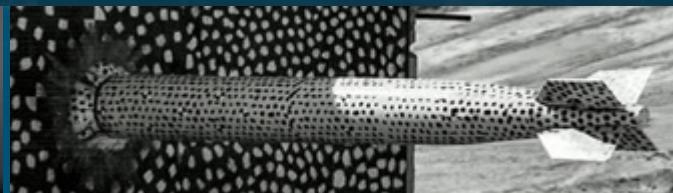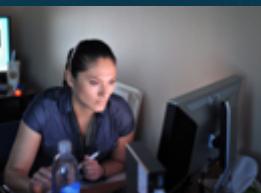# MELCOR for High Temperature Gas-cooled and Fluoride High Temperature Reacotr Modeling

MELCOR Workshop
June 13-17, 2022

PRESENTED BY

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MELCOR HTGR and FHR Modeling and Development Radionuclide Transport – Practice/Exercise

Overview

COR radionuclide transport input structures
- Introduction
- Global diffusional fission product release inputs and practices
- Model-wise diffusional fission product release inputs and practices
- Analytic release model inputs and practices
- Run sequencing inputs and practices

COR radionuclide transport exercises
- Building basic fuel element representations for diffusional fission product release modeling
- Run sequence demonstration
- Use of vectorized control functions

Conclusions

…Inputs and Best Practices…

Conventional Pebble Fuel Element (HTGR/PBR)
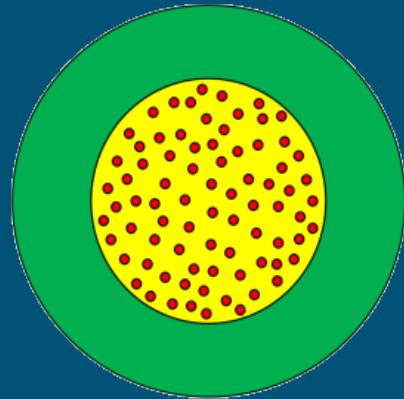
Annular Pebble Fuel Element (FHR)

Prismatic Fuel Element (HTGR/PMR)

| TRISO | **Fuel (FU)** |

| GRAPHITE | **Fuel Extra Material (FUXM)** |

| GRAPHITE | **Matrix (MX)** |

Introduction

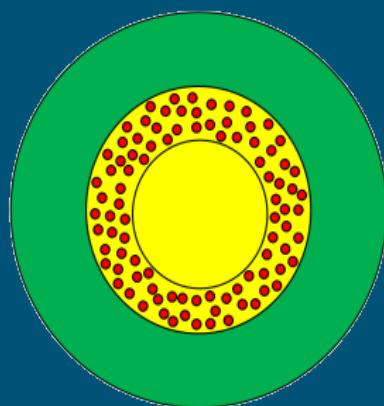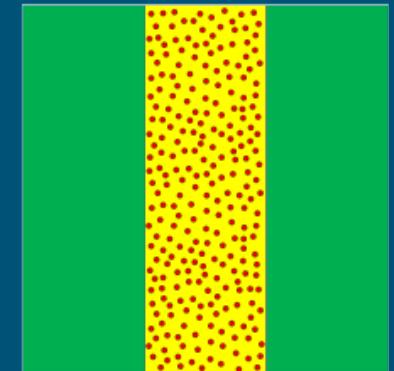Reminder…overall goals of the HTGR fission product release model include:
- Prediction of radionuclide distributions within fuel
- Prediction of radionuclide release from fuel elements to coolant
- Conventional CVH/HS/RN1 takes over once radionuclide inventory escapes COR

A general configuration of the radionuclide release/transport problem includes:
- **Two or more models** representing all cohorts of the TRISO population (e.g. intact, failed)
- **One model** representing the fuel element matrix
- **One or more tracked fission product species** mapped to radionuclide classes
- Global parameters describing the PBR, FHR, or PMR core
- A one-dimensional spherical or cylindrical finite volume solution grid for each defined **model**
- Diffusion coefficient data (Arrhenius temperature relations)
- Miscellaneous data (failure, boundary conditions, sorption isotherms, partition coefficients)

Ascertain radionuclide distribution/release with FV diffusion and/or modified Booth (analytic release model)

