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MELCOR INTEGRATED SEVERE ACCIDENT CODE FOR HIGH TEMPERATURE GAS COOLED REACTOR APPLICATIONS

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ABSTRACT

MELCOR is an integrated severe accident code used for source term analysis that has been developed at Sandia National Laboratories (SNL) for the United States Nuclear Regulatory Commission (USNRC) since the early 1980s. Though MELCOR originated as a light water reactor (LWR) code, development and modernization efforts over the past decades have expanded its application space to non-LWR concepts including High Temperature Gas-cooled Reactors (HTGRs). Current MELCOR development efforts focus on providing the USNRC with the analytical capabilities to support regulatory readiness for licensing non-LWR technologies. Advancements for HTGRs include core heat transfer and thermal hydraulics models and fission product diffusion/release models for TRISO and pebble or prismatic fuel. These models have been successfully exercised in demonstration calculations for the USNRC.

KEYWORDS
MELCOR, TRISO, Pebble, Prismatic

1. INTRODUCTION

The United States Nuclear Regulatory Commission (U.S. NRC) anticipates a near-term regulatory need for non-light water reactor (non-LWR) modeling capabilities to permit mechanistic source term calculations. To ensure a position of regulatory readiness, U.S. NRC has recently supported MELCOR code development initiatives at Sandia National Laboratories (SNL) for non-LWRs to include high temperature gas-cooled reactors (HTGRs) including pebble bed modular reactors (PBMRs) and prismatic modular reactors (PMRs).

Generally, MELCOR development for non-LWRs includes both mathematical physics models and user modeling capabilities. The former refers to mechanistic, systems-level, predictive mathematical models of physical phenomena. The latter refers to freedom afforded the user in probing uncertainties and sensitivities associated with physical phenomena that may not have a rigorous mechanistic and predictive mathematical model available in the code. In most instances and regardless of non-LWR type, existing code infrastructure can be leveraged for purposes of incorporating new physics models and user capabilities. The scope of development activity varies widely by non-LWR type, but thermal hydraulic modeling and radionuclide transport modeling primarily set the HTGR development agenda.

HTGRs (PBRs or PMRs) have - by far - the longest development arc in MELCOR of all the non-LWR types with early efforts dating back to 2006. Nevertheless, development has been most intense in recent years and entails a broad spectrum of thermal hydraulic and radionuclide transport phenomena to include:

- Diffusional fission product release
- Core component conduction (intercell, intracell, boundary)
- Core and control volume convection/flow
- Graphite oxidation
- Point reactor kinetics

This paper endeavors to describe in some detail the mathematical models and user capabilities outlined above. The intention is to summarize the current state of MELCOR HTGR modeling capability.

2. HTGR PHYSICS MODELS AND USER MODELING CAPABILITIES

Aspects of the HTGR MELCOR development agenda are expounded below. For still further details on model mathematics, implementation, and user interfaces, refer to the MELCOR code reference manual [1] and user guide [2]

2.1. Diffusional Fission Product Release

For TRISO fuel and HTGR fuel elements (pebbles or compacts), fission product transport and release to coolant occurs primarily by diffusion. This necessitated a different modeling approach for fission product transport within and release from core structures relative to that traditionally employed in MELCOR for light water reactors.

2.1.1 Introduction

The overarching goals of the HTGR fission product release model are to:

- Predict radionuclide distributions within fuel elements in the core, and
- Predict radionuclide release from fuel elements to coolant

The calculation revolves around a generalized finite volume diffusion solver but has a specialized analytic release model for transient solutions of failed TRISO. A fuel performance and failure modeling capability interfaces with the analytic release model to accommodate a diverse population of TRISO particles. The finite volume diffusion solver and analytic release model together afford the capability to represent entire HTGR fuel elements - consisting of TRISO particles and matrix – for purposes of computing fission product transport and release.

Generally, solution of the diffusional fission product release problem requires:

- User inputs:
  - Two or more “models” representing kinds of TRISO particle in a population
    - At minimum, one model for intact TRISO and one model for failed TRISO
    - Others possible, e.g. defective TRISO
  - A single “model” representing fuel element matrix
  - Geometric configuration of TRISO models and the matrix model
  - One or more tracked fission product species mapped to radionuclide classes
  - Diffusion coefficient data prescribed by tracked fission product species
  - Miscellaneous data (e.g. failure rules)

- The finite volume diffusion solver to perform diffusion calculations within intact TRISO particles and fuel element matrix
- The analytic release model to calculate a time/temperature history dependent release from failed TRISO particles to fuel element matrix
- A methodology for initializing radionuclide distributions within and release from fuel elements at steady state prior to any transient/accident initiating event
- A methodology for establishing a steady-state distribution of radionuclides around the flow loop due to steady-state fuel element release
- A methodology for proceeding with transient diffusion transport/release calculations once an initiating event occurs
- Ancillary capabilities:
    - Approximation of temperature profiles for computing diffusion coefficients
    - Accounting for an initially failed fraction among the TRISO population
    - Accounting for fission product recoil and matrix contamination
    - Accounting for dynamics of intact-to-failed TRISO particle transition
    - Optional partition coefficients and sorption isotherm empirical models

The outcome is a prediction for fission product distribution within and release from fuel elements.

