil the pool water (i.e., no sensible heating is considered so, e.g., a subcooled pool will remain subcooled and its temperature will not change). The LPME model does not consider oxidation of the metallic elements in the ejected debris. If no pool is present, material passes through FDI without any energy removal. At the cavity floor, the material is normally passed to the CAV package (CORCON) by way of the TP interface.

The first step in the LPME calculational sequence involves retrieving the variables describing the debris state entering the model at the beginning of each calculational cycle (timestep). The debris variables are passed from the COR package to the TP package prior to execution of the FDI package, so the values of the variables are current for the timestep. The variables retrieved from the TP package by the FDI package include the mass, composition and temperature of the debris ejected from the vessel during the timestep and the velocity and diameter of the ejection stream (see COR reference manual for a description of the calculation of these variables).

The second step in the LPME sequence is to determine the axial position of the head and tail of the ejected debris with respect to the FDI calculational volume. The user specifies

z_{TOP} and z_{BOT} , the elevation of the top and bottom of the calculational volume, respectively, (which typically are equal to the elevation of the bottom of the reactor vessel and the bottom of the reactor cavity). Then the positions of the head and tail of the ejected debris and its length are given by

$$z_{HEAD} = z_{TOP} - U_f \Delta t \quad (2.1)$$

$$z_{TAIL} = z_{HEAD} + m_f / (\pi D_{f0}^2 \rho_f / 4) \quad (2.2)$$

$$z_{LEN} = z_{TAIL} - z_{HEAD} \quad (2.3)$$

where U_f , m_f , D_{f0} and ρ_f are the velocity, mass, initial diameter (determined by the COR package and equal to the diameter of reactor vessel breach, which may increase if hole ablation occurs) and density of the ejection stream, respectively. Any debris below elevation z_{BOT} accumulates on the cavity floor, and its mass is designated m_{FLR} and given by

$$m_{FLR} = m_f \text{MAX}\{0, \text{MIN}[1, (z_{BOT} - z_{HEAD}) / z_{LEN}]\} \quad (2.4)$$

The portion of m_f that does not reach the floor remains in the FDI calculational volume until the next timestep and is designated m_{CAV} . If there was already mass in the volume (m_{CAV0} from the previous timestep), then it is added to m_{FLR} and deposited on the cavity floor on this timestep. If m_f is zero (i.e., if mass ejection from the vessel has ceased), then any pre-existing m_{CAV0} is transferred to m_{FLR} . If m_f is greater than zero, but z_{HEAD} is greater than z_{BOT} , then only pre-existing m_{CAV0} is deposited on the floor and given by

$$m_{FLR} = \text{MIN}(m_f, m_{CAV0}) \quad (2.5)$$

$$m_{CAV} = m_f + m_{CAV0} - m_{FLR} \quad (2.6)$$

In effect, this means that if mass is being ejected from the vessel but the timestep is too short for newly ejected debris to reach the cavity floor, then pre-existing debris that has not reached the cavity floor is deposited on the cavity floor at a rate equal to the vessel ejection rate, and the newly ejected debris takes the place of the deposited debris. However, as soon as vessel ejection ceases, then all remaining debris that has not reached the cavity floor is immediately deposited in the cavity floor in a single timestep.

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After the mass of debris reaching the floor during the current timestep has been determined, heat transfer to water in the cavity is evaluated. Although the heat transfer occurs during the passage of the debris through the cavity pool, the actual heat transfer associated with a given packet of debris is not transferred to the pool until that packet is deposited on the cavity floor. Debris which does not reach the floor during the current timestep does not participate in heat transfer to the water until a later timestep.

The rate of heat transfer from the debris to the water is determined primarily by the interfacial surface area, which is a function of the debris particle size. The particle size for molten debris particles descending through the cavity pool is given by a modified theoretical correlation for droplet breakup under hydrodynamic force. The original correlation as formulated by Chu [2] for a water/air system is

$$D_f(t) = D_{f0} \exp(-C_1 \tau^{0.772} We^{0.246}) \quad (2.7)$$

We is the Weber number, which is defined by

$$We = \rho_c U_f^2 D_{f0} / \sigma_f \quad (2.8)$$

where ρ_c is the coolant density, U_f , D_{f0} , and σ_f are the velocity, initial diameter and surface tension of the droplets, respectively. τ is the dimensionless time, which is defined by

$$\tau = (U_f t / D_{f0}) (\rho_c / \rho_f)^{1/2} \quad (2.9)$$

where the time of descent, t , is zero when the debris is at the pool surface and increases as the debris descends through the pool. Constant C_1 is taken to be