Inputs and Practices - Global

Globally-applicable parameters apply universally across all models that together comprise fuel elements

COR global inputs COR_DIFF and COR_DIFFGX
- COR_DIFF sets steady-state diffusion stage execution time (calculation occurs in one time-step)
- COR_DIFFG1 for the steady-state burn-up/irradiation time
- COR_DIFFG2 for total numbers of models (all TRISO plus matrix) and total number of tracked species
- COR_DIFFG3 and COR_DIFFG4 for global fuel parameters
  - Number of TRISO particles per fuel element, contamination fraction, recoil fraction
  - Fuel mass per fuel element (i.e. per pebble or per compact)
  - Total FU mass can be used to approximate the number of fuel elements per COR cell and thus the number of TRISO particles
- COR_DIFFG5 for global tracked species parameters
- COR_DIFFG6 for declaration of matrix model number (usually 3) and failed TRISO model number (usually 2)
- COR_DIFFG7 for area scaling if applicable

HTGR Fission Product Release Model Recommendations for Global User Inputs (1/2)

* Text in red indicates any deprecated MELGEN inputs
* Text in green indicates any new information

COR_DIFF

- Generally, make DFLAGS = 1 and start the calculation (EXEC_TSTART) somewhere in problem time prior to the selected time DTIMEONS…this will ensure MELCOR executes the SS DIFF stage at DTIMEONS (which can be given by CF or constant)
- Do the steady-state diffusion calculation at a point in problem time DTIMEONS where an accelerated steady-state run (EXEC_SS) has established constant COR, HS, and CVH temperatures
- Strongly suggest inputs of 'NO' for both MDIFFILE and INITFILE

COR_DIFFG1

- TBURNUP should reflect amount of time for which the core was operating at steady full power prior to the accident/transient in question

COR_DIFFG2

- NREG is the total number of TRISO models plus one for the matrix model. Minimum recommended level of detail is NREG = 3 so that there is space for three models: intact TRISO, failed TRISO, and matrix
- NSPECIES is the total number of tracked fission product species. Note that these species must be mapped to an RN1 class somehow. The bare minimum is NSPECIES = 1 so that at least one species is being calculated.

COR_DIFFG3

- NPARTPFUEL approximates the number of total TRISO particles (i.e. TRISO particles of all kinds be they intact, failed, etc.) in a single fuel element (a pebble or compact)
- Choose/set FRECOIL and FCONTAM to represent the desired amount of allowed fission product recoil and allowed tramp

HTGR Fission Product Release Model Recommendations for Global User Inputs (2/2)

* Text in red indicates any deprecated MELGEN inputs
* Text in green indicates any new information

COR_DIFFG4
◦ Choose/set XFUMASSPFUEL to approximate the mass of fissile material in a single fuel element (pebble or compact)

COR_DIFFG5
◦ Input a table of length NSPECIES with appropriate decay constants for each tracked species (use 0.0 if no decay)

COR_DIFFG6
◦ General recommendation of MFAIL = 2 and MMATRIX set to 1 plus the number of TRISO particle models in the problem, e.g. if intact TRISO is model number 1 and failed TRISO is model number 2, set MMATRIX to model number 3

COR_DIFFG7
◦ AFACTOR is intended to account for deviations in fuel element geometry, so use a scalar other than unity if, e.g., a non-cylindrical fuel compact is being modeled for a PMR. The AFACTOR should then be set to a scalar that makes the cylindrical fuel compact outer surface area equal to the true fuel compact outer surface area

HTGR Fission Product Release Model Recommendations for Model-wise User Inputs (1/2)

* Text in red indicates any deprecated MELGEN inputs
* Text in green indicates any new information

COR_DIFFM1
◦ Enter a descriptive object name for MODNAME and choose a model number NMODEL bearing in mind the global values for MFAIL and MMATRIX
◦ Use 'BOTH' for QOPT
◦ Pick a spherical or cylindrical geometry for NMODEL=MMATRIX according to reactor type, but for all TRISO models of any type, only GEOM='SPH' for spherical geometry is allowed
◦ Use 'SS" for TTYPE