2.1.2 Finite Volume Diffusion

The one-dimensional steady/transient spherical/cylindrical diffusion equation is:

$$\chi \frac{\partial C}{\partial t} = \frac{1}{r^n} \frac{\partial}{\partial r} \left(r^n D \frac{\partial C}{\partial r} \right) - \lambda C + \beta \tag{1}$$

The steady form applies in the context of steady-state initialization of the diffusional fission product release calculation, and the transient form takes over thereafter. Finite difference forms of this equation are written and solved for each applicable model (e.g. intact TRISO, matrix) according to its geometry which generally resembles Figure 1.

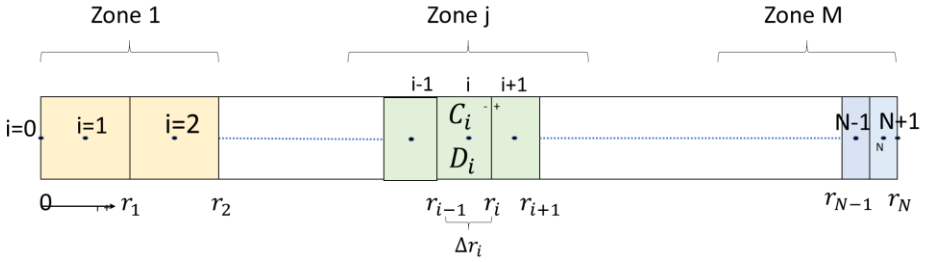

Figure 1. Generic zone-wise nodalization of a model solved with finite volume diffusion

Diffusion coefficients are computed from an Arrhenius equation informed by user input by species:

$$D(T) = D_0 e^{-Q/RT} \tag{2}$$

2.1.3 Run-time sequence

The stages of an HTGR accident/transient simulation employing the diffusional fission product release model are shown in Figure 2. Each stage is briefly summarized. A thermal steady state is first established, then steady-state distributions of radionuclides in core structures and in flow loops are established, then the transient calculation begins.