$$C_1 = 0.171 - 0.149 (\rho_c / \rho_f)^{1/2} \quad (2.10)$$

To provide an easily integrable form for analytic use in MELCOR, Chu's correlation is modified as follows

$$D_f(t) = D_{f0} \exp(-C_1 \tau We^{0.254}) \quad (2.11)$$

with constant C_1 taken to be

$$C_1 = 0.1232 - 0.149 (\rho_c / \rho_f)^{1/2} \quad (2.12)$$

A comparison of Chu's correlation to this modified correlation for the water/air and corium/water systems reveals reasonable agreement [1]. Assuming constant velocity, U_f , Equation (2.11) can be converted to a function of the elevation of the pool surface, Z_{POOL} , as shown below

$$D_f(z) = D_{f0} \exp(-Z) \quad (2.13)$$

for $z_{BOT} \leq z \leq z_{POOL}$ where the variable Z is

$$Z = (C_1 We^{0.254} / D_{f0}) (\rho_c / \rho_f)^{1/2} (z_{POOL} - z) \quad (2.14)$$

Equation (2.13) is valid only as long as the debris remains molten. After the debris solidifies, ($T_f < T_{sol,f}$ as determined by the solution of Equation (2.17) to follow), there is no further breakup, and the heat transfer area is constant.

Another important factor affecting the rate of heat transfer is the heat transfer regime. In the early stage of heat transfer from the debris, the debris temperature is very high; hence, radiation heat transfer would be the dominant heat transfer mechanism. As the debris temperature falls, eventually other mechanisms become important.

Although radiation and conduction through the vapor film occur in parallel, the model incorporated into MELCOR only considers the dominant mechanism at any given time. Hence, the model switches from radiation-dominated to conduction-dominated film boiling heat transfer when the debris temperature falls below the "regime transition temperature". The regime transition temperature, T_{TRAN} , is defined as the temperature at which the net radiation heat flux between the debris and pool is equal to the conduction-dominated film boiling heat flux from the debris to the pool and is given by the solution to the following equation

$$\sigma(T_{TRAN}^4 - T_c^4) = h_{FB}(T_{TRAN} - T_{sat}) \quad (2.15)$$

where σ is the Stefan-Boltzmann constant (and the emissivity is assumed to be unity) and h_{FB} is the conduction-dominated film boiling heat transfer coefficient given by Bromley [3]

$$h_{FB} = (1/2) k_g \{k_g \mu_g D_f (T_g - T_{sat}) / [\rho_g (\rho_c - \rho_g) g i_{fg}]\}^{-1/4} \quad (2.16)$$

where k_g and μ_g are the thermal conductivity and viscosity of the vapor film, respectively, i_{fg} is the latent heat of vaporization of water and g is the acceleration of gravity. To derive

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this equation, it was assumed that the vapor saturation temperature, T_{sat} , the debris diameter, D_f , and the vapor temperature, T_g , are constant. T_g is the arithmetic average of the debris and saturation temperatures. Equation (2.15) can be solved iteratively to yield T_{TRAN} , the heat transfer regime transition temperature.

The rate of change of the debris temperature, T_f , is given by

$$\rho_f c_{vf} (\pi D_f^3 / 6) U_f dT_f / dz = q_{f-c} (\pi D_f^2) \quad (2.17)$$

where c_{vf} is the specific heat capacity of the debris and q_{f-c} is the heat flux from the debris to the coolant. For $T_f > T_{sol,f}$, D_f is given by Equation (2.13); otherwise D_f remains equal to its value at the instant solidification begins. For $T_f > T_{TRAN}$, q_{f-c} is calculated assuming only radiative heat transfer; otherwise, q_{f-c} is calculated assuming only transition film boiling. Equation (2.17) can be integrated from $z = z_{POOL}$ to $z = z_{BOT}$ to yield $T_{f,BOT}$, the debris temperature at the bottom of the coolant pool.

Once the debris temperature at the bottom of the pool is known, the total amount of heat transferred to the pool is given by

$$Q_{f-c} = H_f(T_{f0}) - H_f(T_{f,BOT}) \quad (2.18)$$

where

$$H_f(T) = \sum_{i=1}^{NMAT} [m_{i,FLR} h_i(T)] \quad (2.19)$$

and $h_i(T)$ is the specific enthalpy of debris component i at temperature T . The mass of steam generated by the heat transfer is given by

$$m_{STEAM} = Q_{f-c} / (h_{SCV} - h_{POOL}) \quad (2.20)$$

where h_{SCV} is the specific enthalpy of saturated steam at the total pressure in the FDI control volume and h_{POOL} is the specific enthalpy of the water in the cavity pool. Note that all heat transfer is assumed to generate steam; hence, the pool temperature should not change. If m_{STEAM} exceeds the mass of coolant in the pool, then $H_f(T_{f,BOT})$ and $T_{f,BOT}$ are back-calculated to provide just enough heat transfer to vaporize the mass of coolant in the pool.