COR_DIFFM2
◦ For all TRISO models, NKERN = 1 (innermost zone is the first zone which is the fuel-bearing or kernel zone)
◦ For all TRISO models that have a buffer region, NBUFF ought to be 1+NKERN as the buffer surrounds the kernel
◦ Total number of nodes must be consistent with subsequent model-wise grid geometry input
◦ Ensure FRAC population fraction input is consistent with input for other models that all together comprise the total TRISO population. Note that for the failed TRISO model, population fraction data is given elsewhere (CF or constant can be used for FRAC)

COR_DIFFM3
◦ Choose zone-wise material names that are identified in MP package input
◦ Use QDOT0 of unity in fueled zones and use QDOT0 of zero elsewhere, e.g. in a typical intact TRISO model, the kernel zone should have QDOT0 of 1.0 and all other zones should have a QDOT0 of 0.0

COR_DIFFM4
◦ Give a molecular weight for the material and an initial temperature

HTGR Fission Product Release Model Recommendations for Model-wise User Inputs (2/2)

* Text in red indicates any deprecated MELGEN inputs

* Text in green indicates any new information

COR_DIFFM5

◦ Use the best data available to configure zone-wise diffusion coefficients, or treat them parametrically

◦ Only attempt to configure partition coefficients and sorption isotherms if sufficient data is available to round out the description on subsequent input records (or if probing sensitivities)

COR_DIFFM6

◦ At the "inner" boundary, recommend symmetry (zero flux) conditions for diffusion

COR_DIFFM7

◦ At the "outer" boundary, recommend zero concentration (MOLE 0.0) for diffusion

COR_DIFFM8

◦ According to the partition coefficient formulation and/or the sorption isotherm empirical model, round out the description here

HTGR Fission Product Release Model Recommendations for Other User Inputs

* Text in red indicates any deprecated MELGEN inputs
* Text in green indicates any new information

COR_XPRT

○ Recommend 0 for DFLAGS so that the SS XPRT stage may commence immediately upon the conclusion of the SS DIFF calculation

○ Strongly suggest 'NO' for INITFILE and TRANSFILE

COR_DIFT

○ Recommend 0 for DFLAGT so that the TRANS DIFF/XPRT stage commences upon conclusion of the SS XPRT stage

○ DTIMEONT is the problem time where SS XPRT concludes and TRANS DIFF/XPRT begins, so ensure that by this problem time the requisite CVH/HS/RN1 steady-state has been established (DTIMEONT can be CF or constant)

○ Strongly suggest 'NO' for INITFILE, TRANSFILE, MDIFFILE, FAILFILE

○ GSCALE is a user-imposed scalar on the CVH radionuclide contents and the HS radionuclide depositions upon conclusion of the SS XPRT stage. GSCALE is currently surmised from user input as TBURNUP/(DTIMEONT-DTIMEONS)

○ A CF (to include a vectorized CF) can specify the failed TRISO population dynamics, otherwise a built-in temperature curve can be used

COR_DIFTG1

○ Optionally set a problem time at which the TRANS DIFF/XPRT stage concludes and diffusion is "frozen"

○ Optionally request diffusion time step characteristics that are taken into consideration in view of the COR timestep

COR_DIFTG2

○ Configure analytic release model parameters to treat the failed TRISO model (a few new options to check out)

…Exercise 1 – Building PBR Fuel Elements…

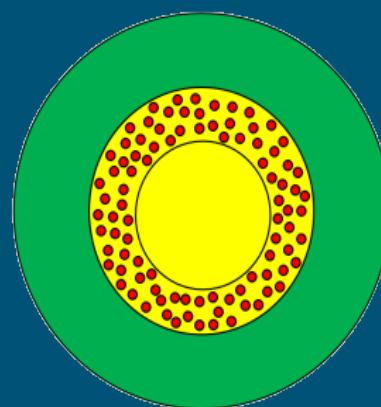**Conventional Pebble Fuel Element (HTGR/PBR)**
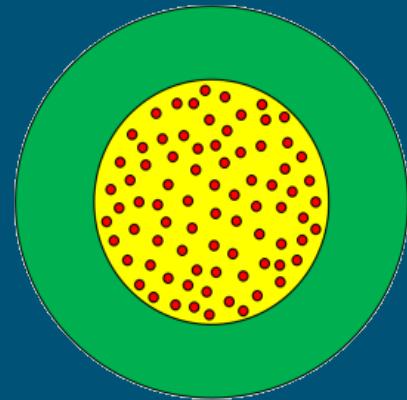
Annular Pebble Fuel Element (FHR)

