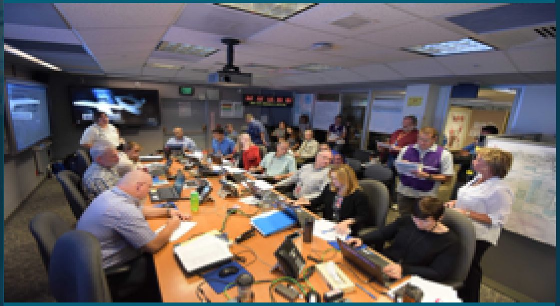
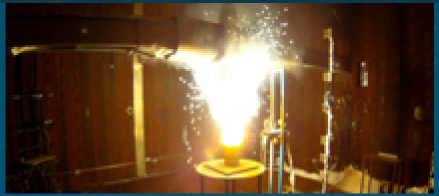
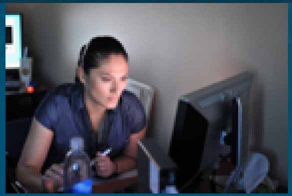
SAND2021-14062PE

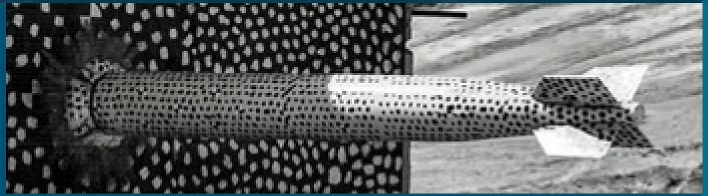
Sandia National Laboratories

MELCOR for High Temperature Gas-cooled Reactor Modeling









Asian MELCOR User Group
November 8-11, 2021

PRESENTED BY

Sandia National Laboratories Technical Staff

U.S. DEPARTMENT OF ENERGY NNSA

MELCOR HTGR Modeling/Development Radionuclide Transport – Theory

Overview

COR radionuclide transport theory

- Introduction
- Aspects of diffusional fission product release calculation
  - Fuel element representation
  - Finite volume diffusion (non-failed TRISO and fuel element matrix)
  - Analytic release model (failed TRISO)
- Solution methodology
  - Accelerated thermal-hydraulic steady state
  - Steady state diffusion stage
  - Steady state transport stage
  - Transient diffusion/transport stage
- Mapping to and consistency with radionuclide (RN1) and decay heat (DCH) code packages
- COR component release and scaling

Conclusions

Introduction

Overall goals of the diffusional fission product release model

- Predict RN distributions within fuel
- Predict RN release from fuel elements to coolant

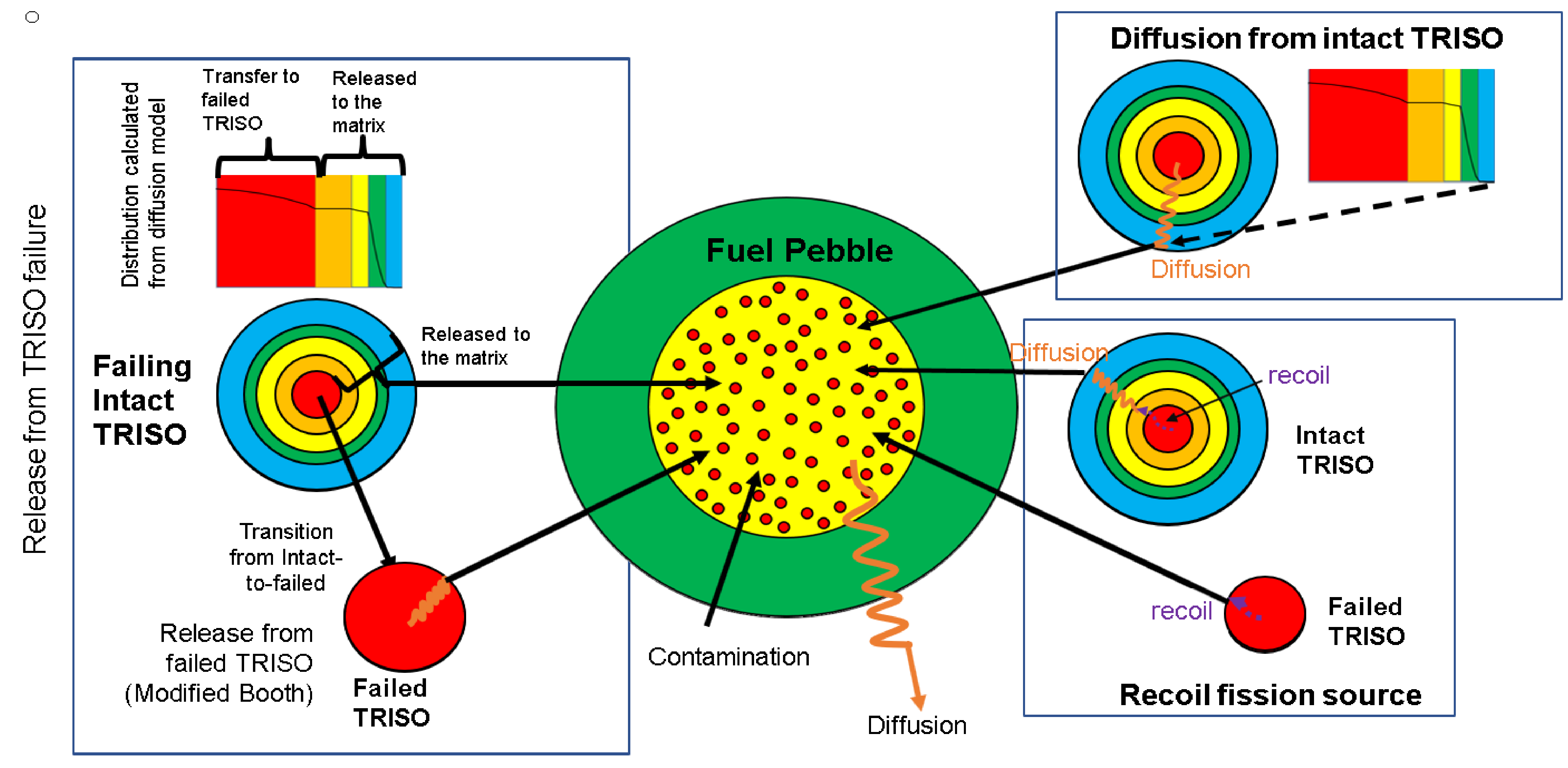
The model thereby facilitates source term calculations for regulatory purposes and risk-informed decision making