Following the calculation of steam generation, the increments to the pool and vapor masses and energies are passed to the CVH package, the debris deposited on the floor at temperature $T_{f,BOT}$ is passed to the CAV package, where core-concrete interactions are modeled, and the radionuclides associated with the debris passed to CAV are transferred from FDI to the radionuclide package.

2.3 High-Pressure Melt Ejection (HPME) Modeling

If the velocity of the molten debris ejected from the reactor vessel exceeds a critical value prescribed by sensitivity coefficient C4602 (with a default value of 10 m/s), or if the user has invoked the stand-alone option for high-pressure melt ejection modeling, then the FDI will be treated by the high-pressure model instead of the low-pressure model.

The parametric high-pressure model requires user input to control both the distribution of debris throughout the containment and the interaction of the hot debris with the containment atmosphere. The processes modeled include oxidation of the metallic components of the debris (Zircaloy, aluminum and steel) in both steam and oxygen, surface deposition of the airborne debris by trapping or settling and heat transfer to the atmosphere and deposition surfaces.

The HPME model does not include a mechanistic debris transport model; rather, the user specifies a set of debris destinations with a corresponding set of transport fractions that prescribe where the ejected debris is assumed to go. The debris destinations may include the atmosphere of any CVH control volume, the surface of any heat structure and cavities defined by the CAV package. The sum of the transport fractions over all the specified control volume atmospheres, heat structure surfaces and cavities must equal one. Transport of the ejected debris to its assumed destinations occurs instantaneously, with no interactions occurring between the point of ejection and the destination sites. As long as the HPME model is active (i.e., as long as the ejection velocity exceeds the LPME/HPME transition velocity prescribed by sensitivity coefficient C4602 or if the user has invoked the stand-alone HPME model), the ejected debris will be partitioned among the destinations as specified by the transport fractions. When the ejection velocity falls below the LPME/HPME transition velocity for non-stand-alone applications, any debris subsequently ejected is passed to the LPME model, which uses LPME model input instead of the HPME transport model to determine the debris destination. However, debris that was transported to the HPME debris destinations before the model transition occurred will continue to be treated by the HPME model.

Debris which is transported to cavity destinations is not treated further by the FDI package; rather, subsequent treatment is provided by the CAV package. As implemented in the HPME model, surface deposition of debris can occur in two distinct ways. Ejected debris which impacts structures prior to any significant interaction with the atmosphere is sourced directly to the destination surface via the user-specified transport fraction for that surface. This process is referred to as trapping in MELCOR. Alternatively, debris which interacts

significantly with the atmosphere should be sourced to the appropriate control volume, in which a user-specified settling time constant will determine the rate of deposition to the specified settling destination (either a heat structure surface or a cavity). This process is referred to as settling in MELCOR.

First-order rate equations with user-specified time constants for oxidation, heat transfer and settling are used to determine the rate of each process. Oxidation of airborne and deposited debris is only calculated if the debris temperature exceeds a minimum value, TOXMIN, which is adjustable through sensitivity coefficient 4609 and has a default value of 600 K. If a pool of water exists in the reactor cavity at the time of debris ejection, then the water is ejected into the droplet field (fog) of the atmosphere at a rate proportional to the rate of injection of the debris into the pool. The proportionality constant is adjustable through sensitivity coefficient C4605 and has a default value of 10. This proportionality constant is strictly parametric and intended for exploratory purposes only. The rate of dispersal of the cavity water may be very important in determining containment loads, if interaction between the debris and cavity water is a primary contributor to the load. Excessive values of this coefficient may disperse the cavity water prematurely and limit subsequent interactions between ejected debris and cavity water, while deficient values will excessively limit the overall interaction of debris and water. Consequently, it is strongly recommended that the effects of variations in the value of this sensitivity coefficient be examined both because of its inherent uncertainty, and because of the large impact it may have on containment loads. The HPME model does not consider any thermal interaction between the ejected debris and the water in the cavity pool such as that described above for the LPME model.