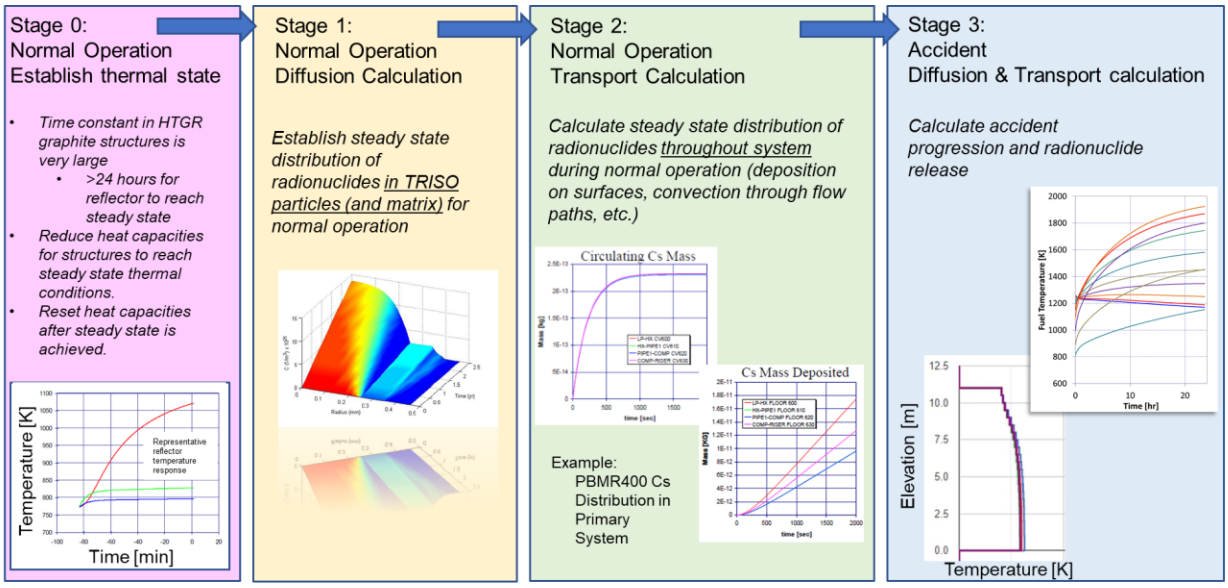

Figure 2. Diffusional fission product release model run sequence in 4 stages

Stage 0 of the run sequence involves no fission product transport/release whatsoever. Instead, the requisite thermal steady state is established as coolant flow, fluid temperatures, and core structural temperatures settle out to constant values while fission thermal energy and decay energy deposition are constant. Stage 0 leads into stage 1 where user input for radionuclide class mass by core cell is leveraged to compute initial radionuclide inventories and distributions in fuel. Steady-state releases from fuel elements are also computed in stage 1 and held constant as stage 2 commences. In stage 2, no new diffusional fission product release calculations occur. Instead, steady-state fuel release rates are held constant and while flow loop radionuclide inventories settle to steady values. At the conclusion of stage 2, steady conditions are established for the thermal hydraulic state of the core, the fuel element radionuclide inventories/distributions, and the flow loop radionuclide inventories/distributions/depositions.

2.1.3.1 Stage 1: steady-state diffusion

Stage 1 (steady-state diffusion) predictions of core fuel element radionuclide distribution and release reflect the combined effects of:

- Radionuclide generation by fission
- Diffusion and its temperature dependence
- Diffusional release, recoil, and contamination if applicable according to user input

Known quantities at the outset of stage 1 include:

- Model noding and geometry,
- Diffusion coefficient data,
- Diffusion equation boundary conditions,
- TRISO population fractions,
- Fuel and matrix temperatures,
- Tracked species radioactive decay constants
- Decay heat (DCH), radionuclide (RN1), and core (COR) code package inputs:
  - DCH/RN1 radionuclide class configurations and total class masses
  - RN1 radionuclide class mass distribution across COR components/cells

Unknown quantities (for all tracked fission product species mapped to RN1 classes) to be solved for during stage 1 include:

- Molar concentrations,
- Volumetric molar generation rates due to fission,
- Matrix model radionuclide inventories,
- Coolant radionuclide inventories,
- Fuel release/transfer rates

Because molar volumetric generation rates due to fission are not known a priori, and because matrix model molar concentration distributions are not known a priori, an iterative method is employed to resolve a self-consistent solution as shown in Figure 3.

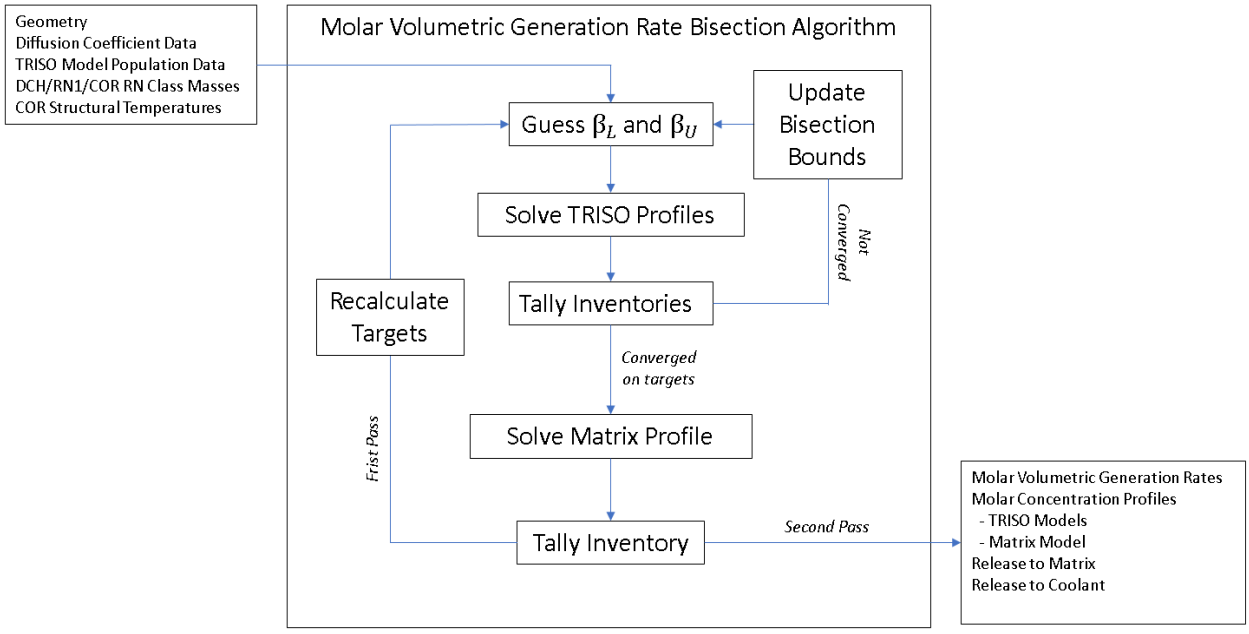

Figure 3. Steady state diffusion stage solution algorithm flow diagram

The method uses molar volumetric generation rate as a bisection variable in an iterative method that seeks molar concentration profiles consistent with known COR cell inventories. The bisection iteration is wrapped in an outer two-iteration loop to predict unknown steady matrix radionuclide

