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Models and Correlations of the DEBRIS Late-Phase Melt Progression Model*

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Abstract

The DEBRIS Late Phase Melt Progression Model is an assembly of models, embodied in a computer code, which is designed to treat late-phase melt progression in dry rubble (or "debris") regions that can form as a consequence of a severe core uncover accident in a commercial light water nuclear reactor. The approach is fully two-dimensional, and incorporates a porous medium modeling framework together with conservation and constitutive relationships to simulate the time-dependent evolution of such regions as various physical processes act upon the materials. The objective of the code is to accurately model these processes so that the late-phase melt progression that would occur in different hypothetical severe nuclear reactor accidents can be better understood and characterized. In this report the models and correlations incorporated and used within the current version of DEBRIS are described. These include the global conservation equations solved, heat transfer and fission heating models, melting and refreezing models (including material interactions), liquid and solid relocation models, gas flow and pressure field models, and the temperature and compositionally dependent material properties employed. The specific models described here have been used in the experiment design analysis of the Phebus FPT-4 debris-bed fission-product release experiment. An earlier DEBRIS code version was used to analyze the MP-1 and MP-2 late-phase melt progression experiments conducted at Sandia National Laboratories for the United States Nuclear Regulatory Commission.

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Models and Correlations of the DEBRIS Late-Phase Melt Progression Model

1. Introduction and Overview

1.1 Introduction

To address important issues related to postulated severe nuclear reactor accidents, Sandia National Laboratories (SNL), under the direction of the United States Nuclear Regulatory Commission (NRC), has been developing various numerical analysis tools. One of these is a computer code called "DEBRIS." DEBRIS contains a collection of models dedicated to treating regions of debris/rubble that may form in the pressure vessel during the late phase of such accidents. This report provides a description of the various models and correlations that are incorporated in the current version of DEBRIS. In particular, the specific models described here have been used in the analysis of the MP-1 and MP-2 late-phase melt progression experiments conducted at SNL for the NRC. In addition, the models have been used most recently for the design phase analyses of the French Phebus Project FPT-4 experiment.

The definition of "model" used here is broad, and includes all aspects of how the physical reality of the problem is represented. The focus of this document is on model description and thus does not provide an *assessment* of the current models. However, Section 6 presents the results of benchmark calculations designed to compare the code results. The results are obtained for a "standard case" with and without a special set of models developed specifically to improve melt relocation models and post-melting energy deposition models.

This section gives a general overview of the DEBRIS computer code, its development, and its current capabilities and limitations. This introduction and overview is intended to provide a useful context for the more specific information that will follow in the succeeding sections.

1.2 Purpose and Objectives of DEBRIS

During the course of a severe reactor accident, material that once was part of a well-defined geometric structure may relocate and form a stationary region that consists of what is often called "debris." This debris may consist of disintegrated fuel rods, control rods, failed structural components, etc., and may be either liquid, partially liquid, or solid. The modeling contained in DEBRIS is designed to represent any such region in which no liquid water is present, and to simulate the time-dependent evolution of such a region as various physical processes act upon the materials. The objective of the code is to accurately model these processes so that the late-phase melt progression that would occur in different hypothetical severe nuclear reactor accidents can be better understood and predicted. In addition, the current computer code implementation of these models has been tailored to facilitate the analysis of the French Phebus FPT-4¹ late-phase melt progression and fission product release experiment to run in the Phebus Facility at

Cadarache, France. Earlier versions of the code were developed and tailored to analyze the MP-1 and MP-2 tests^{2,3}, which were late-phase melt progression experiments conducted at SNL.

1.3 Brief Development History

In response to the accident that happened at Three-Mile Island Unit 2, the NRC organized a broad range of research activities and established some specific goals related to severe reactor accident safety issues. These are described in the report *Nuclear Power Plant Severe Accident Research Plan*.⁴ One of the items identified as essential in realizing these goals was the development of improved computer codes for use in the analysis of severe core-damaging accidents in light-water reactors. In particular, the development of "mechanistic" or "phenomenologically" based models—whose purpose is to provide detailed, best-estimate analysis capabilities—was made a major priority. One of the modeling development efforts that was a direct result of this priority was the MELPROG computer code development effort at Sandia and Los Alamos National Laboratories. DEBRIS is an offshoot of this development effort.

The first documented version of MELPROG was called MELPROG-PWR/MOD0⁵, and consisted of five explicitly coupled modules or sub-codes. One of these modules, called the "DEBRIS" module, was a one-dimensional approach to modeling the formation and behavior of rubble or debris beds throughout the vessel. The next (and final) documented version of MELPROG was designated MELPROG-PWR/MOD1^{6,7}, and contained a completely new "DEBRIS" module, which was a two-dimensional approach based on a porous-media type representation of the debris bed. As part of the development work that went into this revision of MELPROG, a stand-alone version of the DEBRIS module was developed and a number of interesting studies were made (using various versions of this module, see references [8] through [18]). Although NRC funding for the MELPROG code was discontinued after the completion of MELPROG-PWR/MOD1, support of the DEBRIS modeling approach has been maintained by the NRC for the purpose of helping to address late-phase melt progression issues.

Some of the issues related to melt progression in the "late phase" of a light water reactor accident sequence have been addressed by the NRC through a series of two experiments, MP-1² and MP-2³, which were carried out in the Annular Core Research Reactor facility at SNL. The MELPROG DEBRIS module was modified and adapted as a design and analysis tool specifically for application to the MP (melt progression) experiments. It was in this capacity that the DEBRIS code received considerable attention with regard to model improvement and evolved as a useful stand-alone code for analysis of late-phase melt progression.

Further improvement and generalization of the DEBRIS models was undertaken most recently within the framework provided by its application to the design phase of the French FPT-4¹ debris bed experiment. This work is presently ongoing. The French, who committed considerable effort to the development and improvement of the DEBRIS code, have also incorporated the porous media models into their ICARE-2¹⁹ code, which is a separate analytical code development effort. This code has been applied with considerable success to the TMI-2 accident and is being used together with the DEBRIS code for the FPT-4 design phase.

The MERIS code was developed in parallel with the evolution of the DEBRIS code. In recognition of the fact that the porous-media computational algorithms also lend themselves well to early phase application, the MERIS²⁰ code was developed at Sandia originally to treat the early, dry-core, intact-rod phase associated with certain BWR (boiling water reactor) accident sequences. In this capacity the MERIS code was used successfully to analyze the XR²¹ experiments, and has also been used for analysis of the FPT-0, FPT-1²² experiments. Most recently, the MERIS code, because of its three-dimensional (3-D) capability, is also being applied to the FPT-4 experiment in conjunction with the DEBRIS code analysis to explore the possible effects of nonaxisymmetric behavior.

The DEBRIS code represents a stage in the development of the porous media modeling approach to severe accident melt progression. The MERIS code, which makes use of the same computational framework, represents, in effect, a more generalized application of the approach and, thus, the next stage in the development of the porous media methodology. Table 1 outlines a brief comparison of the two codes.

Table 1. Comparison of DEBRIS and MERIS porous media models.

Models	DEBRIS Code	MERIS Code
Geometry	2-D (r,z)	3-D (x,y,z)
Temperature Field	Single control volume temperature for all phases	Separate control volume temperature for each phase
Solid Phase Relocation	YES	NO
Liquid Phase Relocation	YES	YES
Gas Phase Motion	YES	YES
Chemical Reactions	NO	YES
Material Interaction	YES	YES
Interaction Kinetics	NO	YES

It should be noted here that, although much of the discussion that follows seems specifically directed to addressing the application of the DEBRIS code models to experiment analysis, the experiments to which it has been applied as an analytical tool were designed to explore the phenomena associated with full-scale reactor accident conditions. Thus, most of the modeling is useful and directly applicable to full-scale accident situations. For example, the DEBRIS code was recently used as the basis for performing a late-phase melt progression scoping analysis for pressurized water reactors (PWRs).²³ It has also been shown that the implementation of the porous media modeling approach in severe accident codes such as SCDAP/RELAP5 is straightforward²⁴ and provides significant advantages over current models. We note in this context that ad hoc models, and those that are associated with specific experiments are, in general, modular and lend themselves easily to adaptation for full-scale reactor accident application.

The models described here are those that currently exist in a stand-alone version of the DEBRIS computer code that has been tailored and used for both pre-test and experiment design analyses of the FPT-4 experiment to be run at the Phebus facility in Cadarache, France.

1.4 Idealized Representation of a Debris Bed

A basic framework used by the current version of DEBRIS has key elements as outlined below.

1.4.1 Two-Dimensional (r-z) Axisymmetric Domain

In DEBRIS, the region of interest is spatially represented on a two-dimensional (r-z) axisymmetric grid and uses a control volume type discretization scheme. The extent of the physical domain is defined by an axial height H and a radius R . This is illustrated in Figure 1.

Figure 1. Illustration of the axisymmetric grid used in DEBRIS models.

1.4.2 Porous-Media Type Representation

The second key element in the DEBRIS code representation is that the material within the computational domain is treated as a "porous media" containing multiple constituents (for example, uranium dioxide (UO_2), zirconium dioxide (ZrO_2), Zr, and iron (Fe)) in both liquid and solid phases. Specific local geometric features of the debris are not explicitly modeled or tracked in this representation. Instead, only gross characteristics such as local mass fractions and volume fractions (both solid and liquid) are maintained. To account for geometry-specific effects on the various processes modeled (heat transfer, fluid flow, etc.) a specific geometric configuration must be assumed and one characteristic length scale can be used in scaling the geometric properties. For debris beds, an effective particle size (denoted here as D_p) is generally used.

1.4.3 Conservation of Mass, Momentum, and Energy

The third key element of the DEBRIS model is that a specific set of global conservation laws for mass, momentum, and energy must be satisfied for all processes modeled. Each of these equations will be discussed in detail in later sections, but are listed here by way of introduction.

Conservation of Mass (Solid and Liquid Phase)

$$\frac{\partial}{\partial t}(\alpha_l Y_{lj} \rho_{lj}) + \frac{\partial}{\partial t}(\alpha_s Y_{sj} \rho_{sj}) + \nabla \cdot (Y_{lj} \rho_{lj} \bar{u}) + \frac{\partial}{\partial z}(\alpha_s Y_{sj} \rho_{sj} U) = R_j \quad (1)$$

Continuity Equation (Gas Phase)

$$\frac{\partial}{\partial t}(\alpha_g \rho_g) + \bar{\nabla} \cdot (\rho_g \bar{u}_g) = 0 \quad (2)$$

Conservation of Momentum (Liquid and Gas)

$$\bar{u}_l = -\frac{\kappa_l}{\mu_l}(\nabla P_l + g \rho_l) \quad (3)$$

$$\bar{u}_g = -\frac{\kappa_g}{\mu_g}(\nabla P_g + g \rho_g) \quad (4)$$

Conservation of Energy

$$\begin{aligned} \frac{\partial}{\partial t} \left(\sum_{j=1}^{nc} [\alpha_s Y_{sj} \rho_{sj} h_{sj} + \alpha_l Y_{lj} \rho_{lj} h_{lj}] + \alpha_g \rho_g h_g \right) + \nabla \cdot (u_g \rho_g h_g) + \nabla \cdot \left(u_l \sum_{j=1}^{nc} Y_{lj} \rho_{lj} h_{lj} \right) + \\ \frac{\partial}{\partial z} \left(\alpha_s U \sum_{j=1}^{nc} Y_{sj} \rho_{sj} h_{sj} \right) = \nabla \cdot (k_{eff} \nabla T) + [\alpha_s \rho_{s1} h_{s1} + \alpha_l \rho_{l1} h_{l1}] Q + q_c \end{aligned} \quad (5)$$

Note that only one energy equation is currently solved. This is indicative of a basic assumption that the material phases are in local equilibrium, and thus that the thermal state in each control volume can be fully characterized by only one temperature. Also note that a solid material momentum equation is not solved.

Within the constraints imposed by the above-mentioned three elements, a finite set of physical processes is modeled in DEBRIS.

1.5 Basic Processes Modeled

The following generalized processes are modeled within the debris bed:

- 1) internal conduction and radiation heat transfer,
- 2) fission heating,
- 3) melting and freezing,
- 4) UO_2 - ZrO_2 material interactions,
- 5) two-dimensional (r-z) liquid material relocation,

- 6) solid material relocation (settling) in the axial direction, and
- 7) two-dimensional (r-z), two-component gas flow.

In the MP-1 and MP-2 analyses processes 1 through 6 were modeled and for the FPT-4 analysis all seven processes were treated within the debris bed.

The specific models employed to represent these processes are described in detail in Sections 2, 3, and 4. Section 5 describes the material properties used in DEBRIS, and Section 6 contains the results of a limited benchmark calculation.

1.6 Boundary Conditions

In DEBRIS, three types of thermal boundary conditions can be imposed on the region of interest. The first is to specify a given temperature at the boundary, the second is to specify a given heat flux (which could be zero to simulate an adiabatic boundary), and the third is to specify a heat transfer coefficient and a sink temperature. Each of these may be varied spatially and temporally to tailor the boundary conditions to a wide variety of conditions. In addition, a set of special purpose subroutines was written for use in the MP-2 experimental analysis to more accurately model the boundary conditions imposed by the outer cooling water jacket (see Appendix B of reference [3] for a detailed description). The FPT-4 experiment required a number of new models that included a gas-flow inlet condition at the bottom of the debris bed and a radiation boundary condition at the upper surface of the bed.

All liquid velocities are assumed to be zero at all boundaries, thus no liquid or solid mass inflow at boundaries is currently allowed. This is not a strict limitation and can be removed if required.

2. HEAT TRANSFER AND FISSION HEATING

In this section the models used to represent conduction and radiation heat transfer, and the sources of energy as a result of either fission heating or decay heat processes are described.

2.1 Governing Energy Equation

The global energy equation that is solved in DEBRIS can be written as follows:

$$\frac{\partial}{\partial t} \left(\sum_{j=1}^{nc} [\alpha_s Y_{sj} \rho_{sj} h_{sj} + \alpha_l Y_{lj} \rho_{lj} h_{lj}] + \alpha_g \rho_g h_g \right) + \nabla \cdot (u_g \rho_g h_g) + \nabla \cdot \left(u_l \sum_{j=1}^{nc} Y_{lj} \rho_{lj} h_{lj} \right) + \frac{\partial}{\partial z} \left(\alpha_s U \sum_{j=1}^{nc} Y_{sj} \rho_{sj} h_{sj} \right) = \nabla \cdot (k_{eff} \nabla T) + [\alpha_s \rho_{s1} + \alpha_l \rho_{l1}] Q + q_c, \quad (6)$$

where α is a volume fraction of solid s , liquid l , or gas g . Y_{ij} is the volume fraction of phase i (solid s or liquid l) that is occupied by species j , h_{ij} is the enthalpy of species j in phase i , k_{eff} is an effective thermal conductivity which accounts for both conductive and radiative heat transfer in the porous material, Q is the heat source expressed as energy release per unit mass of UO_2 , and q_c is a general heat source term. The seven terms identified in the equation can be described as representing the following:

- term 1: the time rate of change of the energy stored (in liquid, solid, and gas),
- term 2: energy convected by the gas phase,
- term 3: energy convected by liquid motion,
- term 4: energy convected by solid material relocation (not that solid relocation is only in the axial direction),
- term 5: internal conduction and radiation,
- term 6: decay heat generation or fission heating term,
- term 7: a generalized energy source term (oxidation, boundary heat fluxes, etc.).