- Revolves around a generalized finite diffusion solver
- Runs through sequential stages in its solution methodology
- Includes fuel performance and failure modeling capabilities

A general instance of diffusional fission product release entails (best practices)

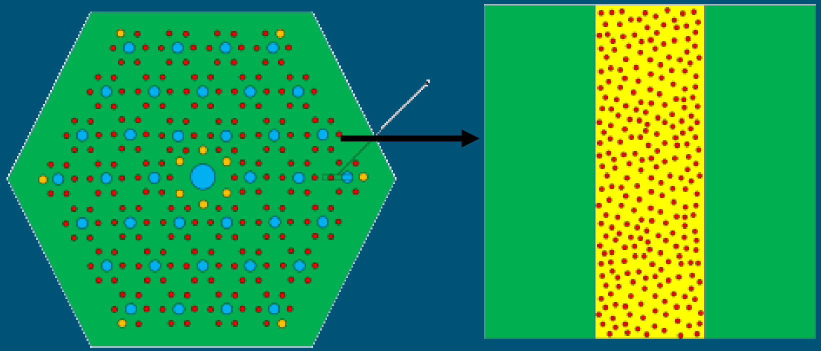
- Two or more “models” representing a type of TRISO particle (intact, failed, defective, etc.)
- A single model representing fuel element matrix
- One or more tracked fission product species that map to RN1 classes
- Solution grids/geometries for each model
- Diffusion coefficient data and other miscellaneous data

…Aspects of Diffusional Fission Product Release Calculation…

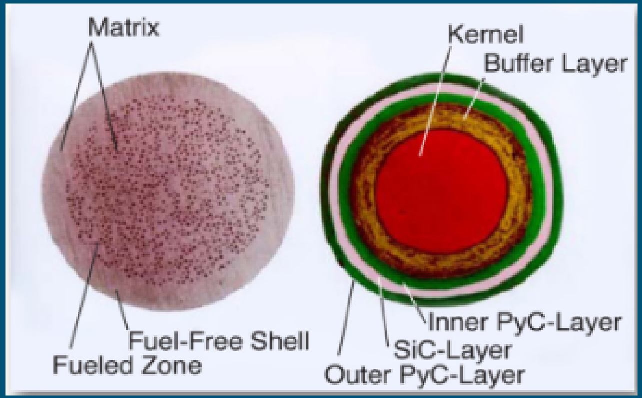


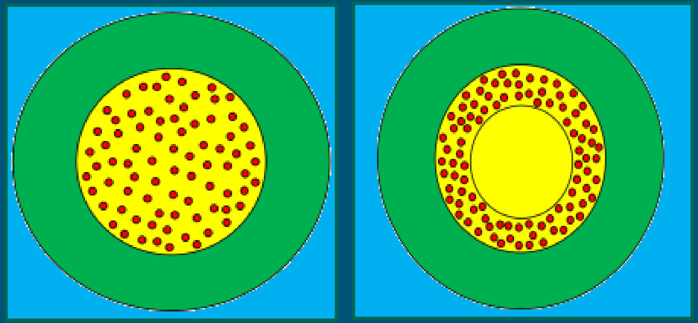
HTGR Fuel Element Representation

PMR fuel elements



PBR fuel elements





* Note pebble fuel element representation applies to any reactor type

TRISO representations (intact, failed) similar for PBR and PMR

Matrix representations different for PBR and PMR

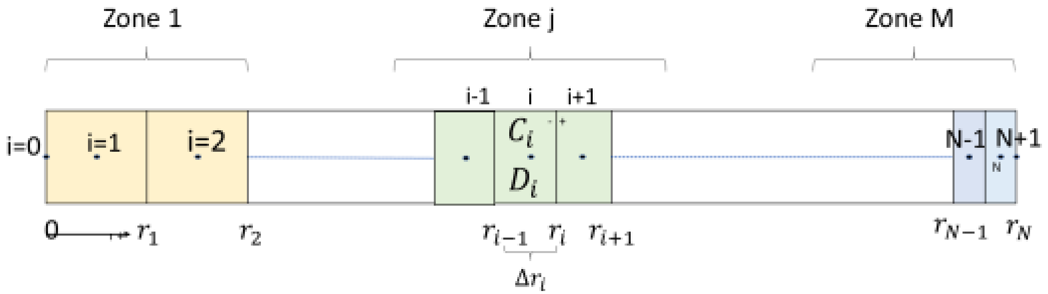
- Denote fueled zones where TRISO resides
- Geometrically describe matrix for diffusion

TRISO per fuel element, total fuel elements per COR cell

Finite Volume Diffusion Solver

One-dimensional finite volume diffusion equation solver illustration: intact TRISO model

- Steady or transient, cylindrical or spherical, generally multiple zones (materials) entailing some number of equally-spaced nodes
- Temperature-dependent diffusion coefficients (Arrhenius form)
- Predict concentrations of each tracked species for model in question and predict diffusional release at model boundary

