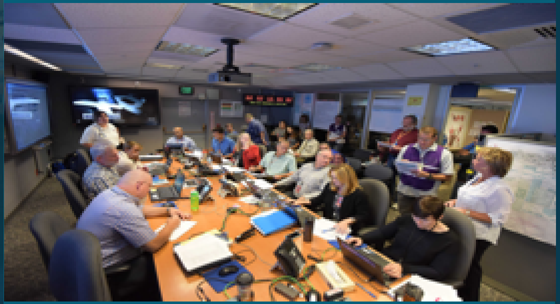
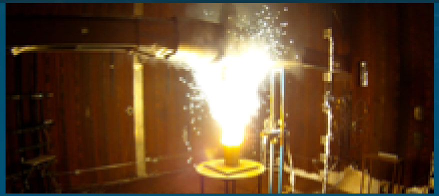
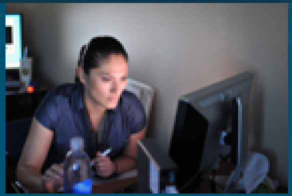
SAND2021-14165PE

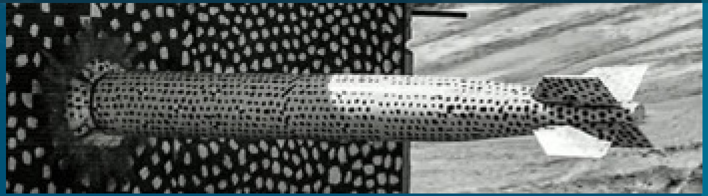
Sandia National Laboratories

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

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MELCOR HTGR Modeling/Development Radionuclide Transport – Practice/Exercise

Overview

COR radionuclide transport input structures

- Introduction/reminder
- 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

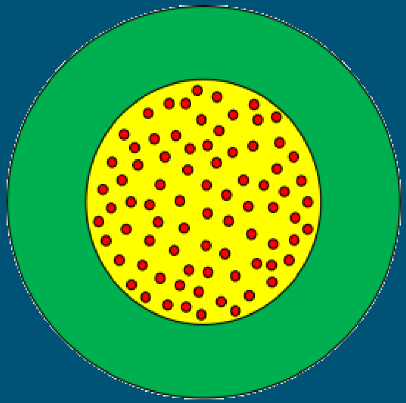
COR radionuclide transport exercises

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

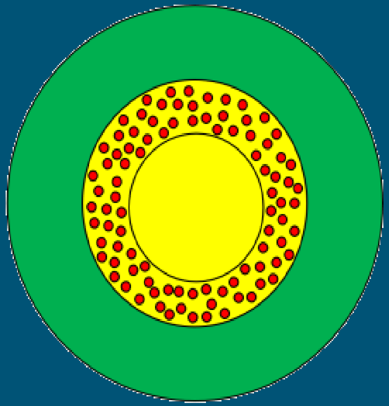
Conclusions

...Inputs and Best Practices...

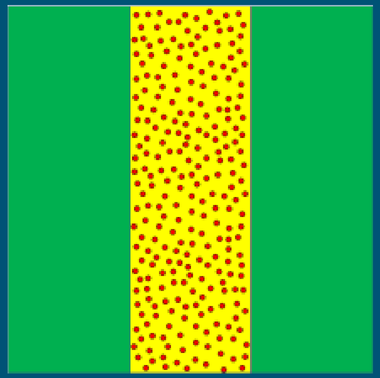
Conventional Pebble Fuel Element



Annular Pebble Fuel Element



Prismatic Fuel Element



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 HTGR (PBR 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

Inputs and Practices - Global

COR_DIFF

- Choose DFLAGS = 1 and start calculation (EXEC_TSTART) prior to DTIMEONS from COR_DIFF
- Do SS DIF at DTIMEONS subsequent to accelerated steady-state run (EXEC_SS)
- Strongly suggest inputs of ‘NO’ for both MDIFFILE and INITFILE (deprecated input acquisition)

COR_DIFFG1

- Burnup time should reflect time for which the core was operating at steady full power prior to accident/transient

COR_DIFFG2

- NREG is the total number of TRISO models plus one for the matrix model
- Recommend NREG = 3 for three models: intact TRISO, failed TRISO, and matrix
- NSPECIES is the total number of tracked fission product species (mapped to an RN1 classes)

COR_DIFFG3

- NPARTPFUEL is the number of total TRISO particles (of all kinds.) in a single fuel element (a pebble or compact)
- FRECOIL and FCONTAM represent fission product recoil and tramp uranium contamination in the matrix