Note that only one energy equation is solved for all three phases, the liquid and the solid phases of the debris bed components and the gas phase consisting of a composite (mixture) gas. This is due to the current assumption that the liquid and solid debris as well as the gaseous components are in local thermal equilibrium (i.e., they have the same temperature at any local position). In terms of liquid/solid equilibrium, this is considered to be a reasonable assumption when melt velocities in the bed are low and the solid surface area per unit volume is large. In terms of gas thermal equilibrium with the liquid/solid components, the accuracy of the approximation depends on particle size, gas flow rate in the bed, and inlet gas temperature. Calculations²⁵ performed to scope the accuracy of the gas-phase equilibrium approximation indicate that for particle sizes in the range up to 1 centimeter (cm) and steam/hydrogen flow rates appropriate for late phase conditions, gas phase temperatures will differ from solid/liquid temperatures by at

most 50 to 80 K in the debris bed temperature range 2000 to 3000 K. For most locations in the bed the temperature differences are significantly less.

2.2 Global Effective Conduction

Term 5 of Equation (6) models the transfer of heat by diffusion-type mechanisms through the use of an effective thermal conductivity, k_{eff} . In DEBRIS, the calculation of k_{eff} is formulated to include the effects of radiation as well as conduction in a potentially three-phase (solid, liquid, gas) region. To account for the dissimilar characteristics of the different regions existing in the MP experiments, three distinct effective thermal conductivity models are incorporated into DEBRIS. These are designed to treat 1) debris bed (particulate) regions, 2) porous but structured regions consisting of control rods, and 3) solid multi-component (crust) regions.

An option is also available in DEBRIS to account qualitatively for the enhanced heat transport associated with the mixing that can occur in a molten pool. This ad hoc model enhances the local thermal conductivity in molten pool regions where the axial temperature gradient is negative (i.e., unstable thermal stratification), with the level of enhancement being a function of a modified Rayleigh number.

2.2.1 Debris Bed Effective Thermal Conductivity

The effective thermal conductivity k_{eff} in a debris bed region is calculated using a method suggested by Imura and Takegoshi²⁶ for particle beds. Radiation heat transfer in the bed is incorporated using the Vortmeyer model²⁷ (parallel conduction/radiation). In this model the effective thermal conductivity is given by

$$k_{eff} = k_{cond} + k_{rad}, \quad (7)$$

where

$$k_{rad} = 4\epsilon_r \sigma \pi d_p T^3 \eta$$

ϵ_r = emissivity of the solid
 σ = Stefan-Boltzmann constant
 d_p = mean particle diameter
 η = an empirical parameter ($\eta = 0.25$ best fit the MP experiments).

In the present model, k_{cond} is assumed to be a weighted combination of contributions from conduction in the solid and liquid, k_o (the solid and the liquid are treated as a single component with a volume-averaged thermal conductivity), and the gas thermal conductivity, k_g . This model can be expressed as

$$k_{cond} = \psi k_g + \frac{1 - \psi}{k_o \omega + k_g (1 - \omega)} k_o k_g, \quad (8)$$

where

$$\omega = 0.3 \alpha_g^{1.6} \left[\frac{k_s}{k_g} \right]^{-0.044}, \quad \psi = \frac{\alpha_g - \omega}{1 - \omega},$$

and

α_g is the volume fraction occupied by gas.

As noted above, the solid and liquid are treated as a single component whose thermal conductivity k_σ is found by volume-averaging the values of the liquid and solid mixture values as follows:

$$k_\sigma = \frac{1}{(\alpha_s + \alpha_l)} \left[\alpha_s \sum_j Y_{sj} k_{sj} + \alpha_l \sum_j Y_{lj} k_{lj} \right], \quad (9)$$

where s and l denote solid and liquid respectively, α denotes volume fraction, and Y is the individual species volume fraction (either liquid or solid).

In the limit as the gas volume fraction goes to zero, both ω and ψ approach zero and consequently, $k_{eff} = k_\sigma$. On the other hand, in the limit as the gas volume fraction goes to one, ψ approaches one and $k_{eff} = k_g$.

Note that Section 2.2.4 describes a further modification of the local thermal conductivity that, if the user so chooses, will potentially enhance the values as calculated here if in a fully dense molten pool region.

2.2.2 Rod Region Effective Thermal Conductivity

Due to the parallel orientation of the fuel rods in this type of region, the effective thermal conductivity in this type of region is anisotropic. From Fouriers Law, a thermal conductivity tensor can be defined by

$$\begin{bmatrix} \frac{q_r}{q_z} \end{bmatrix} = \begin{bmatrix} k_{rr} & 0 \\ 0 & k_{zz} \end{bmatrix} \begin{bmatrix} \partial T / \partial r \\ \partial T / \partial z \end{bmatrix}. \quad (10)$$

In the axial direction, k_{eff} is set equal to k_{zz} , and in the radial direction, k_{eff} is set equal to k_{rr} .

In the axial direction, conduction heat transfer through the gas, conduction through the solid/liquid, and the overall axial radiation heat transport are assumed to occur in parallel. This leads to an expression that can be written as

$$k_{zz} = \alpha_g k_g + (\alpha_s + \alpha_l) k_\sigma + k_{rad,z}. \quad (11)$$

Here, k_g is the thermal conductivity of the gas, k_σ is defined above Equation (9), and the axial radiation component, $k_{rad,z}$, is found as

$$k_{rad,z} = 4\lambda\eta\varepsilon\sigma T^3, \quad (12)$$

where λ is an empirical parameter representing the effective radiation length scale (set equal to 0.016 meters (m) based on MP-2 data), and where

- η = an empirical parameter ($\eta = 0.8$ best fit the MP experiments),
- ε = emissivity (set equal to 0.3),
- λ = an empirical parameter representing the effective radiation length scale (set equal to 0.02 m based on MP-2 data), and
- σ = Stefan-Boltzman constant (5.67×10^{-8} watt (W)/(meter² Kelvin⁴) (W/m²K⁴).

In the radial direction, heat transfer is due primarily to conduction within the gas-solid matrix, and radiation between fuel rods (at high temperature). The model used here is similar to that adopted by Viskanta et al.,²⁸ and can be written in terms of the porosity, $\phi = \alpha_g + \alpha_b$ as

$$k_{rr} = k_f(1 - \sqrt{1 - \phi}) + \frac{k_s}{1 + \frac{k_s(1 - \sqrt{1 - \phi})}{k_f\sqrt{1 - \phi}}} + k_{rad,r} \quad (13)$$

where the radial radiation component, $k_{rad,r}$, is found as per Equation (12) above, with the exception that the empirical parameter, λ , is set equal to 0.0005 m.

2.2.3 Crust Region Effective Thermal Conductivity

In the crust region there is very little pore space and the region is effectively a composite solid. The effective thermal conductivity is, therefore, taken to be the volume average of the conductivities of the various components

$$k_{eff} = \sum_j Y_{sj} k_{sj}, \quad (14)$$

where Y_{sj} is the volume fraction of the j^{th} component. In FPT-4 there are no crust or rod regions, but there is a set of orifice plates that is treated in a similar manner.

2.2.4 Molten Pool Region Effective Thermal Conductivity

An option is now available in DEBRIS to account qualitatively for some aspects of the enhanced heat transport that will occur as a result of buoyancy-driven mixing in a molten pool. In fully dense molten regions where the axial temperature gradient is negative (i.e., unstable thermal stratification), this model calculates a multiplication factor, the value of which represents the magnitude of the effective enhancement to the local effective thermal conductivity. The effective thermal conductivity calculated from Equation (9) is then multiplied by this factor. The basis of this ad hoc model is as follows.

First, it is assumed that an effective thermal conductivity within unstable stratified liquid regions, $k_{eff,pool}$, can be defined as

$$k_{eff,pool} = k_{eff} \left[\frac{Nu_{conv}}{Nu_{cond}} \right], \quad (15)$$

where

Nu_{conv} = the Nusselt number of a horizontal layer of fluid within uniform volumetric heating and with unequal but constant boundary surface temperatures (top and bottom), and

Nu_{cond} = the Nusselt number of a horizontal layer of fluid with uniform volumetric heating and with unequal but constant boundary surface temperatures (top and bottom), but where no fluid motion occurs (i.e., pure conduction regime).

In Equation (15), both Nusselt numbers are defined in terms of the heat transfer at the surface in a standard way such that

$$Nu = \frac{hL}{k} = \frac{Q_w L}{k(T_{max} - T_w)}, \quad (16)$$

where

h = heat transfer coefficient,
 L = distance between the upper and lower surfaces,
 k = thermal conductivity,
 Q_w = heat flux at the surface,
 T_{max} = maximum temperature in the fluid region, and
 T_w = surface temperature.

In DEBRIS, the value of Nu_{cond} is taken as identically equal to two (strictly true only when both top and bottom temperatures are equal), and the value of Nu_{conv} is found from the following correlation derived by Baker:

$$Nu = \frac{.403}{(1 - \eta)} \left[32 Ra_{KG} (1 - \eta)^5 \right]^{.226}, \quad (17)$$

where

$$Ra_{KG} = \frac{g\beta q L^5}{64\alpha vk}, \quad (18)$$

and

g = acceleration of gravity,
 β = coefficient of volumetric expansion,
 q = volumetric heat generation rate,
 k = thermal conductivity of the melt,

L = total height of the fluid layer,
 α = thermal diffusivity,
 ν = kinematic viscosity, and

and where η is defined as a ratio between the positive temperature-gradient-region height, L_0 , to the total height of the pool, L , as is illustrated in Figure 2.

When this option is activated in DEBRIS, each radial ring is treated independently, and Equation (15) is used to modify the value of the effective thermal conductivity in fully liquid regions where the axial temperature gradient is negative.

Figure 2. Illustration of how η is defined.

2.3 Convection

The convective or advective heat transfer processes are modeled for all three phases. The rates of flow for the three phases are calculated separately prior to the solution of the energy equation. For heat transfer resulting from advective liquid and solid motion the liquid/solid mass balance is maintained and the heat transfer process is uncoupled from the conduction/gas-convection calculation. Thus, for each debris bed control volume the mass flow rates of liquid and solid are first determined, the total control volume enthalpy is updated, and from the new total enthalpy the control volume temperature is calculated. Considering two-dimensional flow for a control volume, p , bordered on the left (west), right (east), bottom (south), and top (north) by control volumes w , e , s , and n , respectively, the new total enthalpy, H'_p , at the end of time step, dt , can be written in terms of the total enthalpy at the beginning of the time step, H_p , as

$$\begin{aligned}
 H'_p = H_p + dt \{ & \dot{m}_w h_w - \dot{m}_w h_p - \dot{m}_e h_p + \dot{m}_e h_e \\
 & + \dot{m}_s h_s - \dot{m}_s h_p - \dot{m}_n h_p + \dot{m}_n h_n \}
 \end{aligned}
 \tag{19}$$

Here the function denoted by $\| \|$ returns the value input between the bars if the value is greater than zero and returns zero if the input is less than zero. The mass flow rate at the south boundary of the control volume, for example, is denoted by $\dot{m}_s$, while the specific enthalpy is given by h_s .

Unlike the uncoupled treatment of liquid and solid convection described above, the gas velocities at the control volume boundaries obtained from the solution of the gas phase momentum equations are used to determine the gas-phase convective components, and these are supplied directly to the main heat transfer solver. Thus, gas convection is coupled with conduction and radiation in the DEBRIS code treatment of heat transfer within the debris bed.

2.4 Local Heat Transfer

At a local level (i.e., within a given control volume), the solid, liquid, and gas are assumed to be in local thermal equilibrium. In other words, they share the same temperature. This implies that the rate of heat transfer between the different phases is very high compared to the bed heating rate. If this assumption were to be relaxed, then separate energy equations for the solid, liquid, and gas would need to be solved.

2.5 Radiation Heat Transfer at Boundaries

The MP series experiments did not involve gas flow through the debris bed so that the bed itself was enclosed at all its boundaries by solid structures. In the case of the FPT-4 experiment, however, gas flow enters the lower surface of the bed and exits through the upper surface of the bed into a cylindrical plenum or flow channel that directs the effluent into diagnostic and measurement systems downstream in the Phebus facility. Thus, the FPT-4 debris bed has a free surface at the top of the bed that can radiate to overlying structures. In addition, advective heat transfer in the bed resulting from gas flow prior to the formation of a molten pool, skews the temperature distribution such that the highest temperatures in the bed are achieved near the top surface. Under these conditions radiation from the upper surface of the bed is a key factor in the overall energy disposition.

To calculate the radiative heat flux from the upper bed surface requires a knowledge of the temperatures of the surfaces above the bed in the plenum volume. The problem is complicated by the gas flow out of the bed into the plenum. The gas enters the plenum at or near the temperature of the upper surface of the bed and carries a significant amount of heat into the plenum. Because the gas is composed of steam and hydrogen, the volume above the bed surface is a radiatively participating medium, meaning that the gas absorbs and emits thermal radiation. The net effect is that the heat transfer problem in the upper plenum flow channel is extremely complicated. There are relatively economical methods (Hottel²⁹) for treating the problem if the gas can be assumed to be isothermal or the emission/absorption characteristics of the gas are not strong functions of temperature, but this is clearly not the case for the FPT-4 configuration. A more rigorous solution is possible but computationally prohibitive in terms of computer run time.

The modeling trade-offs in terms of accuracy versus cost involved uncoupling the surface-to-surface radiative transfer from the gas-to-surface radiative transfer. This was implemented in the code by performing a radiation enclosure calculation assuming no absorption/emission in the gas phase and then, in a separate calculation, estimating the radiation exchange between the gas and the walls of the flow channel. The energy and momentum equations for the gas phase are solved using a standard forced-convection finite difference routine that calculates the convective heat fluxes at the channel wall and allows for a volumetric heat source/sink as a result of radiation from the gas to the walls. An implicit finite-difference conduction calculation is performed for the plenum tube structures after the radiative heat fluxes from the bed surface and the combined convection and radiation from the gas volume are calculated. The time step is selected such that the surface and gas temperatures do not change significantly over the time step. This eliminates the necessity for iteration. The radiation enclosure calculations involve the solution of the following set of N equations where N is the total number of absorbing/emitting surfaces.

$$\sum_{j=1}^N \left[\frac{\delta_{kj}}{\epsilon_j} - F_{k \rightarrow j} \frac{1 - e_j}{\epsilon_j} \right] \frac{Q_j}{A_j} = \sum_{j=1}^N (\delta_{kj} - F_{k \rightarrow j}) \sigma T_j^4, \quad (20)$$

where the index k takes on values from 1 to N giving a set of N equations in N unknowns,

and

- δ_{kj} = Kronecker delta
- Q_j = heating rate at the j^{th} surface
- A_j = area of the j^{th} surface
- $F_{k \rightarrow j}$ = radiation configuration factor between areas j and k
- T_j = temperature of j^{th} surface
- ϵ_j = emissivity of j^{th} surface
- σ = Stefan-Boltzmann constant = $5.67 \times 10^{-8} \text{ W/m}^2 \text{ K}^4$

The emissivities are, in general, temperature dependent and differ for each material. The correlations used for the emissivities are given in Section 5.7.

The configuration (form) factors between surfaces are calculated using configuration factor algebra and require only the standard formula for radiation between two facing disks of specific radii to calculate all the necessary factors; ring-to-band, band-to-band, and ring-to-ring. The surfaces are specified as rings representing radial nodes on the debris bed surface and bands that result from axial nodalization of the plenum channel wall.