When the HPME model first initiates direct containment heating in a control volume, the FDI package requests a fallback of the cycle if the timestep exceeds the recommended start-up value prescribed by sensitivity coefficient C4607 (with a default value of 10^{-4} s). The start-up value should be reasonably small both to avoid numerical problems associated with excessive energy transfers to the CVH atmosphere per timestep and to capture the detail associated with the HPME phenomena, which occurs on a time scale comparable to the user-specified time constants for the phenomena. Experience has indicated that for most realistic scenarios, the rapid excursions in pressure and temperature caused by direct containment heating dictate the use of very small timesteps for several cycles following DCH initiation. See the input record SOFTDTMIN in the Executive Package Users' Guide for help with this requirement.

The airborne masses of UO_2 and other materials that neither oxidize nor are the products of oxidation are described by the following first-order linear differential equation:

$$\frac{dm_{i,k}(t)}{dt} = -\frac{m_{i,k}(t)}{\tau_{ST,i}} + S_{i,k} \quad (2.21)$$

where $m_{i,k}(t)$ is the mass of component k in control volume i at time t , $\tau_{ST,i}$ is the time constant for settling in control volume i and $S_{i,k}$ is the constant mass source rate of component k in control volume i associated with the high-pressure melt ejection process. The solution of Equation (2.21) is given by

$$m_{i,k}(t) = [m_{i,k}(t_0) - S_{i,k}\tau_{ST,i}] \exp\left(-\frac{dt}{\tau_{ST,i}}\right) + S_{i,k}\tau_{ST,i} \quad (2.22)$$

where $m_{i,k}(t_0)$ is the mass at arbitrary initial time t_0 and dt is the difference between the final time, t , and time t_0 .

The airborne masses of Zr, Al and steel (the only materials that are oxidized in the presence of oxygen or steam) are described by the following first-order linear differential equation:

$$\frac{dm_{i,k}(t)}{dt} = -\frac{m_{i,k}(t)}{\tau_{SO,i}} + S_{i,k} \quad (2.23)$$

where $\tau_{SO,i}$, the time constant for simultaneous oxidation and settling/trapping, is given by

$$\tau_{SO,i}^{-1} = \tau_{ST,i}^{-1} + \tau_{OX,i}^{-1} \quad (2.24)$$

and where $\tau_{OX,i}$, is the oxidation time constant in control volume i . The solution to Equation (2.23) is identical to Equation (2.22) except that $\tau_{ST,i}$ is replaced by $\tau_{SO,i}$.

The airborne masses of ZrO_2 and other materials that are products of oxidation reactions are given by

$$\frac{dm_{i,k}(t)}{dt} = -\frac{m_{i,k}(t)}{\tau_{ST,i}} + R \frac{m_{i,l}(t)}{\tau_{OX,i}} + S_{i,k} \quad (2.25)$$

where R is the mass of product k formed by the oxidation of a unit mass of reactant l . The solution of Equation (2.25) is

$$m_{i,k}(t) = [m_{i,k}(t_0) - C_1 - C_2] \exp(-dt / \tau_{ST,i}) + C_2 \exp(-dt / \tau_{SO,i}) + C_1 \quad (2.26)$$

where

$$C_1 = (S_{i,k} + RS_{i,i} \tau_{SO,i} / \tau_{OX,i}) \tau_{ST,i}$$

and

$$C_2 = R[S_{i,j} \tau_{SO,i} - m_{i,j}(t_0)]$$

The HPME model contains two options for oxidation modeling. These may be selected independently for each control volume. The first is the sequential oxidation option, in which the order of oxidation is Zr, Al then steel (typical metallic elements associated with reactor cores and/or simulation experiments). This is invoked by specifying a positive value for the oxidation time constant, $\tau_{OX,i}$. The second option is simultaneous oxidation of the metals, which is invoked by specifying a negative value of $\tau_{OX,i}$, in which case the time constant will be equal to the absolute value of $\tau_{OX,i}$. Under normal conditions where the metallic constituents exist in a more or less well-mixed state, the sequential oxidation option is recommended because it is more realistic. Elements with higher oxidation potentials will tend to be preferentially oxidized unless some kinetic limitation exists.

In the sequential oxidation model, a separate oxidation rate is first calculated for each metal independently of all others, with the given value of $\tau_{OX,i}$. Then the mass of metal B consumed will be converted into an equivalent mass of metal A, where metal A is assumed to oxidize in preference to metal B, until all of metal A is consumed. Hence, steel (and Inconel, which is included in the steel mass in the FDI package) will not be consumed until all the Zr and Al have been consumed, and Al will not be consumed until the Zr is exhausted. This implies that the effective time constant for metal A oxidation when metal B is present may be significantly shorter than $\tau_{OX,i}$. The actual values of the effective oxidation time constants will be used in determining the end of timestep airborne mass inventories in Equation (2.23) and Equation (2.26) above.