inventories. For any given tracked fission product species, guesses at upper and lower bounds of fission volumetric molar generation rate are made, and the finite volume diffusion solutions proceed. The resulting molar concentration profiles are appropriately tallied over TRISO and fuel element population in a cell and compared to targets. Upper and lower bounds are then revised as necessary and bisection proceeds. Eventually, a self-consistent set of molar concentration profiles are produced, and fuel element boundary diffusion fluxes to coolant can be predicted.

A representative steady state intact TRISO molar concentration profile for a species representative of the cesium radionuclide class is show in Figure 4 as an illustration of predictive capabilities. A representative steady state matrix (fuel element) molar concentration profile for the same representative species is shown in Figure 5.

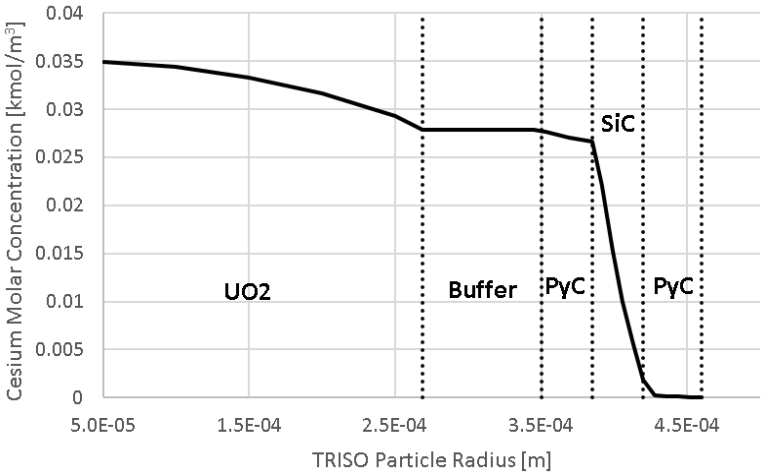

Figure 4. Representative steady intact TRISO concentration profile from finite volume diffusion

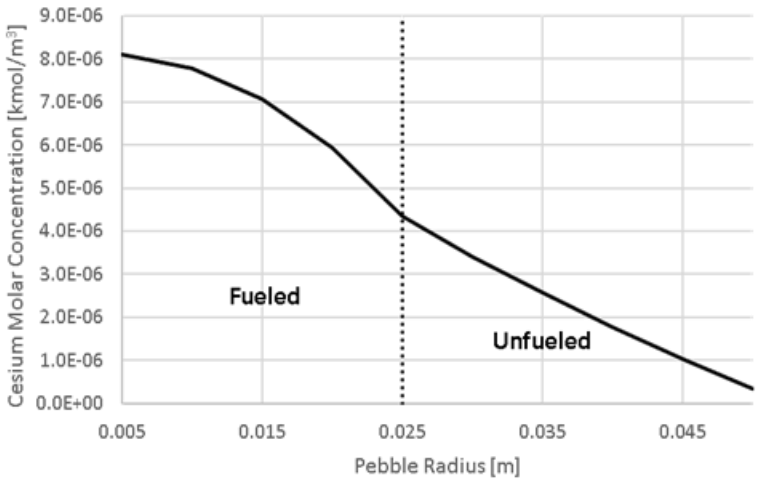

Figure 5. Representative steady matrix concentration profile from finite volume diffusion

Other noteworthy aspects of the diffusional fission product release model include:

- volumetric molar generation rates (fueled matrix zone) due to diffusional release
- volumetric molar generation rates in fuel (TRISO buffer) due to recoil,
- volumetric molar generation rates in fuel (unfueled matrix zone) due to contamination,

Given some release rate from a TRISO model (e.g. intact or failed) due to diffusion, the released inventory is cast as a volumetric molar generation rate uniformly distributed over the matrix kernel (fueled zone of the matrix model). Mathematically, this volumetric generation rate is formulated on a per unit fuel element basis as:

$$\beta_{TRISO-to-matrix,j} = \left(\sum_{m=1}^{M} R_{m,j}\right)\left(\frac{N_p}{V_{matrix\_kernel}}\right) \tag{3}$$