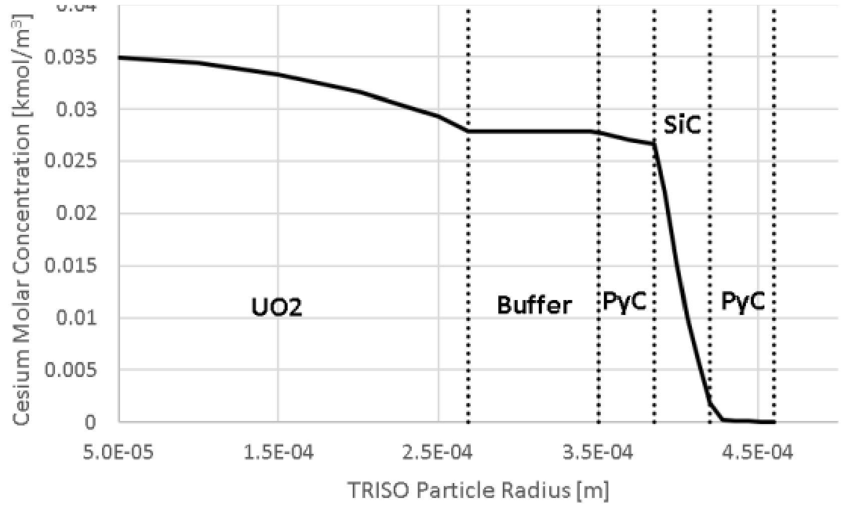


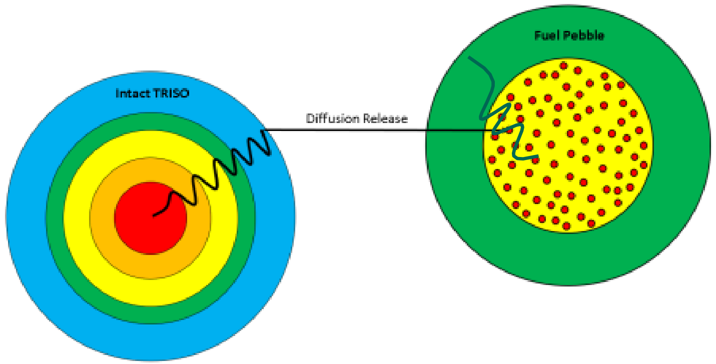
$$\frac{\partial C}{\partial t} = \frac{1}{r^n}\frac{\partial}{\partial r}\left(r^n \mathbf{D}\frac{\partial C}{\partial r}\right) - \lambda C + \beta$$

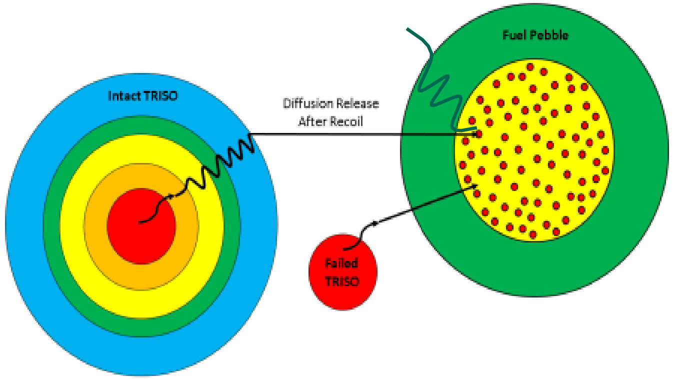
$$D(T) = D_0 e^{-\frac{Q}{RT}}$$

$$\int_{r_{i-1}}^{r_i}\left[\chi\frac{\partial C}{\partial t} = \frac{1}{r^n}\frac{\partial}{\partial r}\left(r^n D\frac{\partial C}{\partial r}\right) - \lambda C + \beta\right]dV \rightarrow \Delta V_i \chi \frac{\partial C_i}{\partial t} = \left(AD\frac{\partial C}{\partial r}\right)_{r_{i-1}}^{r_i} - \lambda C_i \Delta V_i + \beta \Delta V_i$$

Intact TRISO Concentrations







Finite Volume Diffusion Solver

Finite difference equations are obtained by:

- Multiplying the differential equation by an element of volume,
- Integrating over node volume (constant diffusion coefficient and constant source term), and
- Enforcing boundary/interface conditions as appropriate
- Using harmonic mean for effective interface diffusivities

See MELCOR RM

Several boundary conditions possible

- Enforced symmetry at “inner” or “left-hand” boundaries
- User specifies concentration, flux, or mass transfer coefficient at “outer” or “right-hand”

  → Recommendation: a “zero concentration” condition at outer boundary
- Partition coefficients optionally configure concentration jumps at interfaces between grid zones
- Empirical sorption isotherm model can be configured to capture:
  - Coolant boundaries (PMR – coolant holes, PBR – pebble surface)
  - Gas gaps (PMR – gas gap between fuel compacts and hexagonal graphite blocks)

See MELCOR RM

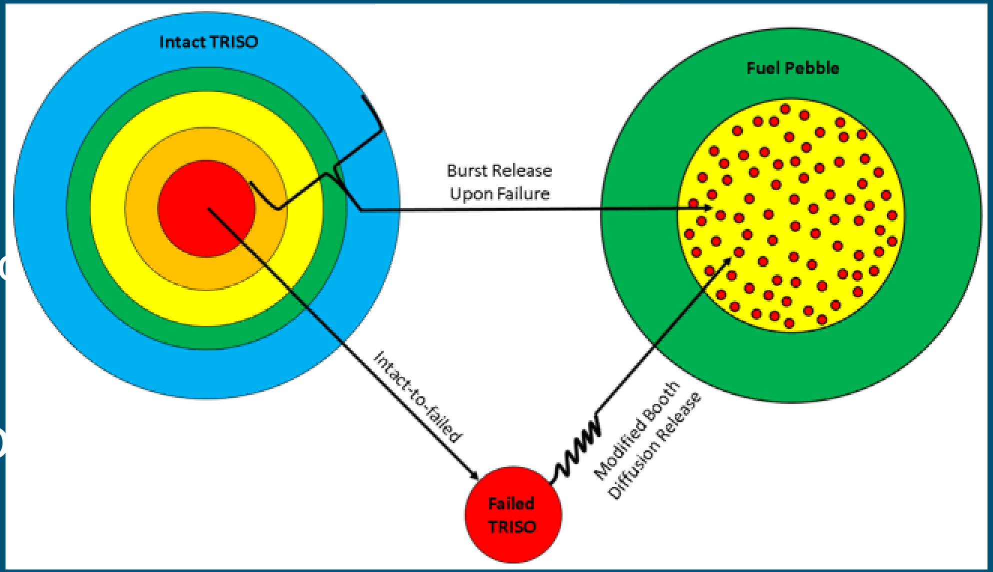
Analytic Release Model

Initially, failed TRISO accounts for some (small) fraction of the overall TRISO population, but during a transient intact TRISO particles generally fail at different times in different core cells