Inputs and Practices - Global

COR_DIFFG4

- XFUMASSPFUEL is the mass of fissile material in a single fuel element (pebble or compact)
-

COR_DIFFG5

- Table of length NSPECIES with radioactive decay constants for each tracked species (use 0.0 if no decay)

COR_DIFFG6

- General recommendation: MFAIL = 2, MMATRIX =3

COR_DIFFG7

- AFACTOR accounts for deviations in fuel element geometry
- Use if a non-cylindrical geometry is being modeled for a PMR. The AFACTOR should then be set to a scalar that makes the idealized cylindrical hex block outer surface area equal to the true hex block outer surface area

Inputs and Practices – Model Specific

Model-wise parameters apply uniquely to their designated models

COR model-wise block inputs COR_DIFFMX…applicable to each model in the problem

- COR_DIFFM1 and COR_DIFFM2 for characteristics of the model (name, number, geometry, materials)
- COR_DIFFM3 for model grid geometry/noding definitions
  - Material and thickness for zones
  - Indicator of fission product source region
- COR_DIFFM4 for zone-wise initialization and information
- COR_DIFFM5 for zone-wise diffusion coefficient Arrhenius parameter definitions

[IAEA TECDOC-0978]

	FP Species							
	Kr		Cs		Sr		Ag	
Layer	D (m^2/s)	Q (J/mole)	D (m^2/s)	Q (J/mole)	D (m^2/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

- COR_DIFFM6, COR_DIFFM7, and COR_DIFFM8 for boundary condition data

Inputs and Practices – Model Specific

COR_DIFFM1

- Descriptive object name for MODNAME, model number NMODEL cannot be MFAIL or MMATRIX
- Use ‘BOTH’ for QOPT
- SPH or CYL for NMODEL=MMATRIX according to reactor type, but all TRISO use GEOM=‘SPH’
- 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 one larger than NKERN
- Total number of nodes must be consistent with subsequent model-wise grid geometry input
- FRAC population fraction input is consistent with input for other models (all together comprise total TRISO population)
- Note failed TRISO model population fraction data is given elsewhere

COR_DIFFM3

- Zone-wise materials should be defined in MP package input
- QDOT0 of unity in fueled zones (TRISO kernel, matrix fueled zone), QDOT0 of zero elsewhere

COR_DIFFM4

- Molecular weight and initial temperature for the material

Inputs and Practices – Model Specific

COR_DIFFM5

- Use the best data available to configure zone-wise diffusion coefficients, or treat them parametrically
- Configure partition coefficients and sorption isotherms if sufficient data is available

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

- Partition coefficient formulation and/or the sorption isotherm empirical model

Inputs and Practices – Analytic Release

COR_DIFT either invokes:

- Built-in empirical model for TRISO failure (intact-to-failed transition), or
- User CF-specified rule(s) for TRISO failure

COR_DIFTG2 configures analytic release parameters for the failed TRISO model

- Activation flag (note activation problem time is on a different record)
- Maximum number of save points allowed
- Other regulators on save point generation (minimum elapsed problem time, minimum required failure fraction change)

Each COR cell has its own time history for analytic release model calculations, but the save point generation criteria are globally applied

Inputs and Practices – Run Sequencing

COR_XPRT

- 0 for DFLAGS so that SS XPRT commences upon conclusion of SS DIFF
- 'NO' for INITFILE and TRANSFILE

COR_DIFT

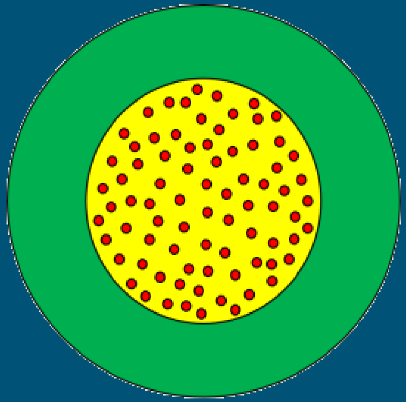
- 0 for DFLAGT so that TRANS DIFF commences upon conclusion of SS XPRT
- DTIMEONT is problem time of SS XPRT conclusion where TRAN DIFF begins, ensure CVH/HS/RN1 steady -state
- 'NO' for INITFILE, TRANSFILE, MDIFFILE, FAILFILE
- GSCALE scales CVH radionuclide contents and HS radionuclide depositions at conclusion of SS XPRT
- Failed TRISO population fraction comes from 'BUILT-IN' plus initial fraction or CF