Recoil in intact TRISO refers to a phenomenon whereby fission products born in the fuel kernel - near the periphery – escape to the buffer region in the process of slowing down and forfeiting their kinetic energy. These fission products essentially bypass any diffusion barrier presented by the fuel kernel and directly enter the buffer. Mathematically, this process is dictated by a recoil fraction and is approximated as a uniform volumetric generation rate in the buffer region:

$$\beta_{m,buffer,j} = \left(\frac{\beta_{m,kernel,j}}{1-f_{rec}}\right)(f_{rec})\left(\frac{V_{m,kernel}}{V_{m,buffer}}\right) \tag{4}$$

Recoil from the bare kernels of the failed TRISO model is possible and is computed similarly. Recoil from failed TRISO must enter the matrix kernel zone, however, because no buffer exists in the context of the bare kernel failed TRISO model. Mathematically:

$$\beta_{m,buffer,j} = \left(\frac{\beta_{mFail,kernel,j}}{1-f_{rec}}\right)(f_{rec})\left(\frac{N_p V_{mFail,kernel}}{V_{matrix\_kernel}}\right) \tag{5}$$

Contamination, e.g from tramp fuel material found outside TRISO particles, is also computed as a uniform volumetric generation rate with the aid of a user-specified fraction:

$$\beta_{TRISO-to-matrix,j} = \sum_{m=1}^{M}\left(\left(\frac{\beta_{m,kernel,j}}{1-f_{rec}}\right)(f_{contam})\left(\frac{N_p V_{m,kernel}}{V_{matrix\_kernel}}\right)\right) \tag{6}$$

2.1.3.2 Stage 2: steady-state transport

Once steady-state COR fuel radionuclide distributions and releases are known, steady flow loop conditions must be ascertained in terms of:

- Radionuclide inventories in control volumes (as aerosols or vapors)
- Radionuclide inventories deposited on heat structures (as aerosols)

For an extent of "pseudo" problem time specified by the user, MELCOR holds COR radionuclide inventories and releases constant while computing control volumes and heat structures. Eventually, steady radionuclide control volume inventories and heat structure surface depositions are established. A scaling factor can be specified by the user to account for steady release over a prescribed burn-up time. The steady control volume and heat structure inventories obtained at the end of steady-state transport pseudo-time are scaled by this factor to obtain end-of-burnup control volume radionuclide inventories and heat structure radionuclide surface depositions.

2.1.3.3 Stage 3: transient diffusion and transport

Once steady-state COR fuel radionuclide distributions, control volume radionuclide inventories, and heat structure radionuclide depositions are all known from the steady-state diffusion and steady-state transport stage executions, the transient diffusion/transport stage may commence. The biggest differences during this stage are:

- failed TRISO diffusional release is computed with the analytic release model, and
- TRISO population fractions are dynamic and evolving (e.g. according to failure rules)

Intact TRISO, any other variety of user specified TRISO, and matrix is still computed with finite volume diffusion but without any molar volumetric generation source terms from fission, recoil, or contamination. Proceeding from transient time zero (not necessarily problem time zero), COR radionuclide inventories and release rates change dynamically along with control volume radionuclide inventories and heat structure radionuclide surface depositions. Presumably, these calculations occur in the context of some transient/accident scenario.

2.1.4 Failed TRISO diffusion and release

Failed TRISO particles release fission product inventory into the fueled zone of the fuel element matrix according to an analytic release model that computes:

- Release from failed TRISO (a modified Booth model instead of finite volume diffusion)
- Intact TRISO failure (built-in rule or user-prescribed rules) including puff/burst release
- Time history effects of failure and release

Release from failed TRISO is an integrated result of particle history described by the convolution integral of failure rate and diffusion release:

$$F_{tot}(t) = \int_0^t \frac{dF_W(t)}{d\tau} F_R(t-\tau)\, d\tau \tag{7}$$

Simplifying the general convolution integral to a summation of time history "save points":

$$F_{tot,j}(t) = \sum_{nc=1}^{ncsave} \left[\left(\frac{df_W}{dt}\right)(f_{R,j})(\Delta t) X_{k,j}\right]_{nc} \tag{8}$$

The failure rate can be approximated from failure rule(s) in place for a given calculation. The failure rule ultimately decides the failed TRISO population fraction in a COR cell. The user can program failure rules via control functions to the desired level of complexity. A simple temperature-dependent built-in model is available for failure fraction. It was derived from historical German fuel performance data and uses the core fuel component temperature:

$$f_W(T) = (2.28109 * 10^{-7}) e^{.00498*(T-273)} \tag{9}$$

The fractional release is predicted by an approximation to a modified Booth prescription [3,4] leveraging a time-averaged reduced diffusion coefficient [1]. The modified Booth prescription for

release fraction of a given radionuclide from an equivalent sphere at some time after irradiation is, according to Lewis [3]:

$$f_R(t) = 6\sum_{n=1}^{\infty}\int_0^t exp\left[-\left(\left(n^2\pi^2\int_0^{\mu} D't'dt'\right)+\lambda\mu\right)\right]D'(\mu)d\mu \tag{10}$$