Continuous release from failed TRISO particles depends

- TRISO failure characterized by intact TRISO failure rules
- Release characterized by failed TRISO population time histo

Finite volume diffusion too mathematically burdenso



Analytic release model integrates over failed TRISO particle diffusion/temperature history

- Analytical diffusion solution (modified Booth with approximations)
- Fresh failures generate burst releases to matrix, and kernel inventories are then subject to diffusional release
- Previously failed TRISO particles continue release

Analytic Release Model

Mathematical ingredients to the analytic release model:

- Modified Booth diffusion equation with approximations
  - Tells the fraction of release from a bare sphere by diffusion
  - Several simplifying assumptions made (*Gelbard)

$$F_R(t) = \begin{cases} 1.0006964\left(\left(\frac{36}{\pi}\right)D't - 3D't\right), & D't < 0.155 \\ 1 - \left(\frac{6}{\pi^2}\right)e^{(-\pi^2 D't)}, & D't \geq 0.155 \end{cases}$$

Gelbard, F. Analytic Modeling of Fission Product Releases by Diffusion from Multi-coated Fuel Particles. SAND2002-3966.

- Time-averaged reduced diffusion coefficient
  - Sum over time history (save points)
  - Units are [1/s] due to division by r^2
  - Arrhenius dimensional diffusion coefficient

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

- Simplified convolution integral of failure and release
  - Time integral ~ sum over discrete historical save points
  - Failed inventory (at point nc) subject to continuous release
  - Time zero ($nc = 1$) at start of transient

$$F_{tot}(t)_j = \int_0^t \frac{dF_W(t)}{d\tau} F_{R,j}(t-\tau)d\tau$$

$$\approx \sum_{nc=1}^{ncsave}\left[\left(\frac{dF_W}{dt}\right)(F_{R,j})(\Delta t)X_{k,int,j}\right]_{nc}$$

- Built-in TRISO failure correlation (optional)

$$f_{fail} = (2.28109 * 10^{-7})e^{(0.00498*(T_{FU}-273.0))}$$

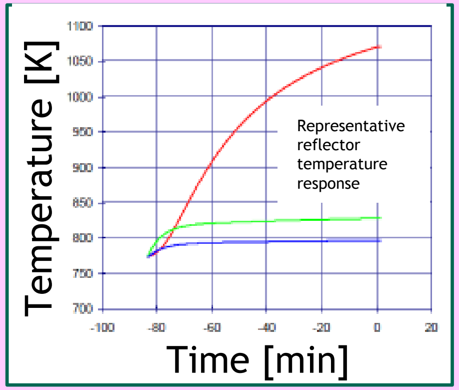
…Solution Methodology…

Stage 0: Normal Operation Thermal Steady State

Large time constant in HTGR graphite structures

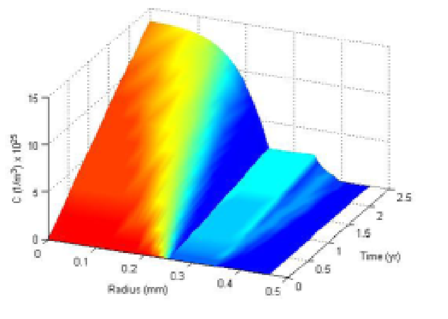
Reduce heat capacities for structures to reach steady state thermal conditions

Reset heat capacities after steady state is achieved.



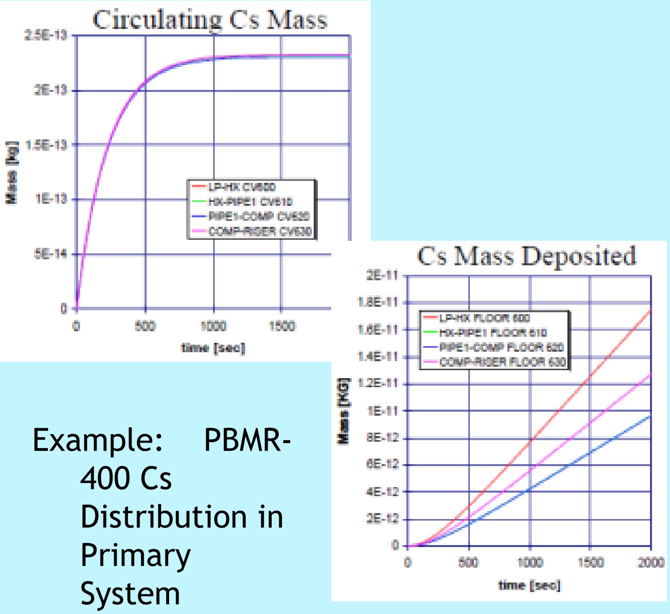
Stage 1: Normal Operation Steady State Diffusion

Establish steady state distribution of radionuclides ***in TRISO particles and matrix***



Stage 2: Normal Operation Steady State Transport

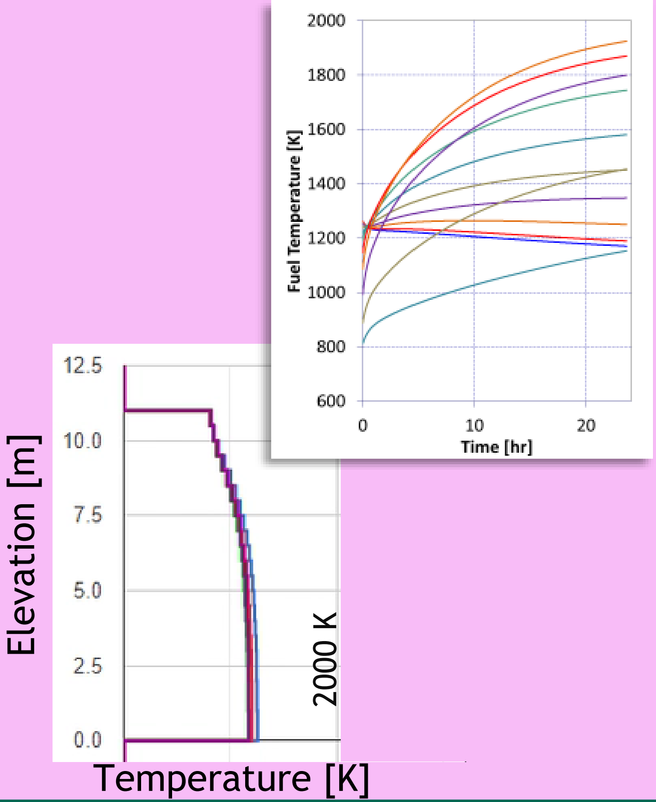
Calculate steady state distribution of radionuclides and graphite dust ***throughout system*** *(deposition, convection through flow paths)*