Both oxidation options are constrained by the availability of oxygen or steam. Oxidation is apportioned between steam and oxygen by their relative mole fractions in the atmosphere. This is a change in MELCOR 1.8.5; previously, the oxygen would react first, followed by steam only after the oxygen had been consumed. Although this assumption probably reflects the relative oxidation potential of oxygen versus steam, it does not consider diffusion transport in the atmosphere and generally resulted in insufficient hydrogen generation during DCH. The relative oxidation effectiveness of oxygen versus steam can

be adjusted through sensitivity coefficient C4610. The default setting of C4610 is 1.0, giving an oxidation ratio proportional to the moles of oxygen divided by the moles of oxygen plus steam:

$$R_{OX} = \frac{W X_{O_2}}{W X_{O_2} + X_{st}} \quad (2.27)$$

where W is the weighting factor given by sensitivity coefficient C4610, X_{O_2} is the moles of oxygen, and X_{st} is the moles of steam in the atmosphere. Making W a large number will weight the oxygen moles and give the previous “oxygen first” behavior. If there is insufficient oxidant to support the calculated rates of oxidation for zirconium and iron, then the zirconium will have first priority. The oxidation reactions will proceed at the start of timestep values of debris temperature in each control volume, and any hydrogen formed by the steam reaction will enter the atmosphere at that temperature.

The temperature of the airborne debris is affected by debris sources, oxidation and heat transfer from the debris to the atmosphere. The temperature of the atmosphere, T_{gas} , is assumed to remain constant and equal to the beginning of timestep value obtained from the CVH package data base. This explicit coupling between FDI and CVH may limit the timestep size during energetic transients, as discussed below. The enthalpy of the airborne debris is given by the solution of the following simple equation:

$$\frac{dH_i(t)}{dt} = \dot{E}_{ox,i}(t) - \dot{Q}_{GAS,i}(t) + S_{H,i} \quad (2.28)$$

where $\dot{E}_{ox,i}(t)$ is the rate of heat generation by the oxidation reaction, $S_{H,i}$ is the enthalpy source rate associated with the HPME source, and the rate of heat transfer to the gas is approximated as:

$$\dot{Q}_{GAS,i}(t) = \frac{Q_g i(t)}{\tau_{HT,i}} = \frac{H_i(T_{dbr}) - H_i(T_{gas})}{\tau_{HT,i}} \quad (2.29)$$

where $Q_g i(t)$ is the enthalpy available for transfer to the gas, $\tau_{HT,i}$ is the user-specified time constant for heat transfer from the airborne debris to the atmosphere in control volume i , $H_i(T_{dbr})$ is the enthalpy content of the debris at its actual temperature, T_{dbr} , and $H_i(T_{gas})$ is the enthalpy content of the debris in equilibrium with the gas at temperature T_{gas} . The solution to Equation (2.28) is given by:

$$H_i(t) = H_i(t_0) + E_{OX,i}(t) - Q_{GAS,i}(t) \quad (2.30)$$

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where $H_i(t_0)$ is the enthalpy of the debris after the addition of the integrated enthalpy source $S_{H,i} dt$ and after adjustments to its composition associated with the oxidation reactions, where $E_{OX,i}(t)$ is the oxidation enthalpy generated between times t_0 and t , and where $Q_{GAS,i}(t)$ is the amount of heat transferred to the gas between times t_0 and t . $Q_{GAS,i}(t)$ is given by

$$Q_{GAS,i}(t) = \int_{t_0}^{t_0+dt} [Q_{g,i}(t) / \tau_{HT,i}] dt \quad (2.31)$$

where the available enthalpy $Q_{g,i}(t)$ increases as a result of oxidation and the addition of high-temperature debris source material and decreases as enthalpy is transferred to the gas. $Q_{g,i}(t)$ satisfies

$$\frac{dQ_{g,i}(t)}{dt} = -\frac{Q_{g,i}(t)}{\tau_{HT,i}} + [Q_{SRC,i} / dt + (E_{OX,i} + Q_{OX,i}) / dt] \quad (2.32)$$

$$Q_{SRC,i} = S_{H,i}(T_{src}) - S_{H,i}(T_{gas})$$

is the available source enthalpy and

$$Q_{OX,i} = H_{OX,i}(T_{dbr}) - H_{OX,i}(T_{gas})$$

is the available enthalpy created by composition adjustments during oxidation. The solution to Equations (2.31) and (2.32) is:

$$Q_{GAS,i}(t) = Q_{OLD,i} [1 - \exp(-dt / \tau_{HT,i})] + [Q_{SRC,i} / dt + (E_{OX,i} + Q_{OX,i}) / dt] \{dt - \tau_{HT,i} [1 - \exp(-dt / \tau_{HT,i})]\} \quad (2.33)$$

where $Q_{OLD,i} = H_i(T(t_0)) - H_i(T_{gas})$ is the initial available enthalpy.