COR_DIFTG1

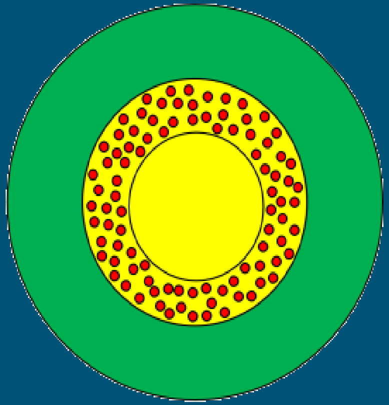
- Optionally set a problem time at which TRANS DIFF concludes and diffusion is "frozen" (no longer updated/calculated)
- Optionally request diffusion time step

…Exercise 1 – Building PBR Fuel Elements…

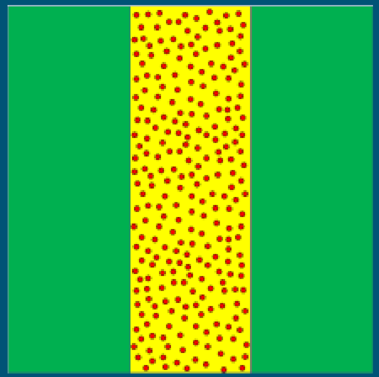
Conventional Pebble Fuel Element



Annular Pebble Fuel Element



Prismatic Fuel Element



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 BOTH SPH SS ! spherical geometry, use T(r) model
cor_diffm2 1 2 0.99999 25
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  2.5   1250.0 ! UO2 molec wght
        2  12.0   0.4   1250.0 ! C molec wght
        3  12.0   10.3  1250.0 ! C molec wght
        4  40.0   168.0 1250.0 ! SiC molec Wght
        5  12.0   10.3  1250.0 ! 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
```

Layer	FP Species Kr D (m²/s)	Kr Q (J/mole)	Cs D (m²/s)	Cs Q (J/mole)	Sr D (m²/s)	Sr Q (J/mole)	Ag D (m2/s)	Ag 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

```
cor_diffm6 6
    1 'Xe'  'FLUX'   0.0
    2 'Cs'  'FLUX'   0.0
    3 'Ba'  'FLUX'   0.0
    4 'I'   'FLUX'   0.0
    5 'Ag'  'FLUX'   0.0
    6 'FLUX'         0.0

cor_diffm7 6
    1 'Xe' 'MOLE'   0.0
    2 'Cs ' 'MOLE'   0.0
    3 'Ba' 'MOLE'   0.0
    4 'I'   'MOLE'   0.0
    5 'Ag' 'MOLE'   0.0
    6 'H'   2.7e4 1250.0
```

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_DIFFM8, 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)
  - Use symmetry conditions at "LHS" inner boundary, use zero concentration conditions at "RHS" outer boundary (all species)

```
cor_diffm1 'FailedTRISO' 2 BOTH SPH SS
cor_diffm2 1 0 5
cor_diffm3 1
        1 'URANIUM-DIOXIDE' 5 250.0e-6 1.0
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

	FP Species							
	Kr		Cs		Sr		Ag	
Layer	D (m^2/s)	Q (J/mole)	D (m^2/s)	Q (J/mole)	D (m^2/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

```
cor_diffm6 6
    1 'Xe'  'FLUX'   0.0
    2 'Cs'  'FLUX'   0.0
    3 'Ba'  'FLUX'   0.0
    4 'I'  'FLUX'   0.0
    5 'Ag'  'FLUX'   0.0
    6 'FLUX'         0.0

cor_diffm7 6
    1 'Xe'  'MOLE'   0.0
    2 'Cs'  'MOLE'   0.0
    3 'Ba'  'MOLE'   0.0
    4 'I'  'MOLE'   0.0
    5 'Ag'  'MOLE'   0.0
    6 'H'   2.7e4 1250.0
```

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)
  - Use symmetry conditions at “LHS” inner boundary, use zero concentration conditions at “RHS” outer boundary (all species)

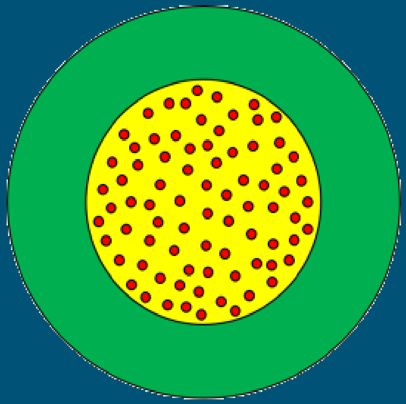
```
! Matrix
cor_diffm1 'Matrix' 3 BOTH SPH SS
cor_diffm2 1 2 10
cor_diffm3 2
          1 'GRAPHITE'  5  2.5e-2 1.0  ! 0.025 m fueled pit of pebble
          2 'GRAPHITE' 10 0.5e-2 0.0  ! 0.03 m pebble outer radius
cor_diffm4 2
          1 12.0 10.0 1250.0
          2 12.0 10.0 1250.0
```

```
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
```