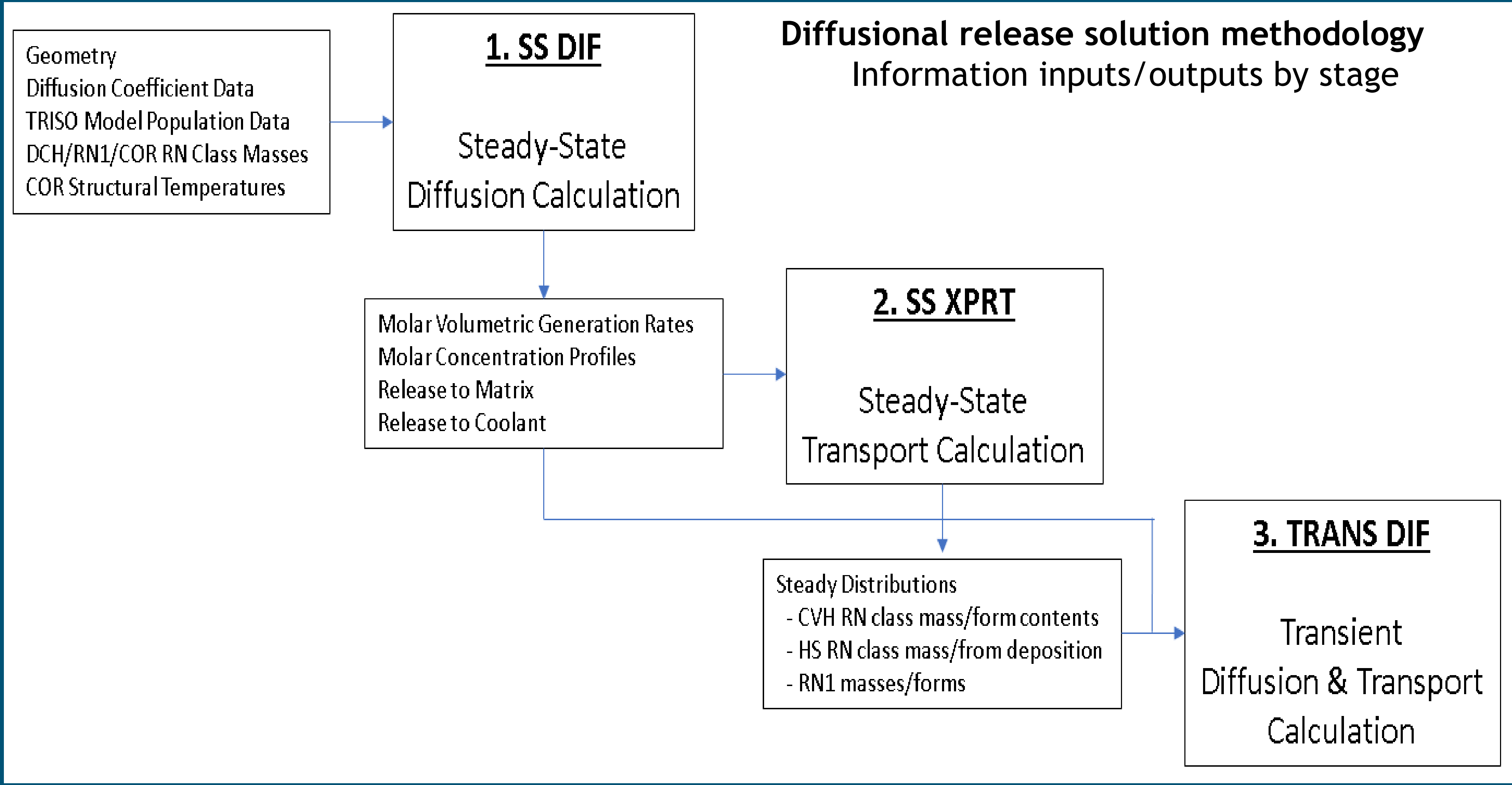
Example: PBMR-400 Cs Distribution in Primary System

Stage 3: Accident Diffusion & Transport calculation

Calculate accident progression and radionuclide release



Solution Methodology – Introduction



Solution Methodology – Accelerated Thermal Steady State Stage

Initial guesses at COR and HS structural temperatures for HTGR calculations may not accurately reflect the steady-state distribution given fission power, decay heat, steady flow, etc.

COR/HS with large thermal inertia require comparatively more computation time to settle into steady distributions

Artificially reduce specific heat capacities (enthalpies) for materials so that temperatures change more quickly given same energy inputs (fission, decay, convection, etc.)

MELCOR can optionally print a file of HS and COR steady-state temperatures (COR_CIT, HS_ND)

Best practice → Whether using accelerated steady state functionality or not, establish steady trends in COR and HS temperatures as well as CVH/FL flows before moving on to the SS DIF stage

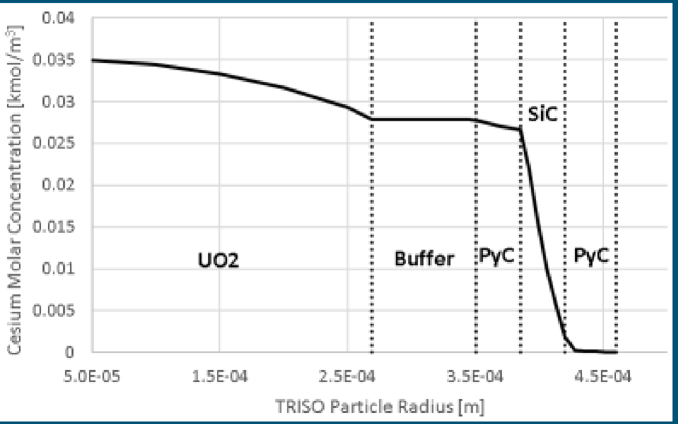
Solution Methodology – Steady State Diffusion Stage (SSDIF)