Gelbard [4] proposes an approximation:

$$f_R(t) = \begin{cases} 1.0006964 * \left(\sqrt{\frac{36\bar{D}'t}{\pi}} - 3\bar{D}'t\right), for\ \bar{D}'t < 0.155 \\ 1 - \left(\frac{6}{\pi^2}\right)e^{-\pi^2\bar{D}'t}, for\ \bar{D}'t \geq 0.155 \end{cases} \tag{11}$$

Equation 11 uses a time-averaged reduced diffusion coefficient that accounts for time/temperature history of the failed TRISO:

$$\overline{D'} = \frac{\sum_{ns=n1}^{ncsave}\left[\left(t_0(nc) - t_0(nc-1)\right)\left(D_0 e^{-Q/T_{nc}}\right)\right]_{ns} + \left(t - t_0(ncsave)\right)D_0 e^{-Q/T_{ncsave}}}{r^2\left(t - t_0(n1)\right)} \tag{12}$$

When intact TRISO particles transition to failed TRISO, the intact TRISO kernel becomes failed TRISO – approximated as bare TRISO fuel kernels - with an inventory subject to release according to the approximate modified Booth model from Equation 11.

All other zones outside the previously intact TRISO kernel immediately release their fission product inventory as a "burst" or "puff" to fuel element matrix. Mathematically, this is affected by summing the known fission product molar inventories of zones outside the previously intact TRISO kernel and casting them in terms of a volumetric molar generation rate when doing a finite volume diffusion solve on the matrix. This is comparable to how intact and failed TRISO diffusional releases to matrix are handled. In any case, proper accounting is made of the number of intact and failed TRISO particles per fuel element and the number of fuel elements per core cell.

2.2. Core Conduction

Core conduction is a major component of HTGR thermal hydraulics. The COR package (MX) and reflector (RF) components were integrated into effective conductivity models that pair with revised core conduction logic to facilitate radial and axial conduction computations in pebble bed and prismatic cores.

2.2.1 Intercell

In context of the COR package and the PBR or PMR reactor types, intercell conduction refers to the conduction heat transfer between similar or dissimilar components in axially or radially

adjacent COR cells. Regardless of the components involved and their relative orientation, MELCOR formulates the conduction heat transfer as an effective conductivity multiplied by the temperature difference between the two components. The effective conductivity is a parallel combination of conductances from each component. For all components other than MX, component conductance is a function of the known material solid conductivity and known component geometry.

For the MX component invoked by PBR and PMR reactor types, the component conductivity model utilizes either:

- The Zehner-Schlunder-Bauer correlation with the Breitbach-Barthels modification (PBR)
- The Tanaka and Chisaka expression (PMR)

The former accounts for combined effects associated with a pebble bed including solid conduction, fluid conduction, and radiation. The latter accounts for combined effects associated with a modular block core with coolant hole perforations including solid conduction, pore conduction, and radiation. Additionally, a term accounting for block-to-block conduction across a gas gap is included. The reader is referred to the MELCOR reference manual and user guide for further information on the mathematical models associated with intercell conduction in HTGRs.

2.2.2 Intracell

In context of the COR package and the PBR or PMR reactor types, intracell conduction refers to the conduction heat transfer between fuel (FU) and MX components in the same COR cell. Physically, this would represent the conduction in a fuel element between a fueled region that hosts TRISO particles and a surrounding unfueled region. Conduction heat transfer is again formulated as a conductance times a temperature difference, but in this case the conductance consists of:

- An FU term depending on geometry and solid material conductivity
- An MX term accounting for geometry, solid material conductivity, and the non-negligible thickness of the unfueled matrix region (note no Zehner-Schlunder-Bauer or Tanaka and Chisaka effective conductivity models are invoked here)
- Another conductance that is a function of radiation, a user-defined gap conductivity term, and a possible user-supplied control function term

The main change for HTGRs in MELCOR involves the MX term which behaves differently from the conventional cladding (CL) component in a light water reactor model.

2.2.3 Boundary

Thermal energy transfer across the core peripheral boundary is a key mode of passive heat removal for HTGRs. In MELCOR, there must exist a mechanism whereby thermal energy can pass from COR structures and exit the COR package entirely. The boundary conduction model facilitates this energy transfer from the outermost ring of a COR nodalization to designated core boundary heat structures.