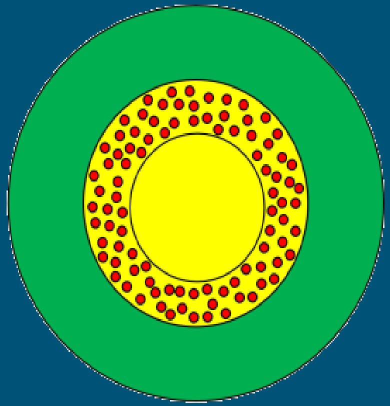
```
cor_diffm6 6
    1 'Xe'  'FLUX'  0.0
    2 'Cs'  'FLUX'  0.0
    3 'Ba'  'FLUX'  0.0
    4 'I'   'FLUX'  0.0
    5 'Ag'  'FLUX'  0.0
    6       'FLUX'  0.0

cor_diffm7 6
    1 'Xe' 'MOLE'   0.0
    2 'Cs' 'MOLE'   0.0
    3 'Ba' 'MOLE'   0.0
    4 'I'  'MOLE'   0.0
    5 'Ag' 'MOLE'   0.0
    6 'H'  2.7e4  1250.0
```

…Exercise 2 – Run Sequence…

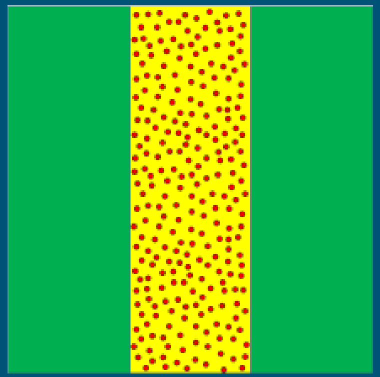
Conventional Pebble Fuel Element



Annular Pebble Fuel Element



Prismatic Fuel Element



TRISO	Fuel (FU)
GRAPHITE	Fuel Extra Material (FUXM)
GRAPHITE	Matrix (MX)

Exercise 2

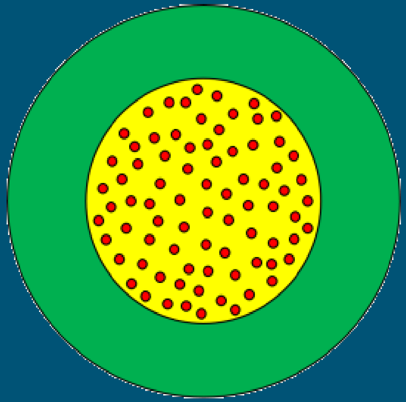
Assume thermal steady state established and illustrate the run sequence of diffusional fission product release

- SS DIF at DTIMEONS within a time-step
- SS XPRT between DTIMEONS and DTIMEONT to establish steady CVH/HS/RN1 conditions (frozen COR release)
- Scaling of SS XPRT steady CVH/HS contents/depositions
- TRANS DIF after DTIMEONT

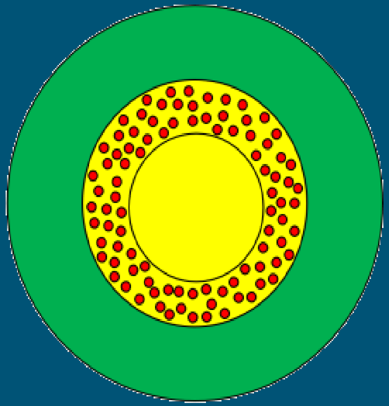
…Demonstration…

…Exercise 3 – Vectorized CFs for Diffusional Fission Product Release…

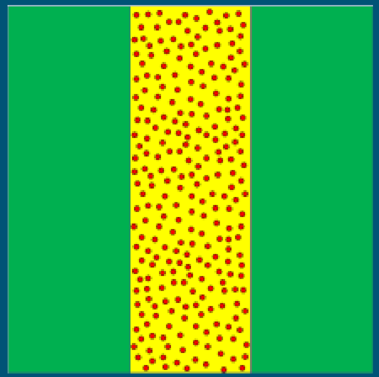
Conventional Pebble Fuel Element



Annular Pebble Fuel Element



Prismatic Fuel Element



TRISO	Fuel (FU)
GRAPHITE	Fuel Extra Material (FUXM)
GRAPHITE	Matrix (MX)

Exercise 3

…Demonstration…

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