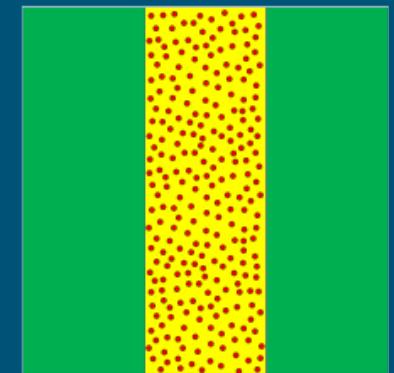**Prismatic Fuel Element (HTGR/PMR)**

TRISO	**Fuel (FU)**

GRAPHITE	**Fuel Extra Material (FUXM)**

GRAPHITE	**Matrix (MX)**

Exercise 1- Intact TRISO

Require a model for intact TRISO to track diffusional release of defined fission product species
- COR_DIFFM1 through COR_DIFFM8, stipulate:
  - Five zones for five TRISO particle layers (kernel is zone 1, buffer is zone 2)
  - Intact TRISO initially comprises 99.999% of total population
  - Choose 25 total nodes across the 5 zones (5 nodes per zone, equally spaced across zone thickness)
  - Use 'URANIUM-DIOXIDE' for kernel material, 'GRAPHITE' for all other zone materials (thermal properties, not diffusion)
  - Furnish Arrhenius diffusion coefficient inputs according to available data (each tracked species, each zone of TRISO)
  - Use symmetry conditions at "LHS" inner boundary, use zero concentration conditions at "RHS" outer boundary (all species)

```
! Intact TRISO
cor_diffm1 'IntactTRISO' 1 ! spherical geometry for model #1 named 'IntactTRISO'
cor_diffm2 1 2 0.99999 25 ! Kernel is zone 1, buffer is zone 2, initial frac, 25 nodes across zones
cor_diffm3 5
        1 'URANIUM-DIOXIDE'     5   250.0e-6  1.0 ! 250 micron outer kernel radius, fueled
        2 'GRAPHITE'           10   95.0e-6   0.0 ! 95 micron thick buffer
        3 'GRAPHITE'           15   40.0e-6   0.0 ! 40 micron thick IPyC
        4 'GRAPHITE'           20   35.0e-6   0.0 ! 35 micron thick SiC
        5 'GRAPHITE'           25   40.0e-6   0.0 ! 40 micron thick OPyC
cor_diffm4 5
        1 270.0 ! UO2 molec wght
        2 12.0  ! C molec wght
        3 12.0  ! C molec wght
        4 40.0  ! SiC molec Wght
        5 12.0  ! C molec wght
```

```
cor_diffm511 'Xe' 5   ! IAEA TECDOC-978 data as Kr/I2
        1 1.3e-12 126000.0 0 ! fuel
        2 1.0e-8   0.0 0        ! porous buffer layer fp recoil
        3 2.9e-8   291000.0 0 ! pyrolytic carbon layer
        4 3.7e+1   657000.0 0  ! SiC
        5 2.9e-8   291000.0 0 ! pyrolytic carbon layer
```

	FP Species							
	Kr		Cs		Sr		Ag	
Layer	D (m²/s)	Q (J/mole)	D (m²/s)	Q (J/mole)	D (m²/s)	Q (J/mole)	D (m2/s)	Q (J/mole)
Kernel (normal)	1.3E-12	126000.0	5.6-8	209000.0	2.2E-3	488000.0	6.75E-9	165000.0
Buffer	1.0E-8	0.0	1.0E-8	0.0	1.0E-8	0.0	1.0E-8	0.0
PyC	2.9E-8	291000.0	6.3E-8	222000.0	2.3E-6	197000.0	5.3E-9	154000.0
SiC	3.7E+1	657000.0	7.2E-14	125000.0	1.25E-9	205000.0	3.6E-9	215000.0
Matrix Carbon	6.0E-6	0.0	3.6E-4	189000.0	1.0E-2	303000.0	1.6E00	258000.0
Str. Carbon	6.0E-6	0.0	1.7E-6	149000.0	1.7E-2	268000.0	1.6E00	258000.0