To estimate the radiative heat transfer rate between the gas phase and the channel wall, which is necessary for calculating the wall temperature, some additional engineering approximations are required. Because the gas temperature is a strong function of position in the plenum flow channel and the transmissivity of steam is also a strong function of temperature, the zoning method of Hottel cannot be used. To achieve a first order approximation for the gas-to-wall radiative heat flux it is assumed that the gas in each axial gas control volume radiates only to the surface immediately adjacent to that control volume. It is further assumed that the gas in each

axial control volume is isothermal, or more correctly, that the gas temperature can be represented by a mean value for the control volume. Then each gas volume can be treated as a small isothermal volume "surrounded" by an enclosure wall that exchanges energy by radiation with the gas in the volume. Using the radiosity at each surface, the energy equation can be written as

$$J_i = \epsilon_i \sigma T_i^4 + \rho_i \sum_{j=1}^N J_j F_{i \rightarrow j} \tau_{ij} + \rho_i \epsilon_g \sigma T_g^4. \quad (21)$$

Equation (21) can be further simplified by assuming that the gas in each axial control volume radiates primarily to its radially bounding surface. This leads to the following expression for the radiosity

$$J_i = \epsilon_i \sigma T_i^4 + \rho_i J_i F_{i \rightarrow i} \tau_{ii} + \rho_i \epsilon_g \sigma T_g^4. \quad (22)$$

Finally, inserting the equation that defines the radiosity into Equation (22), the heat flux at the wall of the i^{th} axial surface along the flow channel that is due to radiation from the gas in the enclosed volume is given by

$$q_{g \rightarrow i} = \epsilon_g \sigma \frac{[\epsilon_i T_i^4 + (\rho_i \epsilon_g + F_{i \rightarrow i} \tau_{ii} - 1) T_g^4]}{1 - \rho_i F_{i \rightarrow i} \tau_{ii}}, \quad (23)$$

where

- $q_{g \rightarrow i}$ = radiative heat flux between the gas and the wall
- ϵ_i = emissivity of the i^{th} surface node
- ϵ_g = emissivity of the gas
- ρ_i = reflectivity of the i^{th} surface
- τ_{ii} = the gas transmissivity over the mean beam length for the i^{th} surface "seeing" itself
- $F_{i \rightarrow i}$ = the radiation form factor for the i^{th} surface "seeing" itself

2.6 Convective Heat Transfer in the Plenum Region

For the FPT-4 experiment the gas flow that exits from the top of the debris bed flows upward through a cylindrical channel that is circular in cross section but varies in radius along the channel. A finite difference method is used to calculate the conductive heat transfer rate within the region that is formed by the structures that lie between the inner surface of this channel and the ultimate heat sink that is the exterior coolant flow. It is necessary to know the temperatures in this region not only for design purposes but also to determine the radiative heat losses from the debris bed upper surface and to estimate the gas temperatures along the channel. It was necessary, therefore, to solve the boundary layer heat transfer equations in the plenum flow channel in order to determine the heat flux at the channel wall.

The solution is somewhat complicated by the fact that part of the total wall heat flux is due to radiation from the gas to the wall and part is from convection from the gas to the wall. The treatment of gas-to-wall radiation was discussed in Section 2.5. Clearly, however, these two processes are coupled. The procedure used here was to estimate the radiative flux separately and simply include the gas radiative heat loss term in the energy equation as a negative source term.

Because the channel is relatively large and the mass flow rates low, the flow is generally laminar. In addition the equations are parabolic, so that a down-stream marching scheme can be used to achieve a solution. A small convection heat transfer code was used that is based on the methods of Patankar and Spalding³⁰ with some minor modifications to perform the gas phase heat transfer calculations. The model adopts an axisymmetrical geometry and expresses the conservation equations in this geometry. The flow is assumed to be a steady, streamline flow around a surface of revolution with the coordinates defined as shown in Figure 3. In this geometry the conservation equations can be expressed as

Continuity

$$\frac{\partial}{\partial x}(\rho ur) + \frac{\partial}{\partial y}(\rho vr) = 0, \quad (24)$$

Momentum

$$\rho u \frac{\partial u}{\partial x} + \rho v \frac{\partial u}{\partial y} = \frac{1}{r} \frac{\partial}{\partial y} \left(r \mu \frac{\partial u}{\partial y} \right) - \frac{dp}{dx} + B_b, \text{ and} \quad (25)$$

Energy

$$\rho u \frac{\partial h}{\partial x} + \rho v \frac{\partial h}{\partial y} = \frac{1}{r} \frac{\partial}{\partial y} \left[r \left(\frac{k}{C_p} \right) \frac{\partial h}{\partial y} \right] + Q_v. \quad (26)$$

In these equations u and v are the streamwise and crosswise velocities, B_x is the body force in the x direction, Q_v is the volumetric heat source, and h is the enthalpy. The continuity equation can be eliminated by performing the standard stream function transformation wherein we define the stream function, Ψ , such that,

$$\frac{\partial \Psi}{\partial x} = -\rho vr, \quad \text{and} \quad \frac{\partial \Psi}{\partial y} = \rho ur. \quad (27)$$

By applying the transformations in Equation (27) to Equations (25) and (26), noting that Equation (27) identically satisfies the continuity Equation (24), and defining a dimensionless stream function

$$\omega = \frac{\Psi - \Psi_I}{\Psi_E - \Psi_I}, \quad (28)$$

Figure 3. Geometry of the plenum region convection calculations.

the momentum and energy equations can both be cast into the general form

$$\frac{1}{\Psi_{EI}} \frac{\partial}{\partial x} (\Psi_{EI} \Phi) + \frac{\partial}{\partial \omega} \left[(a + b\omega) \Phi - c \frac{\partial \Phi}{\partial \omega} \right] = d. \quad (29)$$

In Equation (29), Φ is either the velocity, u , or the enthalpy, h , and Ψ_{EI} is shorthand for $(\Psi_E - \Psi_I)$. In the dimensionless transformation, Equation (28), Ψ_E and Ψ_I are the stream functions at the inner wall and the exterior wall, respectively. The remaining constants in Equation (29) are given by

$$a = -\frac{1}{\Psi_{EI}} \frac{d\Psi_I}{dx}, \quad (30a)$$

$$b = -\frac{1}{\Psi_{EI}} \frac{d\Psi_{EI}}{dx}, \quad (30b)$$

$$c = \frac{1}{\Psi_{EI}^2} r^2 \rho u \Gamma, \quad (30c)$$

$$d = \frac{S}{\rho u}. \quad (30d)$$

In Equation (30c), Γ is a generalized diffusion coefficient (thermal for the energy equation and momentum for the momentum equation) and in Equation (30d), S is a source term with volumetric heat source for the energy equation and terms like the pressure gradient for the momentum equation.

The equations for enthalpy and momentum are discretized into control volumes surrounding mesh points and solved numerically in a downstream marching process in which the region of interest is divided into a grid with the grid length, Δx , specified for each grid in the x direction. The velocity and temperature fields that result from the numerical simulation of the flow channel are then used to calculate the heat fluxes at the wall. The Δx lengths are made to correspond to the same nodalization schemes used in the radiation transfer calculations and the finite difference conduction calculations in the plenum heat structures and the three heat transfer modes are then "soft" coupled (not solved simultaneously). This means that the radiation and convection calculations are performed first assuming the wall temperatures do not change significantly over a time step, and then the conduction calculation is performed assuming that the wall fluxes do not change significantly over the time step. The time step is specified such that these assumptions do not introduce a significant error.

It should be noted that the geometry associated with the plenum flow channel can easily be cast into that depicted in Figure 3 by setting the distance from the axis of symmetry of the interior wall (surface I) equal to zero and making that surface adiabatic with zero cross flow while prescribing the location and the temperatures of the exterior wall (surface E) at each x -location grid point.

2.7 Fission Heating

In DEBRIS, fission heating is treated very simply. In Section 2.1, the fifth term of Equation (6) was described as representing the decay heating generation or fission heating term. This term was written as

$$[\alpha_s \rho_{s1} + \alpha_l \rho_{l1}] Q, \quad (31)$$

where Q is the heat source expressed as energy release per unit mass of species 1 (which is generally defined as UO_2). The value of Q is controlled by the user through various parameters in the input, and may be a function of both spatial location and time. Note that this formulation allows for the local heat generation rate to change as the local effective density (mass fraction) of UO_2 changes as a result of the relocation of either solid or liquid material.

Experiment configurations in which heating is produced by fission power can produce significant power gradients in the debris bed that are due to neutronic "self-shielding." This requires that the resulting spatial and temporal effects on power distribution are properly modeled. The MP-1,2 version of the code utilized a driver-reactor-to-test-section power coupling factor based on neutronic code calculations, together with normalized radial and axial "shape factors," also based on neutronic calculations, to estimate the total power applied to the debris bed and the spatial distribution of the power within the bed. After significant melting and relocation of fissionable material within the bed, the overall coupling factor can change somewhat and the axial "shape factors" can also be affected. In the MP-1,2 experiments these changes in the axial shape factor were addressed by performing neutronic calculations for several stages in the test starting before incipient melting and ending with the final test section configuration. The DEBRIS code models allowed for a number of discrete changes in the axial shape factors at user-specified times. This

option remains active in the current version of DEBRIS, and an additional option is available that maintains the original axial and radial shape factors while adjusting the local power for the effects of self-shielding. The model assumes that there are no temperature or radial shape factors effects and that the UO_2/ZrO_2 fraction remains unchanged. An additional power factor is then applied at each location based on the gas volume fraction that is a measure of the extent of fuel densification. A simple quadratic equation based on three data points, one for the initial bed composition, one for the fully dense configuration, and one for the completely voided configuration, is used to characterize this power factor. Then the self shielding correction is estimated by

$$f_{shield} = C_0 + C_1\alpha_g + C_2\alpha_g^2. \quad (32)$$

Based, for example, on data for the MP-1 experiment in which the local power factor is taken as 1 for the initial porosity of 0.5, 0.4 for the fully dense configuration ($\alpha_s = 0$), and 2.2 for the fully voided configuration ($\alpha_s = 1.0$), the coefficients are determined to be

$$C_0 = 0.4, C_1 = 0.6, C_2 = 1.2.$$

It should be noted these coefficients are appropriate only for the configuration and fuel enrichment specific to the MP-2 test, and would not apply for a debris bed having dissimilar dimensions or fuel enrichment. The shield factor defined above is empirical and would need to be determined using neutronic calculations for each specific configuration.

3. MELTING AND REFREEZING BEHAVIOR

3.1 Overview of the Melting/Freezing Model

The first major assumption affecting the melting and refreezing model used in DEBRIS occurs at the end of each time step when each control volume is assumed to be at thermal equilibrium. This means that each material component within the cell, whether liquid or solid, has the same temperature, T . For a control volume containing "nc" material components (each having a known enthalpy versus temperature relationship $h_j(T)$) and having volume, Vol , the total enthalpy of the material within that control volume, H_{tot} can be expressed as

$$H_{tot} = \left(\sum_{j=1}^{nc} [\alpha_s Y_{sj} \rho_{sj} + \alpha_l Y_{lj} \rho_{lj}] h_j(T) \right) Vol. \quad (33)$$

Given the gross composition and total enthalpy of the control volume, Equation (33) can be solved directly to find the equilibrium temperature, T . In the current version of DEBRIS, standard root-finding techniques are applied because the functional dependence of enthalpy on temperature is, in general, a nonlinear relationship.

If any of the materials is in a phase transition region, the relationship between liquid mass fraction, f_l , and enthalpy must be known to determine the liquid/solid state of each material (i.e., $\alpha_s Y_{sj}$ and $\alpha_l Y_{lj}$). For each pure material, j , the temperature during melting is assumed constant and equal to $T_{melt,j}$, and the relationship between liquid mass fraction and enthalpy while melting is assumed to be of the following form

$$f_{lj} = \frac{\alpha_l Y_{lj} \rho_{lj}}{[\alpha_s Y_{sj} \rho_{sj} + \alpha_l Y_{lj} \rho_{lj}]} = \frac{h_j(T) - h_{j,sol}}{h_{j,liq} - h_{j,sol}}. \quad (34)$$

Furthermore, the relationship between the total material enthalpy and that of the liquid and solid components can be written as

$$h_j = f_{lj} h_{lj} + (1 - f_{lj}) h_{sj}. \quad (35)$$

For a collection of independent materials (i.e., no material interactions), Equations (33) to (35) provide the necessary closure relationships to determine completely the thermodynamic equilibrium state of the multi-component material if the total cell enthalpy and gross material composition are known.

The final topic that must be addressed to describe completely the melting/refreezing model in DEBRIS is the area of material interactions. In DEBRIS, the interactions between materials within a control volume can be treated in either of two ways.

The first option is to assume that no material interactions occur, and thus the materials behave independently from a melting and freezing perspective. This corresponds to the limit where material interaction rates are extremely slow. Under this assumption, Equations (33) to (35) are sufficient to determine completely the solid/liquid state of each material.

The second option is to assume that the system is always in complete thermodynamic equilibrium, and that the melting and freezing behavior follows the pattern determined by equilibrium thermodynamics. This corresponds to the limit where material interaction rates are extremely fast. To treat this case properly, equilibrium phase-diagram information is needed for all possible material combinations. Unfortunately, for multi-component systems these phase diagrams can become extremely complex, and at present only rather limited data are available. Thus the current approach is to deal with a more limited set of binary or pseudo-binary phase diagrams and only treat those material interactions that appear to be of greatest importance. In the MP-1 and MP-2 analysis, the only material interaction modeled was the $\text{ZrO}_2\text{-UO}_2$ reaction, and in this case the system was treated as behaving according to a pseudo-binary phase diagram. As explained in detail in Section 3.2, this provides the key information required to solve for the liquid and solid composition when both ZrO_2 and UO_2 are present (note that all other materials are still treated independently as in option one).

These two limiting behaviors form the basis of the generalized melting and refreezing models used in the current version of DEBRIS.

3.2 $\text{ZrO}_2\text{-UO}_2$ Material Interactions

If thermodynamic equilibrium is assumed (fast reaction rate assumption), then the melting and refreezing models require the use of equilibrium phase-diagram information. In this case the energy equation is first solved at each time step to determine the energy transport and energy input throughout the system. Then, based on the calculated enthalpy in each local control volume, the liquid and solid volume fractions together with the species mass compositions in both the liquid and the solid are found from equilibrium phase-diagram data. For MP-1, the only region to experience melting during the experiment was the debris bed region, which consisted of a heterogeneous mixture of UO_2 and ZrO_2 particles. Thus, the system of interest was the ternary U-Zr-O system.

In the current version of DEBRIS, the ternary U-Zr-O phase diagram is approximated by the pseudo-binary $\text{ZrO}_2\text{-UO}_2$ phase diagram illustrated in Figure 4. The equations defining the solidus and liquidus curves in this approximation are as follows:

$$T_{sol} = \begin{cases} 3023 - 740 m_z + 740 m_z^2, & m_z \leq 0.5 \\ 2973 - 540 m_z + 540 m_z^2, & m_z > 0.5 \end{cases} \quad (36)$$

and

Figure 4. Pseudo-binary phase diagram for the $\text{ZrO}_2\text{-UO}_2$ system used in the MP-1 and MP-2 DEBRIS calculations.

$$T_{liq} = \begin{cases} 2930.5 + 92.5 \cos(2\pi m_z), & m_z \leq 0.5 \\ 2905.5 + 67.5 \cos(2\pi m_z), & m_z > 0.5 \end{cases} \quad (37)$$

where m_z , the mole fraction of ZrO_2 , can be defined as follows in terms of the molecular weights W_1 and W_2 (the subscripts 1 and 2 denote UO_2 and ZrO_2 respectively).

$$m_z = \frac{(\alpha_l Y_{l2} \rho_{l2} + \alpha_s Y_{s2} \rho_{s2}) / W_2}{(\alpha_s Y_{s1} \rho_{s1} + \alpha_l Y_{l1} \rho_{l1}) / W_1 + (\alpha_s Y_{s2} \rho_{s2} + \alpha_l Y_{l2} \rho_{l2}) / W_2} \quad (38)$$

Equations (36) and (37) are convenient approximations of the limited data available in the literature (see, for example, references [31] and [32]).