2.3. Core Convection and Flow

New Nusselt number correlations were included in MELCOR for PBRs representing forced and natural convection from isolated, spherical particles:

$$NU_{forced} = 2.0 + 0.6Re_f^{1/2}Pr_f^{1/3} \quad (13)$$

$$NU_{natural} = 2.0 + 0.6Gr_f^{1/4}Pr_f^{1/3} \quad (14)$$

The conventional Dittus-Boelter correlation applies for the PMR. The user has full access via sensitivity coefficient to all constants and nondimensional number exponents in COR Nusselt number correlations.

Concerning COR convection heat transfer, the MX component is still regarded as non-negligible in terms of its heat transfer resistance. When computing convection heat transfer between an MX component surface and interfacing CVH hydrodynamic material, the heat transfer resistance associated with MX is included in the expression for convection heat transfer rate.

With respect to CVH hydrodynamic material flow through a packed pebble bed, MELCOR accounts for flow resistance and packed bed pressure loss by invoking one of several possible correlations (e.g. Ergun, Achenbach) and casting the flow loss as K-loss. This form is convenient in terms of performing phasic velocity equation solutions.

2.4. Graphite Oxidation

Graphite oxidation is allowed within the generic oxidation framework [1] regardless of component affiliation, i.e. whether the graphite material belongs to MX, RF, or SS. When oxidant (air or water) is present and has access to a component surface, graphite oxidation may proceed according to the built-in graphite oxidation models or another user-specified set of rules. The oxidation rate is subject to diffusion limitations as is generally the case for COR component oxidation.

The reader is referred elsewhere [1] for a description of parabolic kinetics models for graphite oxidation in air or steam. Graphite oxidation yields no solid oxide material within the graphite-bearing core component and produces more than one off-gas. Graphite oxidation by air in a PBR context might follow the gross trends exhibited in Figure 6 for a contrived air ingress scenario. Reactant masses are shown as negative while product masses of carbon monoxide and carbon dioxide are shown as positive. An approximate mass balance is evident. A temperature-dependent empirical model governs the monoxide-to-dioxide molar production ratio at any given problem time and thereby governs the overall oxidation stoichiometry:

$$f = \chi_{CO} \Big/ \chi_{CO_2} = 7396 * \exp\left(-\frac{69604}{8.314 * T_{MX}}\right) \quad (15)$$

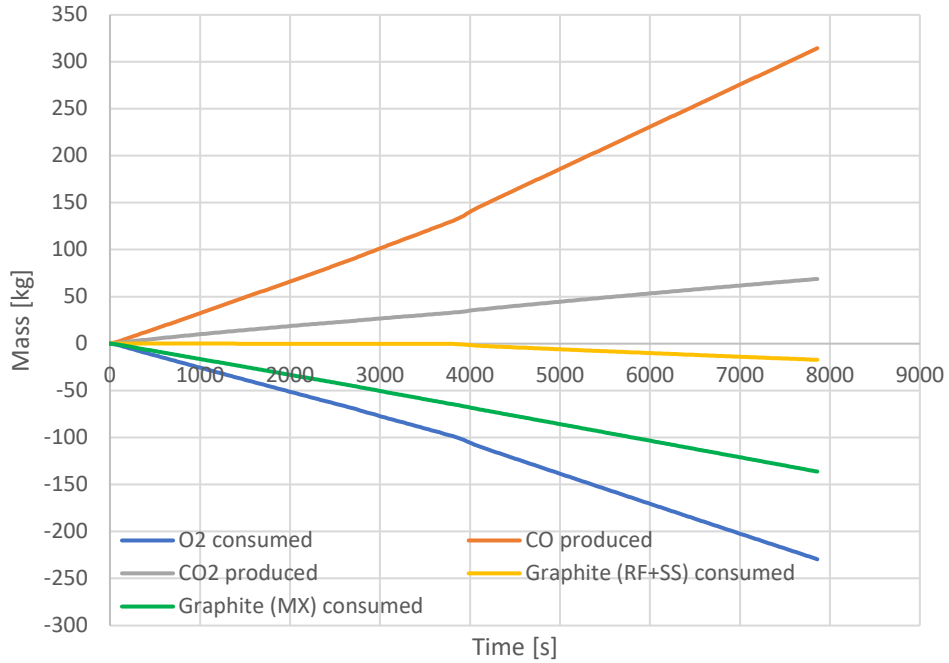

Figure 6. MELCOR prediction of graphite oxidation in a PBR context given dramatic air ingress