Exercise 1- Failed TRISO

Require a model for failed TRISO to track diffusional release of defined fission product species
- Use finite volume solution in SS DIF and pivot to analytic release for TRANS DIFF
- COR_DIFFM1 through COR_DIFFM7, stipulate:
  - One zone for bare kernel representation (kernel is zone 1)
  - COR_DIFT for failed TRISO initial fraction, should be 0.001% since intact is 99.999%
  - Choose 5 total nodes across the kernel zone (equally spaced across zone thickness)
  - Use 'URANIUM-DIOXIDE' for kernel material
  - Furnish Arrhenius diffusion coefficient inputs according to available data (each tracked species)

```
cor_diffm1 'FailedTRISO' 2
cor_diffm2 1 0 5
cor_diffm3 1
       1 'URANIUM-DIOXIDE' 5 250.0e-6
cor_diffm4 1
       1 270.0 2.5 1250.0
cor_diffm521 'Xe' 1
       1 9.38675e-12 126000.0 0
cor_diffm522 'Cs' 1
       1 4.04352e-07  209000.0 0
cor_diffm523 'Ba' 1
       1 1.58853e-02  488000.0 0
cor_diffm524 'I'  1
       1 9.38675e-12 126000.0 0
cor_diffm525 'Ag' 1
       1 4.87389e-08 165000.0 0
```

Note the diffusion coefficients for modified Booth diffusion release (analytic release) are computed from COR_DIFFM5mn for matrix

Exercise 1- Matrix

Require a matrix model to track diffusional release of defined fission product species after release from TRISO

- COR_DIFFM1 through COR_DIFFM8, stipulate:
  - Two zones, one for the fueled zone of the pebble where TRISO resides, one for unfueled shell ("kernel" is zone 1)
  - Choose 10 total nodes across the 2 zones (5 nodes per zone, equally spaced across zone thickness)
  - Use 'GRAPHITE' for both zones (thermal properties, not diffusion)
  - Furnish Arrhenius diffusion coefficient inputs according to available data (each tracked species, each zone)

```
! Matrix
cor_diffm1 'Matrix' 3
cor_diffm2 1 2 10  ! Kernel is zone 1, buffer is zone 2
cor_diffm3 2
      1 'GRAPHITE'  5  2.5e-2   ! 0.025 m fueled pit of pebble
      2 'GRAPHITE' 10 0.5e-2    ! 0.03 m pebble outer radius
cor_diffm4 2
      1 12.0 10.0 1250.0
      2 12.0 10.0 1250.0
```

```
cor_diffm531 'Xe' 2
      1 6.0e-6      0.0 0
      2 6.0e-6      0.0 0
cor_diffm532 'Cs' 2
      1 3.6e-4  189000.0 0
      2 1.7e-6  149000.0 0
cor_diffm533 'Ba' 2
      1 1.0e-2  303000.0 0
      2 1.7e-2  268000.0 0
cor_diffm534 'I'  2
      1 6.0e-6      0.0 0
      2 6.0e-6      0.0 0
cor_diffm535 'Ag' 2
      1 1.6e+00 258000.0 0
      2 1.6e00  258000.0 0
```
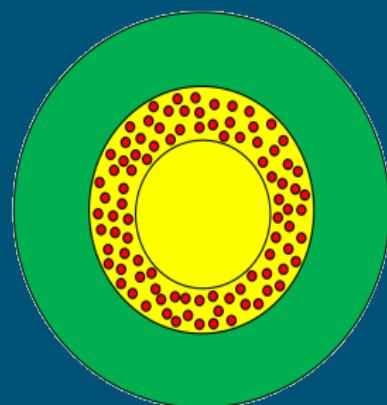
…Exercise 2 – Run Sequence…
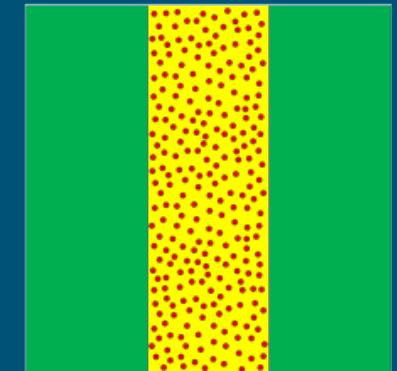
Conventional Pebble Fuel Element (HTGR/PBR)
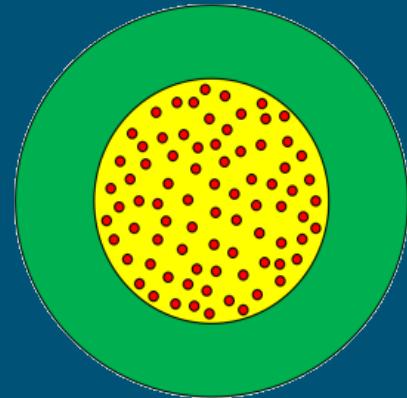
Annular Pebble Fuel Element (FHR)