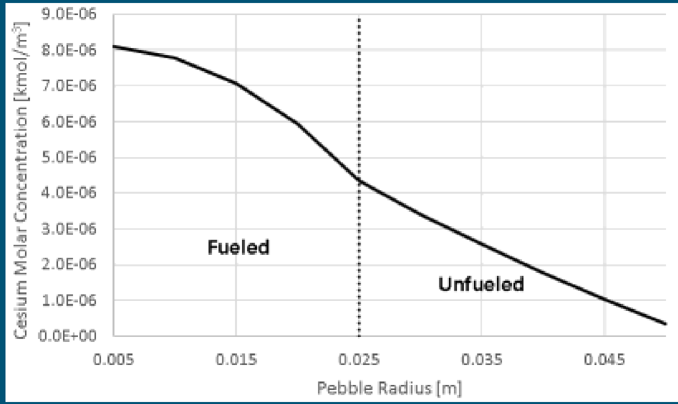
Goal of SS DIF is to generate molar concentration profiles from a steady diffusion treatment

- Each tracked species in each TRISO model (including failed) and in the matrix model
- In each COR cell with diffusion coefficients contingent on temperature
- Assumes a prior set of steady COR structural temperatures (from accelerated steady-state run)

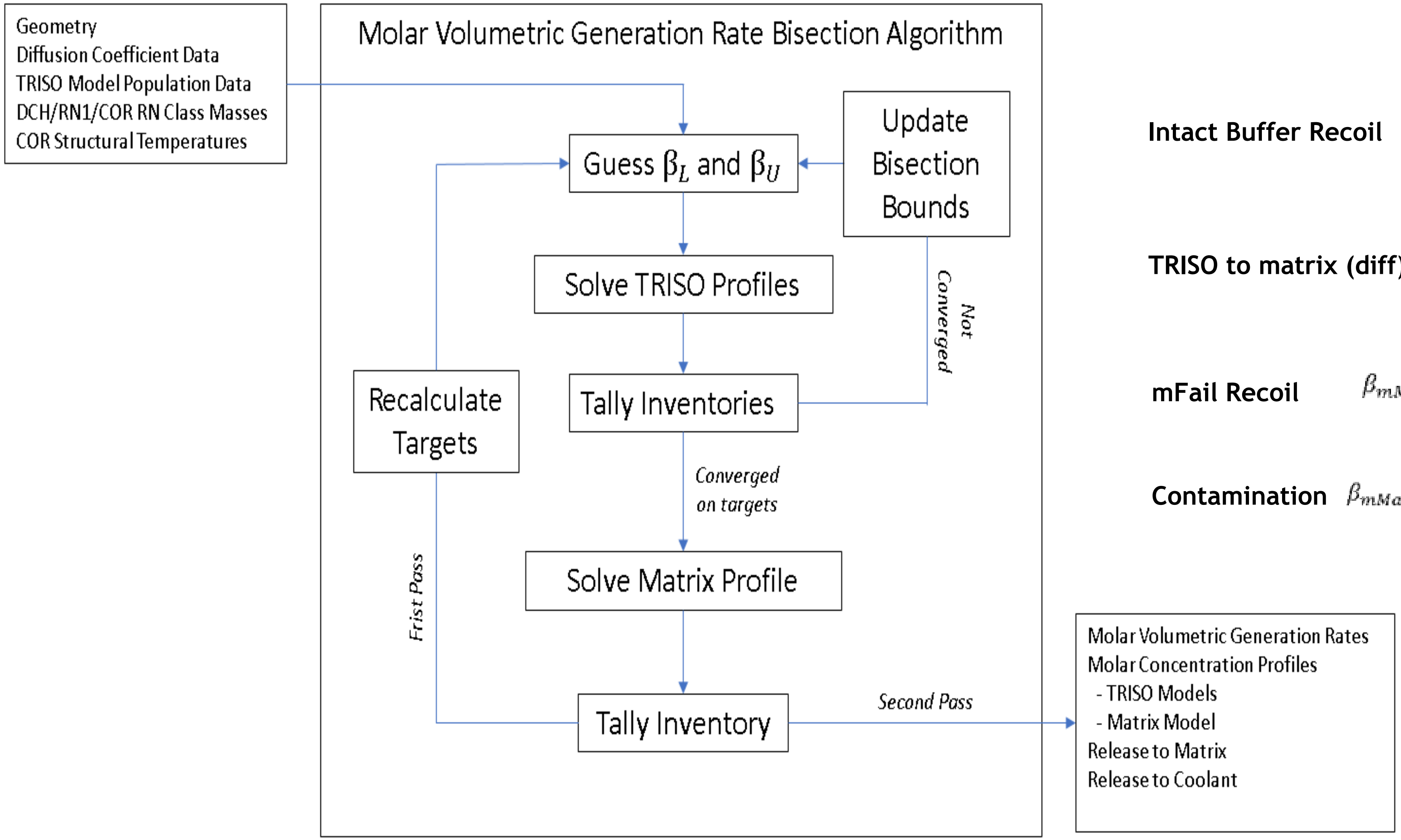
The resulting tracked fission product species concentration profiles:

- Reflect end-of-burnup inventories in TRISO particles and matrix
- Reflect steady-state distributions within fuel, and predict release from fuel
- Are computed with user-defined end-of-burnup inventories (COR/DCH/RN1
- Predict end-of-burnup matrix and coolant inventories
- Reflect several phenomena:
  - Radionuclide generation due to fission and loss due to decay
  - Diffusion and its temperature dependence
  - Leakage and release plus recoil and contamination if applicable





Solution Methodology – Steady State Diffusion Stage (SSDIF)



Source Terms

Intact Buffer Recoil

$$\beta_{m,b,j} = \left[\frac{\beta_{m,k,j}}{1-f_{rec}}\right][f_{rec}]\left[{}^{V_{m,k}}/_{V_{m,b}}\right]$$