The inclusion of the HPME source terms in Equations (2.21) through (2.33) reduces some timestep dependencies that would arise if the sources were added prior to the calculation of oxidation, heat transfer and settling/trapping. After the total enthalpy at the advanced time, t , is determined, it is compared to the enthalpy corresponding to a maximum

permissible temperature, H_{MAX} . If $H_i(t)$ exceeds H_{MAX} , then Equation (2.30) is solved for $Q_{GAS,i}(t)$ with $H_i(t)$ set equal to H_{MAX} as follows:

$$Q_{GAS,i}(t) = H_i(t_0) + E_{OX,i}(t) - H_{MAX} \quad (2.34)$$

so that the heat transferred to the gas is increased sufficiently to limit the advanced time debris temperature to the maximum prescribed value, T_{MAX} . T_{MAX} is given by

$$T_{MAX} = MAX(T_{gas}, T_{dbr}(t_0), T_{dbr}(t'), T4603) \quad (2.35)$$

where T_{gas} is the gas temperature, $T_{dbr}(t_0)$ is the debris temperature at the beginning of the timestep, $T_{dbr}(t')$ the debris temperature after addition of new source material to the initial inventory and T4603 is the temperature limit prescribed by sensitivity coefficient C4603, which normally exceeds the other arguments in the max function of Equation (2.35). The default value of T4603 is approximately equal to the boiling temperature of UO_2 —temperatures much in excess of this value would likely result in very rapid fragmentation of debris droplets and significantly increased droplet-to-gas heat transfer.

After an advanced time temperature for the airborne debris has been determined, the projected change in the CVH atmosphere temperature as a result of direct containment heating during the timestep is calculated. If the change exceeds a value prescribed by sensitivity coefficient C4604 (with a default value of 500 K), then the FDI package requests a fallback with a decreased timestep. This feature provides control over numerical problems associated with excessive energy transfers to the CVH atmosphere. If the value of sensitivity coefficient C4604 is set too high, it is possible that the CVH package will encounter numerical difficulties that cannot be resolved by CVH fallbacks. In practice, the default value was found to prevent numerical problems in CVH without excessively limiting the timestep.

Following the determination of the advanced time temperature for the airborne debris, the advanced time mass equations, Equations (2.21) through (2.26), are used to determine how much material is removed from the atmosphere by settling/trapping. The settled material and its energy content are removed from the airborne inventory and deposited on the appropriate surface specified by user input. After the settling calculation has been performed, the advanced time total airborne mass in each control volume is determined by summing over all components. If the advanced time total airborne mass is insignificant compared to the total mass of material sourced into the control volume atmosphere over the duration of the DCH event, then all of the remaining airborne mass in the control volume is immediately deposited on the appropriate settling surface and a message is issued to notify the user that direct containment heating has ceased in that particular control volume. The ratio used to determine when the airborne mass has become

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insignificant is adjustable through sensitivity coefficient 4606 and has a default value of 0.001. This implies that only 0.1 percent of the mass source will be prematurely deposited, which was judged to be a reasonable compromise between the demands of accuracy and calculational effort.

Deposited Debris

The mass of material k on surface i at time t is given by

$$m_{i,k}(t) = m_{i,k}(t_0) + S'_{i,k} dt \quad (2.36)$$

where

$$S'_{i,k} = S_{i,k} + \sum_j \int_{t_0}^{t_0+dt} [m_{j,k}(t') / \tau_{ST,j}] dt' / dt \quad (2.37)$$

and $S_{i,k}$ is the constant mass source rate of component k to surface i from trapping. The second term on the right-hand side of Equation (2.37) accounts for settling to the surface, where the sum is over all control volumes that have surface i as the user-specified settling surface, and $m_{j,k}(t)$ and $\tau_{ST,j}$ are the airborne mass of component k in control volume j and the settling time constant in control volume j , respectively.