When a control volume containing UO_2 and ZrO_2 reaches a temperature where melting is occurring, the enthalpy function for the two-phase mixture is complicated by the behavior described in the phase diagram. Currently, the DEBRIS modeling does not account for any dissolution energy associated with the material interaction. Given that the control volume is at some temperature, T , the procedure for finding the enthalpy and composition of the $\text{UO}_2\text{-ZrO}_2$ components is as follows:

Step 1 Apply Equations (29) and (30) to find the solidus and liquidus temperatures and verify that $T_{sol} < T < T_{liq}$.

Step 2 Find the composition of the solid by finding where the current temperature isotherm intersects the solidus curve. This is done by inverting Equation (36) and substituting T for T_{sol} as follows

$$m_{z,sol} = \begin{cases} 0.5(1 - \sqrt{1 - (3023 - T)/185}), & m_z \leq 0.5 \\ 0.5(1 + \sqrt{1 - (2973 - T)/135}), & m_z > 0.5 \end{cases} \quad (39)$$

Step 3 Find the composition of the liquid by finding where the current temperature isotherm intersects the liquidus curve. This is done by inverting Equation (37) and substituting T for T_{liq} as follows

$$m_{z,liq} = \begin{cases} \frac{1}{2\pi} \cos^{-1}\left(\frac{T - 9230.5}{92.5}\right), & m_z \leq 0.5 \\ \frac{1}{2\pi} \cos^{-1}\left(\frac{T - 2905.5}{67.5}\right), & m_z > 0.5 \end{cases} \quad (40)$$

Step 4 Find the total liquid and solid mole fractions by applying the lever rule.

$$m_{liq} = \frac{m_z - m_{z,liq}}{m_{z,sol} - m_{z,liq}} \quad (41)$$

$$m_{sol} = 1 - m_{liq} \quad (42)$$

Step 5 Determine the total enthalpy by summing the enthalpies from each of the four components (i.e., solid ZrO_2 , solid UO_2 , liquid ZrO_2 and liquid UO_2). No variation in the enthalpy versus temperature relationships are made from what is used for ZrO_2 and UO_2 elsewhere (see Section 5).

The application of these five steps defines the functional dependence of enthalpy on temperature for any UO_2 - ZrO_2 component that is in the two-phase (melting) region.

4. RELOCATION OF DEBRIS MATERIAL

In this section, the material relocation models that allow for the movement of both liquid and solid debris are described. Briefly stated, the framework for this modeling is a set of mass and momentum conservation equations that are approximately solved on a discrete numerical grid using standard finite difference numerical techniques. These equations were introduced in Section 1, and are now described in greater detail. The models described here allow for fully two-dimensional liquid motion (r-z), but only one-dimensional (z) motion of solid material. In Section 4.1.2, the specific assumptions, correlations, and models employed in the liquid momentum equation are described. In Section 4.1.3, the axial relocation model for solid material is described.

4.1 Conservation Equations for Mass and Momentum

4.1.1 Mass Conservation

Mass conservation equations are solved for each species j present in the debris bed. Balancing the mass stored in a differential control volume, convection by the liquid, convection by the solid (as it settles), and production (or depletion) gives for each species j

$$\frac{\partial}{\partial t}(\alpha_l Y_{lj} \rho_{lj}) + \nabla \cdot (Y_{lj} \rho_{lj} \bar{u}) + \frac{\partial}{\partial z}(\alpha_s Y_{sj} \rho_{sj} U) = -\frac{\partial}{\partial t}(\alpha_s Y_{sj} \rho_{sj}) + R_j, \quad (43)$$

where

- $\bar{u} = (u, v)$ is the two-dimensional liquid superficial velocity vector,
- U = the velocity at which the solid collapses,
- α = a volume fraction,
- Y_{ij} = the volume fraction of phase i that is occupied by material species j ,
- R_j = the rate of production of material species j , and

where the subscripts l and s refer to liquid and solid, respectively.

Note that species diffusion is neglected in Equation (43). Typical diffusivities for liquids near their melting points are on the order of 10^{-9} meter²/second (m²/s)³³. For time scales on the order of 10^3 s, the distance characteristic of diffusion, $(Dt)^{1/2}$, is approximately 10^{-3} m. That is, liquid phase diffusion is only important over length scales comparable to the average particle diameter.

4.1.2 Liquid Momentum Conservation

Liquid flow through the debris bed is modeled based on methods developed for flow through porous media. A two-dimensional (r-z) momentum equation (a modified form of "Darcy's Law") accounts for liquid melt relocation that is a result of both gravity and capillary forces. Because the liquid velocities are assumed to be small, inertial terms (convected momentum) are

neglected. The viscous drag is included by modifying Darcy's Law to account for undersaturated flow.

Balancing viscous drag (which is assumed to vary linearly with velocity), gravity, and changes in pressure gives

$$\rho_l \frac{\partial \bar{u}}{\partial t} + \frac{\mu_l}{\kappa_l} \bar{u} = -(\nabla P_l + \bar{g} \rho_l), \quad (44)$$

where

- ρ_l = the liquid density,
- μ_l = the dynamic viscosity of the liquid,
- κ_l = the relative permeability (modified to account for understaturated flow conditions),
- $\bar{u} = (u, v)$ is the two-dimensional liquid superficial velocity vector
- P_l = the liquid pressure, and
- g = the gravitational acceleration.

Capillary forces enter Equation (44) through the term involving the liquid pressure. Section 4.2 will discuss the details of modeling each of the terms in Equation (44) and review the flow conditions under which it should be valid.

4.1.3 Solid Momentum Conservation

Currently a momentum equation for the relocation of solid debris material is not solved in the DEBRIS relocation modeling. Instead, a simple collapse criteria coupled with the conservation equation is used to determine the axial relocation of solid material. This approach is described in Section 4.3.

4.2 Modeling the DEBRIS Liquid Momentum Equation

Liquid relocation in the debris bed is modeled in DEBRIS by using a modified form of what is often called Darcy's Law. This equation, Equation (44), has been simplified in the MP-1 and MP-2 analysis by assuming that a) transient relaxation times are small relative to the time step taken in the analysis and b) capillary forces in the axial (z) direction are small relative to gravity. Although not used in the FPT-4 calculations, an implicit model that retains the capillary terms in the axial and radial directions and adds a hydraulic head term in the radial direction (for control volumes located in the molten pool region) was added as an alternative option. Both options will be discussed. With these assumptions, the axial and radial momentum equations reduce to the following simple velocity relationships.

$$u = -\frac{\kappa_l}{\mu_l} \left[\frac{\partial P_l}{\partial z} + \rho_l g \right] \quad (45)$$

$$v = -\frac{\kappa_l}{\mu_l} \frac{\partial P_l}{\partial r} \quad (46)$$

In application, these simplified relationships must be contained by a set of limits to prevent the violation of basic physical laws. These include the following:

- 1) the velocity is limited so that more mass cannot leave a control volume in a given time step than is actually there at the beginning of the time step, and
- 2) the velocity is limited so that more mass cannot flow into a control volume than there is space available. (This constraint accounts for the effect of hydrostatic pressure that is not explicitly being modeled. See Section 4.2.2.)

Finally, different schemes are used to account for the radial motion that would naturally equilibrate the top liquid surface level in a pool of melt (by hydrostatic pressure forces). With the explicit solution option, an ad hoc radial relocation model is used that simply identifies molten pool regions and adjusts the adjacent cell saturation levels so that the melt pool liquid level is radially uniform. With the implicit liquid flow model, the hydrostatic head term is incorporated in the equation and the liquid in the pool is allowed to "seek" the appropriate level.

As applied in DEBRIS, Equations (45) and (46) also imply the following assumptions:

- 1) r-z axisymmetric behavior,
- 2) constant species densities,
- 3) low-velocity (laminar) flow through a porous medium, and
- 4) undersaturation effects can be modeled by a relative permeability.

The geometric constraint, item 1, is simply a consequence of the current DEBRIS geometry.

The densities are assumed constant to simplify the equations governing mass conservation. Thus, temperature-induced natural convection buoyancy forces are not currently modeled.

Because the velocity is assumed low, the inertial terms in the momentum equation are neglected and the flow is assumed to be laminar. This assumption requires that the flow Reynolds number (based on the particle diameter) be less than approximately 10 (see reference [34], p. 156);

$$Re = \frac{\rho_l v D_p}{\mu} \leq 10. \quad (47)$$

Also note that because the flow is assumed to exist within a porous solid medium, this modeling approach breaks down if the solid volume fraction becomes too small (due say to melting) over a large portion of the debris bed.

The three terms in Equation (44) affecting the change in velocity represent the viscous friction, $(\mu / \kappa_l) \bar{u}$, pressure forces, $(-\nabla P_l)$, and gravity, $(\bar{g} \rho_l)$. Because both the viscous friction and pressure terms require additional explanation, these will be described in detail in Sections 4.2.1

and 4.2.2. Section 4.2.1 will also include a discussion of the modification to account for undersaturated flow conditions.

4.2.1 Modeling the Viscous Friction Term

The viscous term in Equation (44) varies from the normal term in Darcy's Law by the introduction of a liquid-phase relative permeability, κ_l , which accounts for undersaturated flow conditions. In fully saturated flow, κ_l simply equals the permeability κ and the equation reduces to Darcy's Law. In undersaturated flow, only a fraction of the solid is in contact with liquid and although κ_l is proportional to κ , they are not equal. It can be shown that κ_l depends on the particle diameter, D_p , the porosity, ε , the saturation, S ($S = \alpha/(1-\alpha_s)$), and a critical value of the saturation, S_r , that is often referred to as the residual saturation. The quantity S_r is defined as the threshold value of saturation below which bulk liquid motion ceases.³⁵ When the saturation is below the critical value, the liquid is trapped between the particles by surface tension effects. Liquid will only start to flow when the saturation is increased to the point where these pockets of trapped liquid touch and coalesce.

To calculate the permeability of the bed, κ , DEBRIS uses a correlation by Bird et al.³⁶ that was derived by modeling the porous solid as a bundle of capillary tubes:

$$\kappa = \frac{D_p^2 \varepsilon^3}{150 (1 - \varepsilon)^2}, \quad (48)$$

where ε is the porosity and the factor of 150 is determined empirically.

To calculate κ_l , the current DEBRIS modeling applies the correlation suggested by Reed et al.³⁷ In this formulation

$$k_l = \begin{cases} \kappa S_e^3 & , \text{ for } S > S_r \\ 0 & , \text{ for } S \leq S_r \end{cases}, \quad (49)$$

where the effective saturation, S_e , is defined in terms of a residual saturation, S_r , such that

$$S_e = \frac{(S - S_r)}{(1 - S_r)} \quad (50)$$

and

$$S_r = \begin{cases} \frac{1}{86.3} \left[\frac{\gamma \cos \theta}{\kappa \rho_l g} \right]^{0.263} & ; 0 < \theta < 90^\circ \\ 0 & ; 90^\circ < \theta < 180^\circ \end{cases}, \quad (51)$$

where

- γ = surface tension of the liquid,
- θ = liquid-solid contact angle,
- κ = porosity,
- ρ_l = liquid density, and
- g = gravity.

In a nonwetting system ($90^\circ < \theta < 180^\circ$), $S_r = 0.0$. The dependence of S_r on the porous matrix is contained in the permeability, κ . Increasing the particle diameter or the porosity raises κ and leads to lower values of S_r . For packed beds consisting of small, tightly packed particles, the saturation must be increased to a high value before bulk liquid motion is observed.

4.2.2 Modeling the Liquid Pressure Term

The first key assumption made here is that changes in the gas pressure, P_g , are assumed to be much smaller than changes in capillary pressure, P_c . By definition $P_c = P_g - P_l$ and we can write

$$\nabla P_l = -\nabla P_c. \quad (52)$$

To calculate P_c , DEBRIS applies a relationship suggested by Leverett³⁵, who used dimensional analysis to show that the capillary pressure can be represented as

$$P_c = J\gamma \cos \theta \sqrt{\frac{(1 - \alpha_s)}{\kappa}}, \quad (53)$$

where

- J = an empirical function of saturation (the "Leverett" function),
- γ = surface tension of the liquid,
- θ = liquid-solid contact angle,
- α_s = solid volume fraction, and
- κ = the permeability, κ .

The empirical function J in Equation (53) is found from Hoffman and Barleon³⁸ as

$$J = 0.38[S_e + 0.014]^{-0.27}, \quad (54)$$

where the effective saturation, S_e , is defined above in Equation (50).

Because P_c decreases as the particle diameter, D_p , increases, capillary forces are small in beds with large particles. For $0^\circ < \theta < 90^\circ$, increasing the solid fraction, α_s , or decreasing the saturation, S_e , increases P_c ; capillary forces therefore move liquid into regions of high α_s (low porosity) and low saturation. For $90^\circ < \theta < 180^\circ$, decreasing α_s or increasing S_e increases P_c ; capillary forces therefore move liquid into regions of low α_s (high porosity) and high saturation.

That is, melt tends to agglomerate in a nonwetting system. This effect has been observed in stainless steel-UO₂ beds in both the molten pool (MP) and dry capsule (DC) experiments conducted at SNL (see References [39], and [40]).

4.2.3 Implicit Modeling of Liquid Flow with Capillary and Hydraulic Forces

The implicit solution starts by rewriting the liquid mass equation in terms of the saturation, S , which is defined as the fraction of the pore space that is occupied by liquid. To facilitate the solution the radial and axial flow are separated with the resulting equations

$$\epsilon \frac{\partial S}{\partial t} + \frac{\partial v}{\partial z} = 0 \quad (55)$$

and

$$\epsilon \frac{\partial S}{\partial t} + \frac{1}{r} \frac{\partial}{\partial r}(ru) = 0. \quad (56)$$

The velocities, v and u , are rather complicated functions of the saturation so that the resulting differential equations are nonlinear in S and require an iterative method for solution. Equations (55) and (56) are discretized and the iterative multiple-variable Newton method is used to converge to a solution at each time step. The procedure involves solving a matrix at each iteration. Although the matrix is tridiagonal, and the matrix solution is quite fast, the time stepping control is necessary to achieve a converged solution. Time step control requires subdividing the main DEBRIS time step in the liquid flow calculation and, in addition, if necessary, reducing the main DEBRIS code time step.

For configurations in which gas flow is occurring in the debris bed simultaneously with melt and crust formation, the local gas flow rate can become quite high. To achieve a stable solution in this regime it is necessary to reduce the main DEBRIS code time step to ~ 0.1 s. When the subdivided time step imposed by the implicit liquid flow model is superimposed on this already small time step, a prohibitively long computer run time results. It is not, therefore, recommended that the implicit capillary flow model be used with gas flow configurations.

4.3 Solid Debris Motion Model

The current solid debris motion model conceptualizes solid relocation as a simple "collapse" process that occurs when the solid debris matrix no longer has sufficient structural integrity to support itself. The only mode of solid relocation is one-dimensional, and is allowed to occur only in the downward direction under the influence of gravity. Basically, the model assumes that solid debris will collapse or relocate downward from any given control volume (designated the "donor" cell) into the next lower cell (designated the "receiver" cell) when both the following two criteria are met

- 1) the porosity of the donor cell exceeds a user specified value, ϕ_{crit} , and
- 2) the porosity of the receiver cell exceeds a user specified minimum value, ϕ_{min} .

If these conditions are met, a value for the velocity, U , is calculated such that the transfer of material from the donor cell either increases the porosity of the donor cell to the user-specified maximum value, ϕ_{max} , or decreases the porosity of the receiver cell to the user-specified value ϕ_{min} , whichever criteria is the limiting factor.

Changing the values of ϕ_{crit} , ϕ_{min} , and ϕ_{max} allow for the limited approximation of various solid relocation behaviors. For the MP-1 experiment analysis the following values were found to reproduce the observed behavior; $\phi_{crit} = 0.9$, $\phi_{min} = 0.4$, and $\phi_{max} = 0.999$. Note that the motion of solid debris within the solid/liquid matrix may displace liquid from one control volume to another. If the downward motion of solid debris requires the displacement of liquid, the liquid is constrained to displace upward into the control volume from which the solid debris was relocated.