TRISO to matrix (diff)

$$\beta_{m\_to\_mMatrix,k,j} = \left(\sum_{m=1}^{M}(R_{m,j})\right) * \left(\frac{N_p}{V_{mMatrix,k}}\right)$$

mFail Recoil

$$\beta_{mMatrix\_recoil,k,j} = \left[\frac{\beta_{mFail,k,j}}{1-f_{rec}}\right][f_{rec}]\left[{}^{N_p V_{mFail,k}}/_{V_{mMatrix,k}}\right]$$

Contamination

$$\beta_{mMatrix\_contam,k,j} = \sum_{m=1}^{M}\left(\left[\frac{\beta_{m,k,j}}{1-f_{rec}}\right][f_{con}]\left[{}^{N_p V_{m,k}}/_{V_{mMatrix,k}}\right]\right)$$

Solution Methodology – Steady State Transport Stage (SS XPRT)

With radionuclide distributions and releases known at steady-state (from SS DIF),

- Freeze COR (i.e hold COR constant - including fission product concentration profiles in and releases from fuel)
- Let CVH, HS, and RN1 march through problem time and settle to a steady condition in terms of:
  - CVH/RN1 mass contents (by RN class and by form)
  - HS/RN1 mass deposition (by RN class)

The end-of-burnup steady conditions (pre-transient) are fully resolved after SS XPRT

Run-time of SS XPRT?

- Is implied by the user as the difference between the start of SS DIF and the start of TRANS DIF

  → Best practice: should be as large as necessary for CVH/HS/RN1 to establish a steady state
- Likely does not equal the true burn-up time, so optional scaling on RN1 inventories of CVH and HS deposition surfaces

Solution Methodology – Transient Diffusion/Transport Stage

Radionuclide distributions are known at steady-state (end-of-burnup) throughout the core and flow loop

Switchover to transient mode:

- TRISO (except for the failed model) and the matrix model are treated with transient finite volume diffusion
- Failed TRISO model is treated with the analytic release model (best practice)
- Shifts in TRISO population are allowed (e.g. CF, built-in rules)
- Fission, recoil, and contamination source terms are zeroed
- CVH/HS/RN1 perform normal functions, COR radionuclide inventories allowed to decline

Calculation proceeds:

- Radionuclide diffusion and transport within fuel, release, fuel failure and inventory dynamics
- Radionuclide transport within the flow loop, and
- Thermal hydraulic response

RN1/DCH Mapping and Consistency

Radionuclide classes, total mass, and specific decay powers configured in DCH

RN1 input apportions radionuclide class mass across COR cells by component

Diffusional release model defines tracked species and maps to DCH/RN1 classes:

- Tracked fission product species represents diffusion transport of entire RN class
- Tracked fission product species represents diffusion of a single element in an RN class

Hand-off from COR to CVH/RN1 occurs upon fuel element release to coolant

Radionuclide class release (any class) can come from scaling of any given tracked species

Conclusions

COR PBR/PMR diffusional fission product release theory/physics was reviewed in some detail

Elements of best practice were discussed (refer to EMUG 2021 HTGR modeling best practices presentation)

Key takeaways:

- Understand how to represent HTGR fuel elements
- Understand the solution methodology well enough to navigate its stages
- Understand connections between COR and DCH/RN1 in context of the diffusional fission product release calculation

Back-up Slides

Finite Volume Diffusion Solver

Ill-conditioning has been observed to be a problem for the diffusion solver w/ SOR

Improved direct methodology (new module of linear algebra utilities) implemented as an option or a kick-out when SOR selected and ill-conditioning detected

COR_SC 1801-1804 newly added to toggle diffusion solver options

Most of the time, it seems the molar concentration vector obtained from matrix solve with direct method returns a better approximation (relative to SOR method) to the original source vector when multiplied by the original coefficient matrix

$$\lfloor A \rfloor * \vec{C} = \vec{d}$$

Analytic Release Model Discussion

$$F(t)_{tot,j} = \int_0^t \frac{dF_W(\tau)}{dx} F_{R,j}(t-\tau)d\tau \approx \sum_{nc=1}^{ncsave}\left[\left(\frac{\Delta f_W}{\Delta t} * X\right)_{nc} F_{R,j}(nc, ncsave)\right](\Delta t)$$

$F(t)_{tot,j}$ = Total release fraction from failed TRISO population at time t, species j

$\frac{dF_W(\tau)}{dx}$ = Failure rate of intact TRISO particles (generation rate of failed) at time τ

$F_{R,j}(t-\tau)$ = Fractional release rate of species j from failed TRISO particles at time t given failure occurred at previous time τ

Approximate:

- Time integral by a summation over historical save points in time…generate new save points as user directs
- Failure rate with data (from user or built-in curve) in vicinity of save point nc
- Fractional release with modified Booth model and a time-averaged reduced diffusion coefficient

Quantity $\left(\frac{\Delta f_W}{\Delta t} * X\right)_{nc}$ gives inventory of failed TRISO generated at time corresponding to save point nc

Operate on this inventory with $F_{R,j}(nc, ncsave)$, fractional release at point ncsave of failed TRISO born at point nc

Inventory shifts coincident with save point generation, failed TRISO release is continuous and always allowed to occur

When intact TRISO fails, have puff releases (intact TRISO buffer and outlying zones)

Energy/Temperature for Diffusion Coefficients

Computational grids for all TRISO and matrix models are also used for T(r)

Several scenarios:

- TRISO particles of various possible arrangement/geometry
- Fuel element matrix
  - PMR cylindrical compacts and transformed hex block
  - PBR pebble – conventional arrangement
  - PBR pebble – fueled spherical shell arrangement

Key assumptions:

- Known COR component (FU, MX) temperatures and fission/decay power
- 1-D steady conduction in cylindrical or spherical geometry, with or without heat generation
- Symmetry conditions, interface heat flux continuity and temperature equality