Prismatic Fuel Element (HTGR/PMR)

TRISO	Fuel (FU)

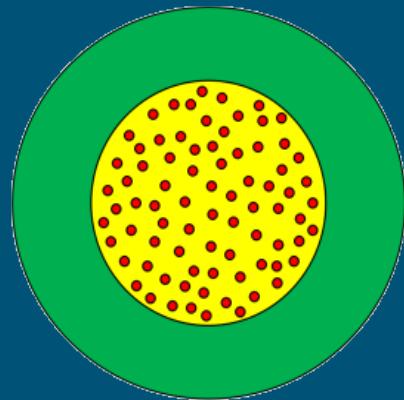| GRAPHITE	Fuel Extra Material (FUXM)

GRAPHITE	Matrix (MX)

Exercise 2

Assume thermal steady state established and illustrate the run sequence of diffusional fission product release

- SS DIF at DTIMEONS within a time-step
- SS XPRT between DTIMEONS and DTIMEONT to establish trends in CVH/HS/RN1 conditions (frozen COR release)
- Optional user-supplied graphite dust generation rate
- Scaling of SS XPRT steady CVH/HS contents/depositions
- TRANS DIF after DTIMEONT approximately coincident with thermal hydraulic transient (e.g. PLOFC)

…Demonstration…

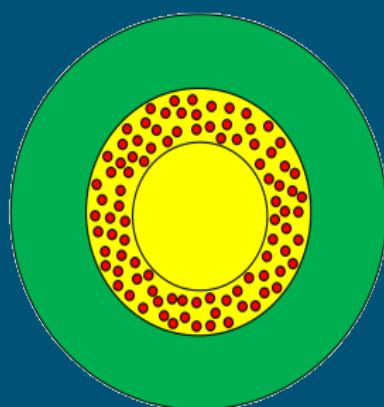# …Exercise 3 – Vectorized CFs for Diffusional Fission Product Release…
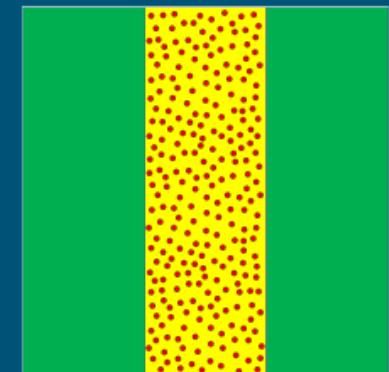
Conventional Pebble Fuel Element (HTGR/PBR)

Annular Pebble Fuel Element (FHR)

Prismatic Fuel Element (HTGR/PMR)

| TRISO | Fuel (FU) |

| GRAPHITE | Fuel Extra Material (FUXM) |

| GRAPHITE | Matrix (MX) |

Exercise 3

…Demonstration of failed TRISO modeling via VCF plus solution/results monitoring…

Exercise 3

…Output Processing (CF arguments and plot variables)…

Conclusions

Reviewed some user input structures and best practice guidelines for diffusional fission product release modeling

Talked through the process of building a fuel element representation (TRISO and matrix) for a PBR

Demonstrated:
  Diffusional fission product release run sequence
  Use of VCFs and CF vector arguments for TRISO failure modeling and results monitoring