4.4 Gas-Phase Flow Model

Explicitly writing out the operators in Equations (2) and (4), the continuity equation and the momentum equations become

$$\frac{\partial(\alpha_g \rho_g)}{\partial t} + \frac{1}{r} \frac{\partial}{\partial r}(r \rho_g v_g) + \frac{\partial}{\partial z}(\rho_g u_g) = 0, \quad (57)$$

$$v_g = -\frac{\kappa_g}{\mu_g} \frac{\partial P}{\partial r}, \quad (58)$$

and

$$u_g = -\frac{\kappa_g}{\mu_g} \left[\frac{\partial P}{\partial z} + \rho_g g \right]. \quad (59)$$

When Equations (58) and (59) are substituted into Equation (57) and the approximation is made that the gas density does not change significantly over one time step, the following partial differential equation in terms of pressure as the single parameter results.

$$\frac{1}{r} \frac{\partial}{\partial r} \left[\frac{r \rho_g \kappa_g}{\mu_g} \frac{\partial P}{\partial r} \right] + \frac{\partial}{\partial z} \left[\frac{\rho_g \kappa_g}{\mu_g} \left(\frac{\partial P}{\partial z} + \rho_g g \right) \right] = 0 \quad (60)$$

The numerical solution to this equation yields the two-dimensional pressure field within the debris bed that is subject to the constraint that the net mass flow rate into each control volume is zero. The density is specified by the ideal gas law based on the temperature at the beginning of the time step. This approximation does not rigorously conserve the gas mass with a net loss of

gas mass taking place over the duration of the run that is equal to the integral over the volume of the difference in density as a result of the difference between the initial and final temperature distributions. This error is quite small compared to the total quantity of gas that passes through the bed over the duration of a typical experiment. This approximation eliminates the necessity for iterations.

When Equation (60) is discretized, it produces the usual banded matrix that results from a two-dimensional formulation. The standard matrix solver produces a reasonably rapid solution for the debris bed pressure field. With the cell-center pressure known, Equations (58) and (59) can be used to calculate the velocity and the mass flow rates at all four control volume boundaries. These velocities are in turn input into the second term of Equation (6) as the convective components of the energy equation.

Similar procedures are used for determining permeability in the Darcy Law formulation for gas flow in a porous media as is used for liquid flow (see Section 4.2) except that gas properties are used. Because the temperature regime of interest in debris bed experiments includes temperatures in excess of 3000 K, it is necessary to address the issue of steam and hydrogen dissociation in determining the thermophysical properties of the component gases. Associated with the dissociation of steam, for example, is the chemical heats of reaction as the water molecule breaks down to H_2 , O_2 , and OH and (if temperatures are sufficiently high) ultimately to nascent hydrogen and oxygen. The net effect of the dissociation reactions is a substantial effective increase in the heat capacity because additional energy must be supplied to the steam molecule to break the chemical bond. This is discussed further in Section 5.8.

5. MATERIAL PROPERTIES

An important part of accurately predicting the physical processes occurring during late-phase melt progression is the accurate description of material properties. In this section the functional relationships used in DEBRIS for calculating the MP-2 late-phase melt progression experiment are described. Additional properties information that was required for the FPT-4 experiment is also included, i.e., gas properties and radiation properties. The properties described here include the thermal conductivity, density, melting temperatures and associated heats of fusion, viscosity, specific heat, enthalpy, and hemispherical total emissivity. The algorithms for determining the absorbing and emitting characteristics of steam are rather involved, and for that reason, they have not been reproduced here. For a description of the methodology see Kreith and Bonn.⁴¹

In general, the properties presented here were obtained from three primary sources. MATPRO⁴² was used preferentially and supplied most of the data for reactor materials, i.e., UO₂, ZrO₂, zircaloy, etc. For materials not available in the MATPRO document, Touloukian⁴³ was used extensively. For specially prepared materials such as the fiber insulation used in the FPT-4 experiment, data supplied by the French were employed in the form of curve fits of the raw data.

In the equations that follow, T denotes temperature in K, and T_0 denotes the initial temperature of the system at the beginning of the calculation.

5.1 Thermal Conductivity

Thermal conductivity for each material is shown in the following equations in units of watt/meter/Kelvin (W/m/K).

UO₂:
$$k_{UO_2} = \frac{A}{\frac{1}{B + CT} + DT^3} \quad (61)$$

For $T < 3023$ K; $A = 100.0$, $B = 4.0$, $C = 2.57 \times 10^{-2}$, $D = 7.3 \times 10^{-13}$
 For $T > 3023$ K; $A = 11.5$, $B = 1.0$, $C = 0$, $D = 0$

ZrO₂:
$$k_{ZrO_2} = A + BT \quad (62)$$

For $T < 2973$ K; $A = 0.835$, $B = 3.62 \times 10^{-4}$
 For $T > 2973$ K; $A = 1.4$, $B = 0.0$

Zircaloy:
$$k_{Zr} = A + BT + CT^2 + DT^3 \quad (63)$$

For $T < 2098$ K; $A = 7.51$, $B = 2.09 \times 10^{-2}$, $C = -1.45 \times 10^{-5}$, $D = 7.67 \times 10^{-9}$
 For $T > 2098$ K; $A = 36.0$, $B = C = D = 0.0$

Stainless Steel: $k_{ss} = A + BT$ (64)

For $T < 1671$ K; $A = 7.581$, $B = 1.89 \times 10^{-2}$
 For $1671 < T < 1727$ K; $A = 610.9393$, $B = -0.342176$
 For $T > 1727$ K; $A = 20.0$, $B = 0.0$

Indium: $k_{ind} = 25.0$ (65)

Tin: $k_{tin} = A + BT + CT^2$ (66)

$A = 101.33$, $B = -0.1825$, $C = 2.166 \times 10^{-4}$

Silver: $k_{sil} = A + BT + CT^2$ (67)

$A = 445.06$, $B = -0.044052$, $C = -2.1635 \times 10^{-5}$

ZrO₂ Fiber Insulation: $k_{ZrO_2F} = A + BT + CT^2 + DT^3$ (68)

$A = 1.84 \times 10^{-1}$, $B = 3.9828 \times 10^{-4}$, -5.6108×10^{-8} $D = 6.24578 \times 10^{-12}$

ThO₂ (Melt Barrier): $k_{ThO_2} = \eta(A + BT + CT^2 + DT^3 + ET^4)$ (69)

For $T < 1900$ K; $\eta = 0.9$
 $A = 27.88269$, $B = -6.720693 \times 10^{-2}$, $C = 7.1066831 \times 10^{-5}$,
 $D = -3.429394 \times 10^{-8}$, $E = 6.2224843 \times 10^{-12}$

For $T > 1900$ K; $\eta = 0.9$
 $A = 0.25$, $B = C = D = E = 0.0$

Tantalum (Liner): $k_{Ta} = A + BT$ (70)

For $T < 600$ K; $A = 75.438$, $B = -1.4226 \times 10^{-2}$
 For $600 < T < 1000$ K; $A = 72.718$, $B = -9.6232 \times 10^{-3}$
 For $1000 < T < 1800$ K; $A = 65.521$, $B = -2.5104 \times 10^{-3}$
 For $T > 1800$ K; $A = 59.699$, $B = 6.9733 \times 10^{-3}$

Helium Gas: $k_{He} = AT^B$ (71)

$A = 2.639$, $B = 0.7085$

5.2 Density

Currently, except for gases, DEBRIS can only treat materials whose densities are assumed constant with temperature. The values used in the MP-1 and MP-2 analysis are listed below in Table 2. Density is given in units of kilogram/cubic meter (kg/m^3).

Table 2. Constant material densities used in DEBRIS for the MP-1 and MP-2 calculations.

Material	Density (kg/m^3)
UO ₂	10,400
ZrO ₂	5840
Zircaloy	6560
Steel	7500
Indium	7300
Tin	6500
Silver	10,500
ZrO ₂ Fiber	1440
ThO ₂	9860
Ta	16,600

5.3 Melting Temperatures and Heats of Fusion

Currently, DEBRIS treats all materials except the UO₂-ZrO₂ compound as melting at a single fixed temperature. For a description of the behavior of UO₂-ZrO₂ during melting see Section 3.2. The melting temperatures and the associated heats of fusion that were used in the MP-1 and MP-2 analysis are listed in Table 3. Units for the heats of fusion are joules/kilogram (J/kg).

Table 3. Melting temperatures and heats of fusion.

Material	Melting Temperature (K)	Heat of Fusion (J/kg)
UO ₂	3023	2.78×10^5
ZrO ₂	2973	7.06×10^5
Zircaloy	2125	2.25356×10^5
Steel	1700	2.80×10^5
Indium	430	2.8465×10^4
Tin	505	6.0278×10^5
Silver	1200	1.0465×10^5

5.4 Liquid Melt Viscosity

A constant liquid melt viscosity (independent of composition and temperature) in Newton seconds/square meter (N s/m^2) was used in the momentum equations for the DEBRIS analysis of MP-2. The value used was

$$\mu = 0.043(\text{N s})/\text{m}^2.$$

Somewhat lower values for the viscosity of molten corium can be found in the literature, and a value of $0.0045 (\text{N s})/\text{m}^2$ has been used, for example, in the FPT-4 calculations.

However, in calculating the Rayleigh number needed by the model to treat the enhanced heat transfer in molten pools (buoyant mixing, see Section 2.2.4), the following equation was used

$$\mu = 9.8 \times 10^{-4} \exp\left(\frac{5620}{T}\right) \quad (72)$$

5.5 Heat Capacity

Heat capacity for each material is shown in the following equations with units of joules/kilogram/Kelvin (J/kg/K).

$$\underline{\text{UO}_2} \quad C_{p\text{UO}_2} = \frac{C_1 e^{C_2/T}}{\left[T(e^{C_2/T} - 1)\right]} + C_3 T + C_4 \frac{e^{C_5/T}}{T^2} \quad (73)$$

$$C_1 = 8.501346 \times 10^7, C_2 = 535.285, C_3 = 2.43 \times 10^{-2}, C_4 = 1.658692 \times 10^{12}, \\ C_5 = 1.896732 \times 10^4$$

$$\underline{\text{ZrO}_2}: \quad \text{For } T < 300 \text{ K} \quad C_{p\text{ZrO}_2} = C_1 + C_2 T + C_3 T^2 \quad (74a)$$

$$\text{with } C_1 = -121.14, C_2 = 3.3651, C_3 = -4.797 \times 10^{-3}$$

$$\text{For } T < 1478 \text{ K} \quad C_{p\text{ZrO}_2} = C_1 + C_2 T + \frac{C_3}{T^2} \quad (74b)$$

$$\text{with } C_1 = 565.0, C_2 = 6.11 \times 10^{-2}, C_3 = -1.14 \times 10^7$$

$$\text{For } T < 2000 \text{ K} \quad C_{p\text{ZrO}_2} = 604.5 \quad (74c)$$

$$\text{For } T > 2000 \text{ K} \quad C_{p\text{ZrO}_2} = C_1 + C_2 T \quad (74d)$$

$$\text{with } C_1 = 171.7, C_2 = 0.2164$$

Zircaloy-4:

$$\text{For } T < 1113 \text{ K} \quad C_{p_{Zr}} = 339.77 \quad (75a)$$

$$\text{For } T < 1233 \text{ K} \quad C_{p_{Zr}} = 676.6 \quad (75b)$$

$$\text{For } T > 1233 \text{ K} \quad C_{p_{Zr}} = 356.98 \quad (75c)$$

$$\text{Steel:} \quad C_{p_{ss}} = A + BX + CX^2 \quad (76)$$

$$A = 326.0, \quad B = 0.298, \quad C = -9.56 \times 10^{-5}$$

$$\text{where: } Z = \min(T, 1558)$$

$$\text{Indium:} \quad C_{p_{ind}} = A + BT \quad (77)$$

$$\text{For } T < 430 \quad A = 196.0, \quad B = 0.14$$

$$\text{For } T > 430 \quad A = 252.0, \quad B = 0$$

$$\text{Tin:} \quad C_{p_{tin}} = A + BT \quad (78)$$

$$\text{For } T < 505 \quad A = 178.67, \quad B = 0.1667$$

$$\text{For } T > 505 \quad A = 257.0, \quad B = 0$$

$$\text{Silver:} \quad C_{p_{sil}} = A + BT \quad (79)$$

$$\text{For } T < 1200 \quad A = 219.766, \quad B = 0.05232$$

$$\text{For } T > 1200 \quad A = 282.55, \quad B = 0$$

ZrO₂ Fiber:

Same as zirconia

$$\text{ThO}_2 \text{ (Melt Barrier):} \quad C_{p_{ThO_2}} = A + BT + \frac{C}{T^2} \quad (80)$$

$$A = 260.0, \quad B = 3.328 \times 10^{-2}, \quad C = -3.5 \times 10^{-6}$$

$$\text{Tantalum:} \quad C_{p_{Tan}} = A + BT \quad (81)$$

$$A = 139.76, \quad B = 1.339 \times 10^{-2}$$

$$\text{Helium} \quad C_{p_{He}} = 5204 \quad (82)$$

5.6 Enthalpy

Enthalpy equations below for each material are in joules/kilogram/Kelvin (J/kg/K).

UO₂:

$$h_{s,UO_2} = \frac{C_1}{C_2} \left\{ \frac{1}{e^{C_2/T} - 1} - \frac{1}{(e^{C_2/T_0} - 1)} \right\} + \frac{C_3}{2} (T^2 - T_0^2) + \frac{C_4}{C_5} (e^{-C_5/T} - e^{-C_5/T_0}) \quad (83)$$

$$h_{l,UO_2} = \begin{cases} h_{s,UO_2} + h_{sl,UO_2}, & \text{for } T \leq T_s \\ h_{s,UO_2}(T = T_s) + h_{sl,UO_2} + Cp_{UO_2}(T - T_s), & \text{for } T > T_s \end{cases} \quad (84)$$

$$C_1 = 8.501346 \times 10^7, C_2 = 535.285, C_3 = 2.43 \times 10^{-2}, C_4 = 1.658692 \times 10^{12}$$

$$C_5 = 1.896732 \times 10^4, h_{sl,UO_2} = 2.78 \times 10^5, Cp = 503.0, T_s = 3023 \text{ K}$$

ZrO₂:

For $T < 300 \text{ K}$

$$h_{s,ZrO_2} = C_1(T - T_0) + \frac{C_2}{2}(T^2 - T_0^2) + \frac{C_3}{3}(T^3 - T_0^3) \quad (85a)$$

$$h_{l,ZrO_2} = 0 \quad (85b)$$

For $300 < T < 1478 \text{ K}$

$$h_{s,ZrO_2} = C_1(300 - T_0) + \frac{C_2}{2}(300^2 - T_0^2) + \frac{C_3}{3}(300^3 - T_0^3) + D_1(T - 300) + \frac{D_2}{2}(T^2 - 300^2) + D_3\left(\frac{1}{T} - \frac{1}{300}\right) \quad (86a)$$

$$h_{l,ZrO_2} = 0 \quad (86b)$$

For $1478 < T < 1479 \text{ K}$

$$h_{s,ZrO_2} = C_1(300 - T_0) + \frac{C_2}{2}(300^2 - T_0^2) + \frac{C_3}{3}(300^3 - T_0^3) + D_1(1478 - 300) + \frac{D_2}{2}(1478^2 - 300^2) + D_3\left(\frac{1}{1478} - \frac{1}{300}\right) + D_4(T - 1478) \quad (87a)$$

$$h_{l,ZrO_2} = 0 \quad (87b)$$

For $1479 < T < 2000$ K

$$h_{s,ZrO_2} = C_1(300 - T_0) + \frac{C_2}{2}(300^2 - T_0^2) + \frac{C_3}{3}(300^3 - T_0^3) + D_1(1478 - 300) + \frac{D_2}{2}(1478^2 - 300^2) + D_3\left(\frac{1}{1478} - \frac{1}{300}\right) + D_4 + D_5(T - 1479) \quad (88a)$$

$$h_{l,ZrO_2} = 0 \quad (88b)$$

For $2000 < T < 2558$ K

$$h_{s,ZrO_2} = C_1(300 - T_0) + \frac{C_2}{2}(300^2 - T_0^2) + \frac{C_3}{3}(300^3 - T_0^3) + D_1(1478 - 300) + \frac{D_2}{2}(1478^2 - 300^2) + D_3\left(\frac{1}{1478} - \frac{1}{300}\right) + D_4 + D_5(2000 - 1479) + D_6(T - 2000) + D_7(T^2 - 2000^2) \quad (89a)$$

$$h_{l,ZrO_2} = 0 \quad (89b)$$

For $2558 < T < 2559$ K

$$h_{s,ZrO_2} = C_1(300 - T_0) + \frac{C_2}{2}(300^2 - T_0^2) + \frac{C_3}{3}(300^3 - T_0^3) + D_1(1478 - 300) + \frac{D_2}{2}(1478^2 - 300^2) + D_3\left(\frac{1}{1478} - \frac{1}{300}\right) + D_4 + D_5(2000 - 1479) + D_6(2558 - 2000) + D_7(2558^2 - 2000^2) + D_8(T - 2558) \quad (90a)$$

$$h_{l,ZrO_2} = 0 \quad (90b)$$

For $T > 2559$ K

$$h_{s,ZrO_2} = C_1(300 - T_0) + \frac{C_2}{2}(300^2 - T_0^2) + \frac{C_3}{3}(300^3 - T_0^3) + D_1(1478 - 300) + \frac{D_2}{2}(1478^2 - 300^2) + D_3\left(\frac{1}{1478} - \frac{1}{300}\right) + D_4 + D_5(2000 - 1479) + D_6(2558 - 2000) + D_7(2558^2 - 2000^2) + D_8 + D_6(T - 2559^2) + D_7(T^2 - 2559^2) \quad (91a)$$

$$h_{l,ZrO_2} = \begin{cases} h_{s,ZrO_2} + h_{sl,ZrO_2}, & \text{for } T \leq T_s \\ h_{s,ZrO_2}(T = T_s) + h_{sl,ZrO_2} + D_9(T - T_s), & \text{for } T > T_s \end{cases} \quad (91b)$$

where

$$\begin{array}{lll} h_{l,ZrO_2} = 7.06 \times 10^5 & T_s = 2973 \text{ K} & \\ C_1 = -121.14, & C_2 = 3.3651, & C_3 = -4.797 \times 10^{-3} \\ D_1 = 565.0, & D_2 = 6.11 \times 10^{-2} & D_3 = 1.14 \times 10^7 \\ D_4 = 48200, & D_5 = 604.5, & D_6 = 171.7 \\ D_7 = 0.1082, & D_8 = 1.02 \times 10^5, & D_9 = 815.0 \end{array}$$

Zircaloy-4:

For $T < 1113 \text{ K}$

$$h_{s,Zr} = A(T - T_0) \quad (92a)$$

$$h_{l,Zr} = 0 \quad (92b)$$

For $1113 < T < 1233 \text{ K}$

$$h_{s,Zr} = A(1113 - T_0) + B(T - 1113) \quad (93a)$$

$$h_{l,Zr} = 0 \quad (93b)$$

For $1233 \text{ K} < T$

$$h_{s,Zr} = A(1113 - T_0) + B(1233 - 1113) + C(T - 1233) \quad (94a)$$

$$h_{l,Zr} = h_{s,Zr} + h_{sl,Zr} \quad (94b)$$

$$h_{sl,Zr} = 225356, \quad A = 339.77, \quad B = 676.6, \quad C = 356.98$$

Steel:

For $T < 1558$

$$h_{s,ss} = A(T - T_0) + \frac{B}{2}(T^3 - T_0^3) + \frac{C}{3}(T^3 - T_0^3) \quad (95a)$$

$$h_{l,ss} = 0 \quad (95b)$$

For $T > 1558$

$$h_{s,ss} = A(1558 - T_0) + \frac{B}{2}(1558^2 - T_0^2) + \frac{C}{3}(1558^3 - T_0^3) + D(T - 1558) \quad (96a)$$

$$h_{l,ss} = h_{s,ss} + h_{sl,ss} \quad (96b)$$

$$h_{sl,ss} = 28000, \quad A = 326.0, \quad B = 0.298, \quad C = -9.56 \times 10^{-5}, \quad D = 558.228$$

Indium:

For $T < 430$

$$h_{s,ind} = \frac{A}{2}(T^2 - T_0^2) + B(T - T_0) \quad (97a)$$

$$h_{l,ind} = h_{s,ind} + h_{sl,ind} \quad (97b)$$

For $T > 430$

$$h_{s,ind} = h_{s,ind}(T = 430) + C(T - 430) \quad (98a)$$

$$h_{l,ind} = h_{s,ind} + h_{sl,ind} \quad (98b)$$

$$h_{sl,ind} = 28465.0, \quad A = 0.14, \quad B = 196.0, \quad C = 252.0$$

Tin:

For $T < 505$

$$h_{s,tin} = \frac{A}{2}(T^2 - T_0^2) + B(T - T_0) \quad (99a)$$

$$h_{l,tin} = h_{s,tin} + h_{sl,tin} \quad (99b)$$

For $T > 505$

$$h_{s,tin} = h_{s,tin}(T = 505) + C(T - 505) \quad (100a)$$

$$h_{l,tin} = h_{s,tin} + h_{sl,tin} \quad (100b)$$

$$h_{sl,tin} = 60278.0, \quad A = 0.1667, \quad B = 178.67, \quad C = 257.0$$

Silver:

For $T < 1200$

$$h_{s,ag} = \frac{A}{2}(T^2 - T_0^2) + B(T - T_0) \quad (101a)$$

$$h_{l,ag} = h_{s,ag} + h_{sl,ag} \quad (101b)$$

For $T > 1200$

$$h_{s,ag} = h_{s,ag}(T = 1200) + C(T - 1200) \quad (102a)$$

$$h_{l,ag} = h_{s,ag} + h_{sl,ag} \quad (102b)$$

$$h_{sl,ag} = 104650, \quad A = .05232, \quad B = 219.766, \quad C = 282.55$$

5.7 Emissivities

Four materials may be involved as significant radiating surfaces in the FPT-4 experiment, urania, zirconia, thoria, and inconel. The general form used in DEBRIS for expressing the temperature-dependent hemispherical total emissivity is

$$\varepsilon = c_0 + c_1T + c_2T^2 + c_3T^3, \quad (103)$$

where T is the surface temperature and the c_i are the material-specific coefficients. Table 4 provides the values of the coefficients for each of these materials for specific temperature ranges.

Table 4. Emissivity correlations for radiating materials.

Material	Temp Range (K)	c_0	c_1	c_2	c_3
UO ₂	<2100	0.85	0.0	0.0	0.0
	2100-2485	1.666667	-3.88889E-4	0.0	0.0
	>2485	0.7	0.0	0.0	0.0
ThO ₂	<1850	0.3	0.0	0.0	0.0
	1850-3050	-1.809198	8.48006E-5	1.127375E-6	-3.0337E-10
	>3050	0.3	0.0	0.0	0.0
ZrO ₂	<3000	0.1686524	1.337360E-4	9.997673E-8	-3.5847E-11
Inconel	<1500	0.85	0.0	0.0	0.0

5.8 Gas Properties

Figure 5 shows the effects of temperature on the composition of initially pure steam. This information was obtained from studies done by Vargaftik⁴⁴ that show that there is a strong effect on both heat capacity and thermal conductivity resulting from molecular dissociation. The effects are due to the fact that the chemical reactions have associated heats of reaction that have the net effect of increasing the amount of heat that is required to raise the gas temperature.

Figure 5. Components of steam decomposition.

The equilibrium compositions are also pressure dependent. The data shown in Figure 5 are given at a pressure of 2.0 bars (the FPT-4 experiment condition). In addition, the presence of hydrogen will affect the degree of decomposition of steam. Hydrogen itself dissociates in the same temperature range and, for a completely rigorous treatment of steam/hydrogen mixtures, thermodynamic calculations must be performed to accurately determine the gas composition as a function of temperature, pressure, and initial composition. In the present application such detail is not justified and the individual properties are calculated with the simplifying assumption that the presence of one component does not affect the degree of decomposition of the other, and thus, of its predicted properties.

The effects of dissociation as seen in Figure 5, begin to become important for temperatures above ~2000 K. Thus, the data provided by Vargaftik for heat capacity, thermal conductivity, and viscosity of steam and hydrogen have been curve fit over two temperature ranges, 400 to 2000 K and 2000 to 4000 K. For functional uniformity all regressions were done to a 5th order polynomial.

$$\Phi = \sum_{i=0}^5 \phi_i T^i, \quad (104)$$

where Φ represents the physical property and the ϕ_i denote the regression coefficients. The coefficients for the various properties regressions are summarized in Tables 5 and 6. The units in these tables are heat capacity, C_p (J/kg/K), thermal conductivity, k (W/m/K), and dynamic viscosity, μ (N s/m²)

Table 5. Thermal properties of steam.

Φ	$\Delta T(K)$	ϕ_0	ϕ_1	ϕ_2	ϕ_3	ϕ_4	ϕ_5
C_p	400-2000	2.43281E+3	-2.65291E+0	4.82819E-3	-2.94503E-6	5.92810E-10	3.84134E-14
C_p	2000-4000	1.04947E+6	-1.95960E+3	1.45206E+0	-5.32990E-4	9.69592E-8	-6.9475E-12
k	400-2000	4.138730E-2	-1.21437E-4	1.706034E-7	1.75789E-10	-2.0582E-13	5.38074E-17
k	2000-4000	1.13299E+2	-2.36603E-1	1.959813E-4	-8.01286E-8	1.61082E-11	-1.2604E-15
μ	400-4000	-1.00477E-5	6.85513E-8	-3.4674E-11	1.76294E-14	-4.9290E-18	5.00005E-22

Table 6. Thermal properties of hydrogen.

Φ	$\Delta T(K)$	ϕ_0	ϕ_1	ϕ_2	ϕ_3	ϕ_4	ϕ_5
C_p	400-2000	1.30987E+4	8.83675E+0	-2.14624E-2	2.457188E-5	-1.24145E-8	2.35600E-12
C_p	2000-4000	3.45125E+5	-1.28922E+3	1.53570E+0	-8.07025E-4	1.953696E-7	-1.7531E-11
k	400-2000	-2.56005E-2	9.81746E-4	-1.34823E-6	1.444623E-9	-7.5379E-13	1.51992E-16
k	2000-4000	-2.99464E+2	4.82411E-1	-2.87129E-4	7.501744E-8	-7.3917E-12	6.84149E-17
μ	400-4000	3.482335E-6	1.912529E-8	-7.5242E-13	-3.1495E-15	1.56114E-18	-2.0837E-22

6. Benchmarking Calculations

Although it is not within the scope of this report to verify or validate the DEBRIS code modeling, a specific requirement for incorporation of the implicit fluid flow model was that it be benchmarked against the existing explicit model. Both the explicit and the implicit flow models were described in some detail in Section 4. The chief modeling differences between the two approaches, other than the numerical solution technique, are the inclusion in the implicit technique of the capillary force terms. The capillary force terms allow for motion of molten material as a result of capillary pressure and the radial motion of molten material as a result of pressure head differences at the surface of the molten pool.

For most cases of interest where the mean debris bed particle size is larger than about 2 millimeters (mm), it has been assumed that gravitational forces dominate capillary forces and that the latter can be ignored in the solution, while still achieving a relatively good characterization of debris bed melt relocation. It can be shown, however, that if the melt is assumed to wet the solid, in locations where there exists a large saturation gradient, the local capillary forces may be sufficiently high to compete with gravitational forces and, in particular, contribute strongly to melt flow in the radial direction.

The explicit method utilized a somewhat nonphysical model that assumed radial flow velocities at the surface of the molten pool to be infinite, in effect resulting in an instantaneous equilibration of the liquid surface level in each radial node within the molten pool. In the implicit method this assumption is not made. Rather, a pressure difference resulting from hydraulic head between adjacent control volumes is approximated, finite flow velocities between control volumes are calculated, and the liquid level is allowed to approach the appropriate level with the transient effects retained.

6.1 Description of Test Case

The purpose of this section is to present the results of a comparison between calculations performed using the explicit and implicit melt flow models as described above. The baseline case configuration for the FPT-4 experiment was selected as the test case. The FPT-4 experiment will consist of a debris bed containing a mixture of ~4.8 kg of partially crushed, irradiated fuel pellets, and ~1.2 kg of crushed and oxidized zircaloy cladding to simulate a configuration that is likely to develop during the "late phases" of a nuclear reactor accident. The bed will be contained within a cylindrical region bounded by a thorium melt barrier and several zirconia fiber insulation layers in the radial direction and a series of orifice blocks that support the bed from below. The entire assembly is contained within an inconel tube that provides mechanical constraint. The tube is cooled on the outside by reactor coolant flow that, within the coolant flow path geometry, is highly turbulent. The orifice blocks below the bed are provided with a large network of small flow channels that supply a mixture of steam and hydrogen to the bottom of the bed. The steam, after flowing through the bed, emerges at the upper surface of the bed where it is carried downstream to the diagnostic and measurement equipment in the Phebus facility. The bed dimensions are 6.8 cm in diameter by ~36 cm in height. Because the implicit

model requires extremely small time steps, particularly with concurrent gas flow, gas phase flow has been suppressed for the test case.

Because it is not the purpose here to examine the actual absolute values of parameters, temperatures, pressures, flow rates, etc., but rather to compare specific parameters related to melt relocation, it is not necessary to present a detailed description of the test case configuration beyond the cursory description given above. It is obvious that the final disposition of debris bed components is the appropriate metric for assessing the differences in melt relocation models. Therefore, the results will be depicted in terms of the spatial distribution of debris bed materials at the end of the simulation period.

6.2 Results of Comparisons

The approach taken here is to subject the test section model to a power deposition duty cycle that generates fission heating within the debris bed (Figure 6) using both of the melt flow models (explicit and implicit) and then to compare the results. The "stair step" power profile used is similar to those used in the MP-1 and MP-2 experiments and that will be used in the FPT-4 experiment. The power duty cycle is not identical to that proposed for the actual experiment, but is suitable for purposes of comparison. The power cycle is designed to raise the debris bed temperature at an average rate of about 1K/s up to the bed melting temperature and then to proceed to an end-of-simulation configuration in which about half of the original debris is molten.

The degree of debris relocation and the disposition of the relocated debris for the explicit and implicit calculations are presented in Figures 7 and 8, respectively. These two plots describe the location of material in terms of the material volume fraction that is the sum of the liquid and the solid debris volume fractions. There are several differences in the characteristics of the two cases. The implicit case appears to show a somewhat larger degree of melting in the radially central portion of the bed leaving a larger, essentially voided cavity above the molten pool (Figure 8). There is a relatively small radial gradient in volume fraction for the explicit case compared to the implicit case with a gradual increase in volume fraction from 0.1 to 0.4 over 2.5 cm. The gradient in the implicit case is generated over the same volume fraction range in only about 0.5 to 1.0 cm of the melt zone. A key observation, however, is the rather prominent formation in the implicit case of a densified zone or crust "enclosing" the voided region especially in the radial direction. This crust is formed as a result of the radial flow of material under the influence of capillary forces that is modeled in the implicit but not in the explicit formulations. A slight densification is also observed on the "roof" of the voided cavity indicating that some minor relocations resulting from capillary pressure are predicted to actually occur counter-directional to gravity flow.