Energy/Temperature for Diffusion Coefficients

Cylindrical geometry

$$k\frac{d}{dr}\left(r\frac{dT}{dr}\right)+r\dot{q}=0$$

$$\bar{T}(R_i<r<R_o)=\frac{\int_0^{2\pi}\int_{R_i}^{R_o}\big(T(R_i<r<R_o)\big)r\,dr\,d\theta}{(\pi)\left(R_o^2-R_i^2\right)}$$

$$T(r)=A\ln(r)+B-\frac{\dot{q}r^2}{4k}\quad OR\quad T(r)=A\ln(r)+B$$

Spherical geometry

$$k\frac{d}{dr}\left(r^2\frac{dT}{dr}\right)+r^2\dot{q}=0$$

$$\bar{T}(R_i<r<R_o)=\frac{\int_0^{2\pi}\int_0^{\pi}\int_{R_i}^{R_o}\big(T(R_i<r<R_o)\big)r^2\sin\theta\,dr\,d\theta\,d\phi}{\left(\frac{4\pi}{3}\right)\left(R_o^3-R_i^3\right)}$$

$$T(r)=\frac{A}{r}+B-\frac{\dot{q}r^2}{6k}\quad OR\quad T(r)=\frac{A}{r}+B$$

Energy/Temperature for Diffusion Coefficients

TRISO particle treatment…series of conduction equations yields $T(r), q''(r)$

$$
T(r) = \begin{cases}
\dfrac{C_1}{r} + C_2 - \dfrac{\dot{q} r^2}{6k}, & r \le R_{f,o} \quad (n = 1) \\
\dfrac{C_3}{r} + C_4, & R_{f,o} \le r < R_{f2,o} \quad (n = 2) \\
\cdots & \\
\dfrac{C_{2n-1}}{r} + C_{2n}, & R_{f(n-1),o} \le r < R_{fn,o} \quad (n) \\
\cdots & \\
\dfrac{C_{2N-1}}{r} + C_{2N}, & R_{f(N-1),o} \le r < R_{fN,o} \quad (n = N)
\end{cases}
$$

$$
q''(r) = \begin{cases}
\dfrac{k_1 C_1}{r^2} + \dfrac{\dot{q} r}{3}, & r \le R_{f,o} \quad (n = 1) \\
\dfrac{k_2 C_3}{r^2}, & R_{f,o} \le r < R_{f2,o} \quad (n = 2) \\
\cdots & \\
\dfrac{k_n C_{2n-1}}{r^2}, & R_{f(n-1),o} \le r < R_{fn,o} \quad (n) \\
\cdots & \\
\dfrac{k_N C_{2N-1}}{r^2}, & R_{f(N-1),o} \le r < R_{fN,o} \quad (n = N)
\end{cases}
$$

Enforce a symmetry condition, interface conditions, and let $T(r = R_N) = T_{FU}$

Derive equations for constants of integration that can be solved algorithmically

[illegible] = 0 ; [illegible] = ([illegible] ,)(+) + [illegible] ; [illegible] = [illegible]

[illegible] = [illegible] ( ) ; [illegible] = (,)([illegible] − [illegible]) + [illegible]

$$C_{2N} = T_{FU} - {C_{2N-1}}/{R_{fN,o}}$$

Energy/Temperature for Diffusion Coefficients

Fuel matrix treatment (conventional PBR pebble fuel as illustrative example)

$$T(r) = \begin{cases} \frac{C_1}{r} + C_2 - \frac{\dot{q}r^2}{6k_f}, r \leq R_{f,o} \\ \frac{C_3}{r} + C_4, \quad R_{pb} \geq r > R_{f,o} \end{cases} \qquad q''(r) = \begin{cases} \frac{k_f C_1}{r^2} + \frac{\dot{q}r}{3}, r \leq R_{f,o} \\ \frac{k_m C_3}{r^2}, \quad R_{pb} \geq r > R_{f,o} \end{cases}$$

Conditions:

$$\bar{T}(r) = \begin{cases} T_{FU} = \left(\frac{3}{4\pi R_{f,o}^3}\right)\left(\int_0^{2\pi}\int_0^{\pi}\int_0^{R_{f,o}} \left(\frac{C_1}{r} + C_2 - \frac{\dot{q}r^2}{6k_f}\right) r^2 \sin\theta \, dr \, d\theta \, d\phi\right) \\ T_{MX} = \left(\frac{3}{4\pi\left(R_{pb}^3 - R_{f,o}^3\right)}\right)\left(\int_0^{2\pi}\int_0^{\pi}\int_{R_{f,o}}^{R_{pb}} \left(\frac{C_3}{r} + C_4\right) r^2 \sin\theta \, dr \, d\theta \, d\phi\right) \end{cases}$$

$$q''(r = 0) = 0$$

$$q''(r = R^-{}_{f,o}) = q''(r = R^+{}_{f,o})$$

Solution:

- Calculate pebble center and pebble surface temperatures directly
- Calculate a fueled region surface temperature by blending predictions from both profiles
- March through the grid and fill in temperatures according to profile prescriptions

Energy/Temperature for Diffusion Coefficients

$$T_{CL} = T(r=0) = T_{FU} + \left(\dot{q}R_{fo}^2 \Big/ 10k_{fu} \right)$$

$$T_{pb} = T(r=R_{pb}) = T_{MX} + \left(\dot{q}R_{fo}^3 \Big/ 3k_{mx} \right)\left(\frac{1}{R_{pb}} - \left(\frac{3}{2}\right)\left(\frac{R_{pb}^2 - R_{fo}^2}{R_{pb}^3 - R_{fo}^3}\right) \right)$$

$$T_{fo} = T(r=R_{fo}) = \left(\frac{T_{pb} + \left(\dot{q}R_{fo}^3 \Big/ 3k_{mx} \right)\left(\frac{1}{R_{fo}} - \frac{1}{R_{pb}} \right)}{2} \right) + \left(\frac{T_{CL} - \left(\dot{q}R_{fo}^2 \Big/ 6k_{fu} \right)}{2} \right)$$

$$T(r) = \begin{cases} T_{\mathrm{fo}} + (T_{CL} - T_{fo})\left(1 - \left(\frac{r}{R_{fo}}\right)^2\right), & r \le R_{f,o} \\ T_{pb} + (T_{fo} - T_{pb})\left(\left(\frac{1}{r} - \frac{1}{R_{pb}}\right) \Big/ \left(\frac{1}{R_{fo}} - \frac{1}{R_{pb}}\right) \right), & R_{pb} \ge r > R_{f,o} \end{cases}$$