For UO_2 and other materials not associated with oxidation, the settling term is given by

$$\int_{t_0}^{t_0+dt} m_{j,k}(t') dt' / \tau_{ST,j} = m_{j,k}(t_0) [1 - \exp(-dt / \tau_{ST,j})] + S_{j,k} \{ dt - \tau_{ST,j} [1 - \exp(-dt / \tau_{ST,j})] \} \quad (2.38)$$

For metals that oxidize, the settling term is given by

$$\int_{t_0}^{t_0+dt} m_{j,k}(t') dt' / \tau_{ST,j} = (\tau_{SO,j} / \tau_{ST,j}) (m_{j,k}(t_0) [1 - \exp(-dt / \tau_{SO,j})] + S_{j,k} \{ dt - \tau_{SO,j} [1 - \exp(-dt / \tau_{SO,j})] \}) \quad (2.39)$$

which reduces to Equation (2.38) if $\tau_{OX,i} \gg \tau_{ST,j}$, because in that case $\tau_{SO,j} \approx \tau_{ST,j}$ as shown by Equation (2.24). For oxidation products, the settling term is given by

$$\begin{aligned}
 \int_{t_0}^{t_0+dt} m_{j,k}(t') dt' / \tau_{ST,j} = m_{j,k}(t_0) [1 - \exp(-dt / \tau_{ST,j})] + S_{j,k} \{ dt - \tau_{ST,j} \\
 [1 - \exp(-dt / \tau_{ST,j})] \} + R \{ (\tau_{SO,j} / \tau_{OX,j}) [m_{j,l}(t_0) + S_{j,l} (dt - \tau_{SO,j} \\
 - \tau_{ST,j})] - [m_{j,l}(t_0) - S_{j,l} \tau_{ST,j}] \exp(-dt / \tau_{ST,j}) + ([\tau_{SO,j} / \tau_{ST,j}] \\
 [m_{j,l}(t_0) - S_{j,l} \tau_{SO,j}] \exp(-dt / \tau_{SO,j}) \} \quad (2.40)
 \end{aligned}$$

where material *l* is the metal from which the oxide is formed and *R* is the mass of product *k* formed by the oxidation of a unit mass of material *l*.

The energy of the deposited debris is calculated with equations almost identical to Equations (2.28) through (2.35) except the source term $S_{H,i}$ also includes the enthalpy associated with debris settling. It is assumed that the enthalpy of the settled debris is equal to the end of timestep value calculated with Equation (2.30). The settled mass with the end of step enthalpy is applied to the deposition surface during the timestep at a constant rate as implied by Equation (2.36). The other difference between the treatment of the energy of airborne and deposited debris concerns heat transfer. As discussed above, the user specifies a time constant for heat transfer from the airborne debris to the atmosphere. However, for heat transfer from deposited debris to the structure, a different approach is taken. Because the CVH package does not recognize the deposited debris temperature as the effective surface temperature, in order to effectively simulate the heat transfer from the hot debris to the CVH pool and/or atmosphere associated with the surface, it is necessary to couple the debris temperature tightly to the HS surface temperature that CVH does recognize.

The debris temperature and HS surface temperature will be tightly coupled if the effective heat transfer coefficient from the debris to the surface, h_{SRF} , is large compared to the heat transfer from the surface to the first interior node in the structure, which is given by $k_{HS,1} / \Delta x_{HS,1}$ (structure thermal conductivity divided by the node thickness). In order to generate a large value of h_{SRF} , a very small time constant equal to the minimum of half the surface oxidation time constant and a value of 0.001 s is used to calculate the amount of heat transfer from the debris to the deposition surface using the analog of Equation (2.33) for heat transfer to surfaces. The value obtained is then used to determine h_{SRF} as follows:

$$h_{SRF} = Q_{SRF,i}(t) / (A_{SRF} \Delta T dt) \quad (2.41)$$

where A_{SRF} is the surface area of the structure, ΔT is the difference between the beginning of timestep debris temperature and the structure surface temperature and Q_{SRF} is the value obtained from the analog of Equation (2.33). This value will almost always exceed the value of $k_{HS,1} / \Delta x_{HS,1}$. In fact, the value of h_{SRF} may be large enough to induce oscillations in the structure surface temperature because of the explicit coupling between