Figures 9 and 10, which show the distribution of molten material within the debris bed for these two cases, emphasize the final important difference. For this particular power level, the implicit case (Figure 10) does not appear to form an extended molten pool. The melt appears to form a very small, fully dense region (at about the 2-cm radial and 46-cm axial location) with the remaining melt distributed in approximately the same general area as predicted by the explicit

Figure 6. Power history for explicit-implicit comparison.

Figure 7. Material disposition for explicit flow model.

Figure 8. Material disposition for implicit flow model.

Figure 9. Melt disposition for explicit flow model.

Figure 10. Melt disposition for implicit flow model.

case (Figure 9) but in a less dense configuration. For the explicit case, a well-defined molten pool ~2 cm deep forms at the 43-cm level and extends from the radial center out to about 2.5 cm radially. It is presumed that the limited extent of the molten pool as predicted by the implicit case is due, in part, to the quantity of melt that is transported radially outward, and resolidified to form an extensive radial crust. This material apparently becomes unavailable for incorporation into the molten pool.

The overall test section temperature response for the implicit and explicit cases are presented in Figures 11 and 12. Except for the temperature contours in the immediate vicinity of the molten pool, the two profiles are quite similar. The 2800 K contour in the explicit case (Figure 11) extends downward somewhat farther than for the implicit case (Figure 12) showing the somewhat greater downward penetration and extent of the molten pool for the former case.

Treatment of capillary forces in the momentum equations appears to produce a somewhat different disposition of material in the debris bed. In general, although the quantity of material melted is not substantially different, part of this melt is transported outward toward the radial boundary and resolidifies there to form a crust. This material is not available for inclusion in the molten pool and the result is a somewhat less extensive pool region.

The implicit model appears to provide some improvement in the resolution of material distribution. However, this increase in resolution comes at the price of a significantly increased computer run time. For example, using a 12-by-50-node (radial-by-axial) mesh, the explicit case ran in less than 1 day on a Unix HP-755. The implicit case had run 300 s of real time after a week of computer time when it was terminated. It is estimated that approximately one month of computer time would be required to complete the case. The analysis presented here was performed by reducing the mesh to 6 radial by 25 axial nodes and reducing the convergence criterion in the implicit solver by two orders of magnitude. These steps achieved run times for the implicit case that were less than a week, but also reduced the spatial resolution and the computational accuracy.

It is possible to incorporate the capillary force model into the current explicit computational algorithm with a significantly reduced run-time penalty, and this may be the appropriate approach in view of the results reported here that tend to suggest that this phenomenon may have significant effects on debris-bed melt relocation.

There are currently no experimental results with similar particle size distributions that can unambiguously confirm the formation of a radial crust as predicted by the implicit model with capillary flow. The MP-1 and MP-2 tests were run without gas flow, but they were more heavily insulated in the radial direction and had a significantly lower boundary heat sink capacity than does the FPT-4 test section. The result was that these tests were nearly one-dimensional with the debris bed melting all the way out to the radial melt barrier. The small quantity of unmelted material remaining near the radial boundary of the bed adjacent to the voided zone in the MP tests did not, however, appear to exhibit an increase in density that could have indicated a radial crust formation. The MP experiments were performed with a mean particle diameter of 2 mm and would have been more likely to exhibit such a crust formation because of the smaller particle size used in those tests compared to the FPT-4 simulation (4-mm particle diameter).

Figure 11. Temperature response for the explicit flow model.

Figure 12. Temperature response for implicit flow model.

Thus, the magnitude of the capillary effects on melt relocation and the importance of modeling these effects have not been firmly established at this time.

Finally, it is not clear that this phenomenon would be more or less significant in full-scale reactor analysis. The much larger volumes involved in reactor accident analysis lead to a more two-dimensional melt zone than have been simulated in debris bed experiments to date, and this configuration may be more likely to display the capillary effects if they are present. On the other hand, there is likely to be a more heterogeneous particle size distribution with perhaps large local differences that might make capillary effects less significant and perhaps less important in terms of large-scale melt relocation. The presence of a strong radial heat sink that is common to the MP and FPT debris bed experiments is certainly not a prototypic configuration in the reactor accident environment. This would tend to suggest that the radial crust formation that is predicted to occur as a result of the combined effects of capillary flow and a radial temperature gradient in the experiments may be much less significant in reactor safety considerations.

References

1. J. Bussac and H. Holtbecker, The PHEBUS FP In-Pile Test Programme, *International Conference on Thermal Reactor Safety (NUCSAFE 1988)*, ANS/ENS; Avignon, France, October 1988.
2. R.D. Gasser, R.O. Gauntt, and S. Bourcier, *Late Phase Melt Progression Experiment -- MP-1, Results and Analysis*, NUREG/CR-5874, SAND92-0804, Sandia National Laboratories, Albuquerque, NM, 1993.
3. R.D. Gasser, R.O. Gauntt, and S. Bourcier, *Late Phase Melt Progression Experiment -- MP-2, Results and Analysis*, NUREG/CR-6167, SAND93-3931, Sandia National Laboratories, Albuquerque, NM, to be published.
4. United States Nuclear Regulatory Commission, *Nuclear Power Plant Severe Accident Research Plan*, NUREG-0900, Washington, D.C., 1983.
5. W.J. Camp, et al., *MELPROG-PWR/MOD0: A Mechanistic Code for Analysis of Reactor Core Melt Progression and Vessel Attack Under Severe Accident Conditions*, NUREG/CR-4909, SAND85-0237, Sandia National Laboratories, Albuquerque, NM, 1987.
6. S.S. Dosanjh, ed., *MELPROG-PWR/MOD1: A Two Dimensional, Mechanistic Code for Analysis of Reactor Core Melt Progression and Vessel Attack Under Severe Accident Conditions*, NUREG/CR-5193, SAND88-1824, Sandia National Laboratories, Albuquerque, NM, 1989.
7. R.C. Schmidt, P.T. Giguere, T.J. Heames, and S.S. Dosanjh, *MELPROG PWR/MOD1 Models and Correlations*, SAND89-3123, Sandia National Laboratories, Albuquerque, NM, June 1992.
8. S.S. Dosanjh, *On the Melting and Refreezing of Porous Media*, NUREG/CR-5028, SAND87-1976, Sandia National Laboratories, Albuquerque, NM, October 1987.
9. S.S. Dosanjh, *Melt Progression in Severely Damaged Reactor Cores*, NUREG/CR-5029, SAND87-2384, Sandia National Laboratories, Albuquerque, NM, December 1987.
10. S.S. Dosanjh, *On the Melting of Reactor Core Particle Beds*, *25th National Heat Transfer Conference*, Houston, TX, July 1988.
11. S.S. Dosanjh and R.O. Gauntt, *MELPROG Debris Meltdown Model and Validation Experiments*, *25th National Heat Transfer Conference*, Houston, TX, July 1988.
12. S.S. Dosanjh, *Melt Progression in Core Debris Beds*, *ANS 1988 Annual Meeting*, San Diego, CA, 1988.

13. S.S. Dosanjh, *Relocation of Metallic Constituents in Core Debris Beds*, NUREG/CR-5109, SAND88-0535, Sandia National Laboratories, Albuquerque, NM, 1988.
14. S.S. Dosanjh, A Detailed Mechanistic Analysis of Core Debris Melt Progression Behavior in LWR's - The MELPROG DEBRIS Module, *ENS/ANS International Conference on Thermal Reactor Safety*, Avignon, France, October 1988.
15. S.S. Dosanjh, Melt Propagation in Dry Core Debris Beds, *Nuclear Technology*, Vol. 88, No. 1, pp. 30-46, October 1989.
16. S.S. Dosanjh, Melt Propagation in Porous Media, *Int. J. Heat and Mass Transfer*, Vol. 32, No. 7, pp. 1373-1376, 1989.
17. S.S. Dosanjh, Melting and Refreezing of Porous Media, *Int. J. Heat and Fluid Flow*, Vol. 10, No. 4, December 1989.
18. S.S. Dosanjh, *Melt Progression, Oxidation, and Natural Convection in a Severely Damaged Reactor Core*, NUREG/CR-5316, SAND88-3476, Sandia National Laboratories, Albuquerque, NM, 1990.
19. R. Gonzalez, P. Chatelard, and F. Jacq, *ICARE2 - A Computer Program for Severe Core Damage Analysis in LWRs, ICARE2, Version2 Mod1, Users Manual*, Institut de Protection et de Surete Nucleaire, Department de Recherches en Securite, CEA, France, July 1993.
20. R.C. Schmidt, *MERIS: A Model for Melt Relocation in Core Structures of Nuclear Reactors During Severe Accident Conditions*, Report prepared for the United States Nuclear Regulatory Commission Office of Nuclear Regulatory Research, Sandia National Laboratories, Albuquerque, NM, October 1993.
21. R.C. Schmidt, *Analysis of the XR-1 and XR-2 Melt Progression Experiments with the MERIS Computer Code: Results and Assessment of Models*, Report prepared for the United States Nuclear Regulatory Commission Office of Nuclear Regulatory Research, Sandia National Laboratories, Albuquerque, NM, January 1996.
22. R.C. Schmidt, *Analysis of the PHEBUS FPT-0 (Post-test) and FPT-1 (Pre-test) Experiments with MERIS*, Report prepared for the United States Nuclear Regulatory Commission Office of Nuclear Regulatory Research, Sandia National Laboratories, Albuquerque, NM, June 1996.
23. R.C. Schmidt and L.L. Humphries, *Late-Phase Melt Progression Scoping Analysis and Sensitivity Studies for PWRs*, NUREG/CR-6296, SAND92-2837, Sandia National Laboratories, Albuquerque, NM, December 1996.
24. R.C. Schmidt and T.J. Heames, *A Work Plan for the Development of a Porous Media Based Late Phase Melt Progression Module for SCDAP/RELAP5*, Report prepared for the United

States Nuclear Regulatory Commission Office of Nuclear Regulatory Research, Sandia National Laboratories, Albuquerque, NM, October 1994.

25. N.E. Bixler, R.D. Gasser, R.O. Gauntt, and T. Heames, *Design Studies and Performance Analysis for the Phebus FPT-4 Experiment*, Sandia National Laboratories, Albuquerque, NM, November 1996.
26. S. Imura and E. Takegoshi, Effect of Gas Pressure on the Effective Thermal Conductivity of Packed Beds, *Heat Transfer Japanese Research*, Vol. 3, No. 4, p. 13, 1974.
27. D. Vortmeyer, Radiation in Packed Solids, *Proc. 6th Int. Heat Transfer Conference*, Toronto, Vol. 6, pp. 525-539, 1978.
28. R. Viskanta, S. Chellaiah, and M.K. Moallemi, *Thermal Analysis of Core Barrel Heating and Coolant Recirculation During Core Uncovery in PWR Accidents*, EPRI NP-5586, Research Project 1760-3 Final Report, Purdue University Heat Transfer laboratory, West Lafayette, IN, 1987.
29. H.C. Hottel and A.F. Sarifim, *Radiative Transfer*, McGraw-Hill Publishing, New York, NY, 1967.
30. S.V. Patanker and D.B. Spalding, *Heat and Mass Transfer in Boundary Layers*, 2nd ed., Intertext, London, England, 1970.
31. D.L. Hagrman, *Zircaloy - UO₂ - Steam Interactions*, Report prepared for the U.S. Nuclear Regulatory Commission, EG&G Idaho, Inc., Idaho Falls, ID, September 1985.
32. K.A. Romberger, C.F. Bates, Jr., and H.H. Stone, Phase Equilibrium Studies in the UO₂-ZrO₂ System, *Journal of Inorganic and Nuclear Chemistry*, Vol. 29, pp. 1619-1630, 1966.
33. C.A. Wert and R.M. Thomson, *Physics of Solids*, Second Edition, McGraw-Hill Book Co., New York, NY, pp. 71-72, 1970.
34. A.E. Scheidegger, *The Physics of Flow Through Porous Media*, Third Edition, p. 156, University of Toronto Press, Toronto, Canada, and Buffalo, NY, 1974.
35. M.C. Leverett, Capillary Behavior in Porous Solids, *Pet. Trans. AIME*, 142, pp. 152-169, 1941.
36. R.B. Bird, W.E. Stewart, and E.N. Lightfoot, *Transport Phenomena*, John Wiley and Sons, Inc., New York, NY, p. 119, 1960.
37. A.W. Reed, et al., *DCC-1/DCC-2 Degraded Core Coolability Analysis*, NUREG/CR-4390, SAND85-1967, Sandia National Laboratories, Albuquerque, NM, October 1985.

38. G. Hofmann and L. Barleon, Reduced Coolability of Particle Beds as a Result of Capillary Effects at Horizontal Phase Boundaries, *Proceedings of the International ANS/ENS Topical Meeting on Thermal Reactor Safety*, San Diego, CA, February 2-6, 1986.
39. J.T. Hitchcock and J.E. Kelly, Post-Test Examinations of the In-Pile Molten Pool Experiments, *Trans. Am. Nucl. Soc.* 43, p. 515, 1982.
40. C.P. Fryer and J.T. Hitchcock, *Postirradiation Examination of the DC Melt Dynamics Experiments*, NUREG/CR-4625, SAND86-1102, Sandia National Laboratories, Albuquerque, NM, July 1988.
41. F. Kreith and M.S. Bohn, *Principles of Heat Transfer*, 5th Edition, West Publishing Co., New York, NY, pp. 619-628, 1993.
42. J.K. Hohorst, ed., *SCDAP/RELAP/MOD2 Code Manual, Vol. 4: MATPRO-A Library of Material Properties for Light-Water-Reactor Accident Analysis*, NUREG/CR-5273-Vol. 4, T190-008333, United States Nuclear Regulatory Commission, Washington, DC, February 1990.
43. Y.S. Touloukian, Editor, *Thermophysical Properties of High Temperature Solid Materials*, Thermophysical Properties Research Center, Purdue University, West Lafayette, IN, 1967.
44. N.B. Vargaftik, *Handbook of Physical Properties of Liquids and Gases: Pure Substances and Mixtures*, 2nd Edition, Hemisphere Publishing Corp., New York, NY, 1975.