2.5. Point Reactor Kinetics

To facilitate MELCOR modeling of anticipated transient without scram (ATWS) scenarios, a point reactor kinetics model was added. The formulation is along the lines of a standard textbook approach with six delayed neutron precursor groups:

$$\frac{dP}{dt} = \left(\frac{\rho - \beta}{\Lambda}\right) P + \sum_{i=1}^{6} \lambda_i Y_i + S_0 \tag{16}$$

$$\frac{dY_i}{dt} = \left(\frac{\beta_i}{\Lambda}\right) P - \lambda_i C_i, \quad for\ i = 1 \ldots 6 \tag{17}$$

Nuclear kinetics data is open to user sensitivity coefficient controls as are all reactivity feedback models. The solution methodology employs high-order Pade approximants to a matrix exponential to inform particular and homogeneous solutions. Considerable improvements were recently made to the algorithm numerics. A representative result from the MELCOR point reactor kinetics model is shown in Figure 7 for a PBR type reactor subject to a \$0.50 reactivity insertion.

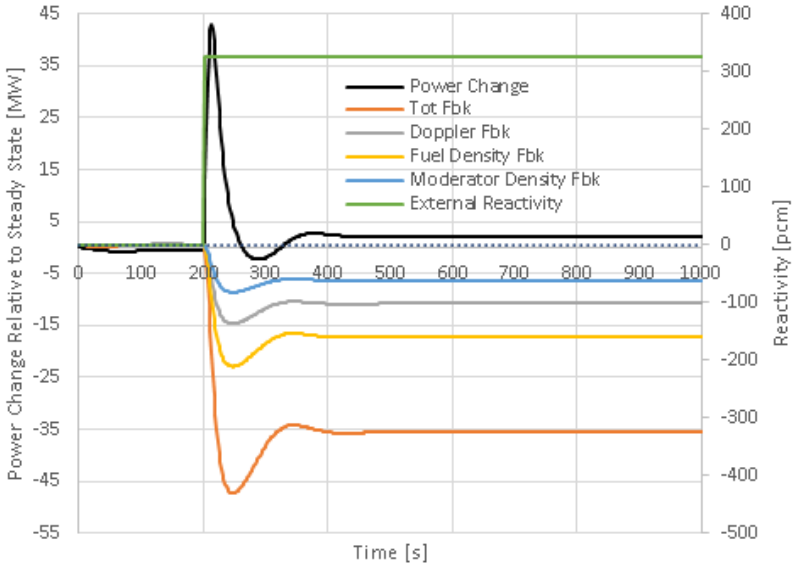

Figure 7. PRK model prediction for a PBR subject to \$0.50 reactivity insertion

3. CONCLUSIONS

Recent MELCOR non-LWR development has covered various reactor concepts and has added several physics models and modeling capabilities to help meet anticipated regulatory needs. In the realm of HTGRs, thermal hydraulics models related to core conduction, convection/flow, graphite oxidation, and point reactor kinetics have been added. A diffusional fission product release model was also added to facilitate mechanistic source term calculation.

NOMENCLATURE

Variables

χ = Multiplier (0 for steady-state diffusion, 1 for transient diffusion) | Mole fraction [-]
C = Molar concentration [kmol/m^3]
t = Time [s]
r = Radial coordinate [m]
D = Diffusion coefficient [m^2/s]
λ = Decay constant [1/s]
β = External source [kmol/m^3/s] | Delayed neutron fraction [-]
F = A fractional quantity clarified by subscript (e.g. total release, failure, Booth release)
τ = Dummy time integration variable [s]
Δt =Timestep [s]
X = Molar inventory, failed TRISO kernel [kmol]
T = Temperature [K]
μ = Dummy variable of integration
n = Term counter in infinite series sum
D' = Reduced diffusion coefficient [1/s]
$\bar{D}'$ = Time-averaged reduced diffusion coefficient [1/s]
D_0 = Arrhenius equation precoefficient [m^2/s]
Q = Arrhenius equation activation energy [J/mol]

R = Gas constant = 8.314 [J/mol/K]
$ncsave$ = Total number of save points in time history tracking of failed TRISO
t_0 = Time at which save point is written [s]
f = Stoichiometric ratio CO-to-CO_2
P = Thermal power due to fission [W]
$\rho = \frac{k-1}{k}$ = Reactivity for k the effective multiplication factor [$\delta k/k$ or pcm]
Λ = Neutron generation time [s]
S_0 = Thermal power generation rate due to neutron source [W/s]
Y = Precursor power [W]

Subscripts

i = Delayed neutron precursor group indicator
0 = Indicates an initial value
j = tracked species index
k = kernel
W = Indicates failure (F_W)
R = Indicates release (F_R)
tot = Indicates total release (F_{tot})

Superscripts

n = Geometry indicator, = 1 for cylindrical, = 2 for spherical

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