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FDI and HS packages. Therefore, a limit is placed on the value of h_{SRF} . If h_{SRF} exceeds a maximum value, $h_{SRF,max}$, specified by sensitivity coefficient 4608 (default value 1000. W/m²-K), then the value of Q_{SRF} is reduced by the ratio $h_{SRF,max} / h_{SRF}$ to limit it to the value consistent with $h_{SRF,max}$. Whenever, the Q_{SRF} is limited by $h_{SRF,max}$ the direction of heat transfer (i.e., debris-to-surface or surface-to-debris) is compared to the direction from the previous timestep. If the direction is alternating, this probably indicates that the surface temperature has been driven into an oscillation about the debris temperature because the timestep exceeds the stability limit associated with the explicit coupling between the FDI and HS packages. In such cases, FDI requests a system fallback with the timestep reduced by a factor of one half. Normally, the value of $h_{SRF,max}$ should be chosen large enough to promote rapid equilibration of the debris and surface temperatures, yet not so large as to induce instability in the surface temperature for reasonable values of the timestep. Users should refer to the HS Reference Manual for a further discussion of stability/accuracy concerns associated with structure nodalization and timestep size.

If the MELCOR RadioNuclide (RN) package is active, then FDI will call RN1 of the RN Package anytime fuel is moved so that the associated radionuclides can be moved simultaneously. Furthermore, the decay heat associated with the radionuclides will be deposited in the appropriate location.

3. Sensitivity Coefficients

For convenient reference, the sensitivity coefficients for the FDI package are summarized below, taken from the FDI Reference manual.

Sensitivity Coefficients	Definition
C4602	Vessel ejection velocity at transition between high- and low-pressure ejection modeling. (default = 10., units = m/s, equiv = none)
C4603	Airborne debris temperature above which oxidation energy is deposited directly in the atmosphere—approximate vaporization point. (default = 3700., units = K, equiv = none)
C4604	Maximum change in the temperature of the CVH atmosphere permitted without a timestep cut. (default = 500., units = K, equiv = none)
C4605	Ratio of the mass of water ejected from a pool into the reactor cavity atmosphere to the mass of the debris injected from the vessel into the cavity pool. (default = 10., units = none, equiv = none)

Sensitivity Coefficients	Definition
C4606	Ratio of the current airborne debris mass to the integrated airborne debris mass source in a control volume below which the mass will be deposited onto the settling surface associated with the control volume—deactivates DCH when the remaining airborne mass becomes insignificant.
	(default = 0.001, units = none, equiv = none)
C4607	Initial timestep size for HPME initiation.
	(default = 0.0001, units = s, equiv = DTHPME)
C4608	Maximum debris-to-surface heat transfer coefficient.
	(default = 1000., units = W/m ² -K, equiv = HTC MAX)
C4609	Minimum temperature for oxidation.
	(default = 600., units = K, equiv = TOXMIN)
C4610	Oxygen-steam oxidation weighting factor.
	(default = 1., units = none, equiv = none)

4. Discussion and Development Plans

The simple direct containment heating model described above in Section 2.3 is not intended to predict all details of DCH events from first principles. Nodalization requirements would be much greater than normal MELCOR models. Rather, it is intended to allow users to evaluate the overall effect of varying the relative rates of the most important processes controlling DCH loads.

HPME model results are sensitive to the relative values of $\tau_{OX,j}$, $\tau_{HT,j}$ and $\tau_{ST,j}$ specified by the user for each control volume. Reasonable values for these time constants can be obtained in basically two ways. First, results from detailed codes such as CONTAIN can be used to obtain appropriate values; or, second, reasonable assumptions concerning particle sizes and velocities in conjunction with simplified hand calculations can yield a range of time constants in the correct range. In most cases, this second method should be adequate for parametric PRA studies. Specified time constants of less than 10^{-6} s will be reset to that value to avoid potential numerical problems associated with vanishing time constants. For time scales of interest, a time constant of 10^{-6} s implies an essentially instantaneous process (i.e., instantaneous complete oxidation, instantaneous thermal equilibration with the atmosphere or instantaneous settling).

Users are cautioned that the absence of mechanistic debris transport in the HPME model currently limits the scope of phenomena that may be investigated. Specifically, decoupling the debris transport from the vessel blowdown precludes accurately investigating effects associated with the coherence between the debris and steam ejection. If the severity of the DCH threat is primarily limited by the amount of thermal and chemical energy available in the ejected debris, then the model should prove useful. However, if the threat is primarily

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limited by the amount of steam that has an opportunity to interact with the airborne debris, then the model may fail to capture the important phenomena and can underpredict the DCH load. The user should suspect that this condition may exist whenever the following two conditions hold:

- (1) Most of the debris is specified to not reach the main volume of the containment.
- (2) In the cavity and/or subcompartment volumes which are specified to receive most of the debris, maximum gas temperatures approach the initial debris temperature and/or oxidant concentrations ($O_2 + H_2O$) fall to low levels during the time period that airborne debris concentrations are relatively high.

References

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