APPENDIX A

Simplified Listing of the DEBRIS Subroutine Calling Sequence

1) Problem set-up and initialization

Call INPUT open files and read input deck. Initializes all needed variables

2) March through time

```

do 50 ii=1,isteps
time=time+dt
Call POWER                    Find the current reactor power level
if(NPC.eq.0)                    NPC=0 explicit melt flow model, NPC=1 implicit melt flow model
Call PROP                    calculate cell saturations, and permeabilities (for explicit melt flow
                             calculation)

else
Call PROPPS                    calculate cell saturations, capillary pressure, and permeabilities (for
                             implicit melt flow calculation)

endif
Call TINFIN                    input time dependent gas flow rate, temperature and composition
Call EQNSTATE                    calculate the gas phase cell densities
Call HCPST                    calculate gas phase  $C_p$  and enthalpy
Call GFLOW                    calculate cell pressures and gas flow rates
Call PROP2                    calculate cell thermal conductivities, specific heat and heat generation
                             (for bed and test section structures)

Call PROP3                    calculate cell thermal conductivities, specific heat (for plenum region
                             structures)

Call HTCOEF                    calculate boundary heat transfer coefficients and sink temperatures
Call RADTOP                    calculate radiation from bed surface to plenum structures
Call ADVECT                    calculate convective and radiative heat transfer from gas to plenum
                             wall

Call HTRAN                    calculate effective heat transfer coefficients ( $k/dx$ ) between cells in the
                             bed and test section structures

Call HTRANP                    calculate effective heat transfer coefficients ( $k/dx$ ) between cells in the
                             plenum region

Call TEMPER                    solve conduction/convection equation for new interum temperatures
                             "Tn" in the bed and test section structures (not final)

Call TEMPERP                    solve conduction equation for new interum temperatures "Tpn" in the
                             plenum region structures (not final)

Call HNEW                    Calculate new cell enthalpies "hn" based on temperatures form
                             TEMPER

```

Call HEATOUT
 Call RESETH
 Call RESET(1)
 Call SOLFAL
if(NPC.eq.1)

do imvt=1,nstep

Call PROP2
 Call FLOWZPC
 Call TNEW
 Call XENERG

Call PROP2
 Call FLOWRPC
 Call TNEW
 Call XENERG
 Call TNEW

end do

else

Call FLOWZ
 Call TNEW
 Call FLOWR
 Call TNEW

endif

c

Check if time to stop by assessing various values. If time to stop, jump out of do-loop

c

If time to print

Call SPRINT
 Call EPSCON
 Call TIMPNT
 Call XMASS

Calculate various energy balance quantities for conservation checks
 update the enthalpies h with the newly calculated enthalpies Hn
 update temperatures with newly calculated interum temperatures Tn
 calculate solid relocation

NPC=0 explicit melt flow model, NPC=1 implicit melt flow model
implicit melt flow model

(subdivide the time step for flow calculation)

(same as above)

calculate (implicit) axial melt relocation

calculate final (end of time step) cell temperatures and composition

check energy balance (iterate over previous 4 Calls if energy balance criterion not met)

(same as above)

calculate (implicit) radial melt relocation

(same as above)

(same as above)

(same as above)

explicit melt flow model

calculate (explicit) axial melt relocation

(same as above)

calculate (explicit) radial melt relocation

(same as above)

write out selected axial and radial temperature profiles and total matrix

write out selected the porosity and mass concentrations

write out various temperatures and energy balance values

calculate the total mass in the system of each of the seven material species

endif

50 continue

3) Stop Calculation

80 Call PRINT
 Call XMASS

write out complete data set to unit 11

calculate the total mass in the system of each of the seven material species

Call RSTART

write out everything needed to restart the calculation later

end

APPENDIX B

Brief Description of DEBRIS Subroutines and Functions

Name	Type	Description
DEBRIS	program	main driver routine
INITIAL	block data	initializes various data
INPUT	subroutine	opens files and reads input deck. Initializes lots of variables
PROP	subroutine	calculates residual and effective saturations (sr and se), and the axial and radial permeabilities (cfz and cfr) for explicit melt relocation model
PROPPS	subroutine	calculates residual and effective saturations (sr and se), the capillary pressure (pc) and the axial and radial permeabilities (cfz and cfr) for implicit melt relocation model
TINFIN	subroutine	extrapolates from a set of input data that specify the time-varying test section gas flow rate, gas inlet temperature, pressure, and composition ($H_2O(v)$, H_2)
EQNSTATE	subroutine	uses the ideal gas law to estimate the gas density in each control volume based on the temperature, pressure and composition ($H_2O(v)$, H_2)
HCPST	subroutine	calculates the specific heat and enthalpy of the gas phase based on temperature and composition ($H_2O(v)$, H_2)
GASPROP	subroutine	calculates the gas phase transport properties (viscosity and thermal conductivity) based on temperature and composition ($H_2O(v)$, H_2)
GFLOW	subroutine	calculates the pressure at the center of each control volume and the mass flow rates at the boundaries of each control volume based on the mass flow rate of gas into the bottom of the debris bed and the pressure prescribed at the top of the debris bed
SETTLE	subroutine	previously did the calculation for the solid material relocation. Is still called after calling SOLFAL, but only the first 20 or so lines are used - which zero some arrays and check for liquid
FLOWZ	subroutine	explicitly calculates the axial relocation of the liquid melt, including the convection of species without capillary forces
FLOWZPC	subroutine	implicitly calculates the axial relocation of the liquid melt, with capillary forces
FLOWR	subroutine	explicitly calculates the radial relocation of the liquid melt, including the convection of species without capillary forces
FLOWRPC	subroutine	implicitly calculates the radial relocation of the liquid melt, with capillary forces and hydraulic pressure head
XENERG	subroutine	calculates the total energy in the melt phase before and after melt relocation to check the energy balance

TNEW	subroutine	calculates a new cell temperature and liquid/solid composition based on the total cell enthalpy and composition
ESCAL	subroutine	calculates a new cell porosity and saturation
RESET	subroutine	updates the temperatures t with the newly calculated temperatures t_n . Also (for $n=0$), will extrapolate forward in time to estimate a new temperature, and eliminate negative porosities.
RESETH	subroutine	updates the enthalpies h with the newly calculated enthalpies h_n .
PRINT	subroutine	writes out complete data to unit 11, and some special data to unit 14 (special MP PIE file)
SPRINT	subroutine	writes out selected axial and radial temperature profiles at specified times during a run. Also writes the entire temperature matrix to unit 20
SGTSLR	subroutine	a tridiagonal matrix solver. Only called once, and that is in subroutine FLOWR
PROP2	subroutine	calculates the thermal conductivities (both k_r and k_z), the heat capacity, and the internal heat generation in each node based on the temperature, composition, reactor power and shape factor for the debris bed and most test section structures. Note, this routine includes a model to account for pool convection effects (sub.CONVECT)
PROP3	subroutine	calculates the thermal conductivities (both k_r and k_z), the heat capacity, and the internal heat generation in each node based on the temperature, composition, and shape factor for the structures in the exit gas plenum
CONVECT	subroutine	modifies the axial and radial heat transfer coefficients in cells with a molten pool in order to help account for pool convection
SUMY	subroutine	sums the species volume fractions to see if they equal 1.0. Only called in the input file to check the input
FKCAL1	function	calculates the thermal conductivity of the UO_2 , ZrO_2 , Zr , Fe mixtures, in the MP1 debris bed
FKCAL2	function	calculates the thermal conductivity of the UO_2 , ZrO_2 , Zr mixtures in the MP1 crust region. Ron notes that this is a volume average method
FKCAL3	function	calculates the thermal conductivity of the UO_2 , Zr mixture in the MP1 rod region using a correlation that appeared to give good results in the TAC2D analysis for the rod region
FKCAL4	function	calculates the thermal conductivity of Stainless steel
FKCAL5	function	calculates the thermal conductivity of ZrO_2 Fiber Insulation
FKCAL6	function	calculates the thermal conductivity of Thoria
FKCAL7	function	calculates the thermal conductivity of Tantalum
FKCAL8	function	calculates the thermal conductivity of "stagnant Helium gas" by calling GASCON
FKCAL9	function	calculates the thermal conductivity of Aluminum
FKCAL10	function	calculates the specific heat of Tungsten
CPCAL5	function	calculates the specific heat of ZrO_2 Fiber Insulation

CPCAL6	function	calculates the specific heat of Thoria
CPCAL7	function	calculates the specific heat of Tantalum
CPCAL8	function	calculates the specific heat of "stagnant Helium gas"
CPCAL9	function	calculates the specific heat of Aluminum
CPCAL10	function	calculates the specific heat of Tungsten
GASCON	function	calculates the thermal conductivity of the gas space. In the MP-1 experiment the gas is helium
KUO2	function	calculates the thermal conductivity of 95% theoretical density UO2
KZRO2	function	calculates the thermal conductivity of Zirconia (ZrO ₂)
KZR	function	calculates the thermal conductivity of Zircaloy
HTRAN	subroutine	calculates the "effective heat transfer coefficients" (i.e., k/dx) between control volumes. The arrays found are HTB(j,i), HTT(j,i), HTL(j,i), and HTR(j,i)
HTRANP	subroutine	calculates the "effective heat transfer coefficients" (i.e., k/dx) between control volumes in the plenum region. The arrays found are HTPB(j,i), HTPT(j,i), HTPL(j,i), and HTPR(j,i)
CP1	subroutine	calculates the specific heat capacity of both liquid and solid UO2. Called from PROP2
CP2	subroutine	calculates the specific heat capacity of both liquid and solid ZrO2. Called from PROP2
CP3	subroutine	calculates the specific heat capacity of both liquid and solid Zircaloy. Called from PROP2
CP4	subroutine	calculates the specific heat capacity of both liquid and solid Stainless Steel 316. Called from PROP2
CP5	subroutine	calculates the specific heat capacity of both liquid and solid Indium. Called from PROP2
CP6	subroutine	calculates the specific heat capacity of both liquid and solid Tin. Called from PROP2
CP7	subroutine	calculates the specific heat capacity of both liquid and solid Silver. Called from PROP2
HTCOEF	subroutine	this subroutine calculates the radial heat transfer coefficient between the MP-X test package and the cooling heat exchanger. Also calculates the local coolant sink temp. Called from DEBRIS
TEMFLW	subroutine	reads the coolant inlet temperature and flow rate at various times from an external file (unit 7). Called from INPUT
GAP	subroutine	assigns gap thicknesses to each control volume boundary. Arrays given values are GAPL(j,i), GAPR(j,i), GAPB(j,i), GAPT(j,i). These values are only used in subroutine HTRAN when calculating the effective heat transfer coefficients between cells
ADVECT	subroutine	solves the momentum and energy equations for laminar forced convection in the exit gas plenum using the Patankar formulation. Also estimates the radiative heat transfer from the gas to the plenum wall

RADTOP	subroutine	solves the set of radiation enclosure equations to determine the radiation heat fluxes between the debris bed upper surface and the structures associated with the exit gas plenum
FORM	subroutine	calculates the radiation configuration factors between surface areas in a constant diameter cylindrical enclosure. Called from RADTOP
CONFAC	subroutine	calculates the radiation configuration factors between surface areas in a varying diameter (generated by a surface of rotation) cylindrical enclosure. Called from RADTOP
TEMPER	subroutine	solves for new temperatures based on the conduction/convection heat transfer part of the energy equation using an ADI type method. Called from DEBRIS after calling HTRAN
TEMPERP	subroutine	solves for new temperatures based on the conduction heat transfer part of the energy equation for the plenum region using an ADI type method. Called from DEBRIS after calling HTRANP
TRIDAG	subroutine	the tridiagonal matrix solver called from TEMPER
POWER	subroutine	determines the current reactor power level by interpolating from the time/power table read in through subroutine POWIN. Called from DEBRIS
POWIN	subroutine	reads in the reactor time/power table from an external file (unit 8)
HNEW	subroutine	calculates the new total enthalpy in each cell ($HN(i,j)$) after the conduction heat transfer calculation is completed. Called from DEBRIS
DNSTY	subroutine	calculates the "cell density" of each of the seven material species currently modeled (i.e., kg of species n per m ³ - within the cell) Includes both solid and liquid. Called from DEBRIS. Results used in calling subroutine TNEW
TIMPNT	subroutine	utility subroutine to write out various quantities at a specified print interval. Units 90 and 91; as many as 50 temperatures at specified locations (up to 25 in each file), Units 94, 95, and 96; various energy and heat balance quantities. Called from DEBRIS
HEATOUT	subroutine	calculates the following energy balance related quantities. totout = integrated heat lost through boundary (kJ) totfiss = integrated fission heating in bed+crust+rods (kJ) totbed = integrated increase in bed+crust+rods enthalpy (kJ) totgam = integrated gamma heat in structures (kJ) totstret = integrated increase in structures enthalpy (kJ) toth2o = integrated gamma heat in coolant (kJ) qstore = energy stored as an increase in enthalpy qinfiss = sum of fission heat ($q(j,i)$) in the heated region qingam = sum of the fission heat ($q(j,i)$) in the non heated structure region qintot = qinfiss + qingam totin = totfiss + totgam totbal = totbed + totstret + totout

RSTART	subroutine	writes out everything needed in order to restart the calculation from a particular point in time. Called at the end of a calculation from DEBRIS
EPSCON	subroutine	at specified times, this writes out the porosity and mass concentrations at specified locations in the debris, crust, and rod regions. Called from DEBRIS
PHASE	subroutine	based on temperature and composition, uses an approximation to the UO ₂ -ZrO ₂ Pseudo-binary phase diagram to determine fractions of UO ₂ and ZrO ₂ that are liquid and fractions which are solid.
AXLSHAPE	subroutine	at specified times in the MP calculations, this routine is called to change the axial power shape as a result of material relocation. Called from DEBRIS
SOLFAL	subroutine	calculates solid relocation
XMASS	subroutine	calculates the total mass in the system of each of the seven material species. Called from DEBRIS
ENTHUO2	subroutine	calculates the enthalpy of UO ₂ as a function of temperature. Returns both an enthalpy of the solid (HS) and an enthalpy of the liquid (HL)
ENTHZRO2	subroutine	calculates the enthalpy of ZrO ₂ as a function of temperature. Returns both an enthalpy of the solid (HS) and an enthalpy of the liquid (HL)
ENTHZR	subroutine	calculates the enthalpy of Zircaloy as a function of temperature. Returns both an enthalpy of the solid (HS) and an enthalpy of the liquid (HL)
ENTHSS	subroutine	calculates the enthalpy of stainless steel as a function of temperature. Returns both an enthalpy of the solid (HS) and an enthalpy of the liquid (HL)
ENTHAG	subroutine	calculates the enthalpy of silver as a function of temperature. Returns both an enthalpy of the solid (HS) and an enthalpy of the liquid (HL)
ENTHIN	subroutine	calculates the enthalpy of Indium as a function of temperature. Returns both an enthalpy of the solid (HS) and an enthalpy of the liquid (HL)
ENTHSN	subroutine	calculates the enthalpy of Tin as a function of temperature. Returns both an enthalpy of the solid (HS) and an enthalpy of the liquid (HL)
ENTHGAS	subroutine	calculates the enthalpy of the gas as a function of temperature. Bases on a constant Cp (value of CPGAS)
ENTHALP1	subroutine	calculates the enthalpy of a mixture of materials given the temperature, volume fractions (both solid and liquid), porosity, and saturation. <u>Non-phase diagram melting</u>
ENTHALP2	subroutine	calculates the enthalpy of a mixture of materials given the temperature and knowing that melting is occurring on the UO ₂ /ZrO ₂ phase diagram

ENTHALP3	subroutine	calculates the liquid and solid enthalpies of a mixture of materials given the temperature, volume fractions (both solid and liquid), porosity, and saturation. <u>Non-phase diagram melting</u>
ENTHSCOP	subroutine	calculates the enthalpy at a specific temperature - i.e., the melting temperatures, to scope the enthalpy
BRACKET1	subroutine	narrows the bracket T1,T2 in which the root is located for entry into ZBRENT root finder. <u>Used for non-melting cases.</u> Called from TNEW
BRACKET2	subroutine	narrows the bracket T1,T2 in which the root is located for entry into ZBRENT root finder. <u>Used for phase diagram melting.</u> Called from TNEW
ZBRENT	subroutine	given bracket temperatures, this routine uses "Brent's" method to find a root of the enthalpy function. Called from TNEW to find new temperature, eps, S, Ys1, Ys2, Yl1, and Yl2

In addition to the subroutines described above, a number of subroutines have been appropriated from the standard SLATEC mathematics library that solve the matrix equations for cases in which the matrices are not tridiagonal. In particular, the system of finite difference equations that describe the two-dimensional pressure field in the debris bed with gas flow (in subroutine GFLOW) are banded and require a banded matrix solver. Also, the system of equations that describe the radiative wall heat fluxes in an enclosure (subroutine RADTOP) yields a general matrix (generally all nonzero elements) that requires a general matrix solver. These routines are

DGBCO	subroutine	computes the LU factorization and condition of a banded matrix
DGBSL	subroutine	computes the solution to the banded system of equations using the LU decomposition generated by DGBCO
DGECO	subroutine	computes the LU decomposition and condition for a general matrix
DGESL	subroutine	computes the solution to the general system of equations using the LU decomposition generated by DGECO

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