KENO-VI modeling of double heterogeneous reactor systems using TRISO fuel

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ORNL is managed by UT-Battelle, LLC for the US Department of Energy

2nd SCALE Users’ Group Workshop
August 27–29, 2018, ORNL
Outline

• Introduction
  - What are double heterogeneous systems?
  - What are the challenges for modeling these systems?

• Modeling double-het systems with SCALE/KENO-VI

• SCALE hands-on: Part 1 (together)

• SCALE hands-on: Part 2 (alone)

• Other SCALE capabilities for double-het systems

• Outlook to SCALE 6.3
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Double heterogeneous systems

Tristructural (TRISO) fuel particle

- Outer pyrolytic carbon layer (OPyC, 30-60 μm)
- Silicon carbide (SiC) layer (30-50 μm)
- Inner pyrolytic carbon layer (IPyC, 30-60 μm)
- Graphite buffer layer (80-150 μm)
- Fuel kernel (200-800 μm diameter)
  UCO – UO₂, UC, UC₂

(1) Fuel pebble

Uranium Oxycarbide (UCO) Kernel
- 10% enrichment

TRISO Particle
- UCO kernel encased in carbon and ceramic layers
- 0.4 mm in diameter

Fuel Pebble
- TRISO particles embedded in graphite
- 25,000 TRISO particles per pebble

Pebble Bed
- 170,000 pebbles per Xe-100 reactor

Double heterogeneous systems

(2) Prismatic fuel block with fuel compacts

(3) Plate fuel

Figure: Courtesy of H. Gougar, NEAMS presentation, January 24, 2016.

Double heterogeneous systems

- Renewed interest in advanced reactor systems:
  - High temperature gas-cooled reactors (HTGRs); pebbles, prismatic blocks
  - Fluoride salt-cooled high-temperature reactors (FHRs); pebbles, plates, etc.
  - Other designs

- Characteristics:
  TRISO fuel, graphite moderator, helium or molten salt cooled

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Modeling challenges of double-het systems

- TRISO particles are randomly dispersed in a graphite matrix

- Criticality calculations:
  - Using continuous-energy (CE) cross section data
    → We can model everything explicitly
  - Using multigroup (MG) cross section data
    → Problem-independent MG cross sections must be shielded
Modeling challenges of double-het systems

- Continuous-energy calculations:
  
  a) Simplify TRISO particles distributed in array
     
     • Relatively easy to model
     • Allows for neutron streaming paths
     • Particle clipping recommended to be avoided (adds another unrealistic element and fuel mass might be incorrect)
     • Particles closer together to keep overall packing fraction correct $\Rightarrow$ larger local packing fraction
     • Some codes: on-the-fly random placement of the TRISO particle within its lattice cell
Modeling challenges of double-het systems

• Continuous-energy calculations:
  
b) Define every single randomly picked position of TRISO particles in fuel region
  • A larger modeling effort is required
  • Code might have issues determining initial neutron distribution → some effort has to be spent on defining source
  • An extremely long computation time is required, depending on the number of particles
  • This model is closer to reality, but it still has simplification (cf. particle packing fraction is different in outer zone of fuel pebble)
Multigroup calculations:

- Generic MG cross sections must be corrected for self-shielding effects in a given application:
  1. TRISO particle in graphite matrix, embedded in fuel pebble/rod/plate
  2. Fuel component in lattice
- MG calculations allow for simple modeling and fast computation time
- However, approximation is used, so it always must be validated
Modeling challenges of double-het systems

• Self-shielding:

Undiluted absorber (pure absorber)

\[ \sigma(E) \]

\[ \Phi(E) \]

Average Group Cross-section = \( \sigma_g = 3 \text{ b} \)

Impact of resonance absorption on neutron spectrum

\[ \frac{(E-E_0)}{(\Gamma_t/2)} \]
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• **Modeling double-het systems with SCALE/ KENO-VI**

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Modeling double-het systems with SCALE

- Criticality calculations with the 3D Monte Carlo code KENO-VI using either CE or MG data
- KENO-VI is used via the CSAS6 sequence that automates the cross section processing
CSAS6 criticality safety sequence

CE mode

SCALE driver and CSAS6

Input

KENO-VI

END

MG mode

SCALE driver and CSAS6

Input

XSProc

KENO-VI

END

Cross section preparation, including self-shielding calculation

Monte Carlo criticality calculation
CSAS6 criticality safety sequence

• General structure of CSAS6 input:
  - title
  - cross section library
  - composition
  - cell data for MG self-shielding (only for MG mode)
  - parameters for Monte Carlo calculation
  - geometry description
  - array if applicable (e.g., in CE)
  - boundary condition (always a good idea)
  - end statements

```plaintext
=csas6
  title
  library
  read composition
  ... end composition
  read celldata
  ... end celldata
  read parameter
  ... end parameter
  read geometry
  ... end geometry
  read array
  ... end array
  read bounds
  ... end bounds
end data
end
```
SCALE cross section libraries

• Continuous-energy:
  - ENDF/B-VII.0 (ce_v7.0_endf)
  - ENDF/B-VII.1 (ce_v7.1_endf)

• Multigroup:
  - ENDF/B-VII.0: 238-group (v7-238)
  - ENDF/B-VII.1: 56g, 252g (v7.1-56, v7.1-252)

Use of ENDF/B-VII.1 data is strongly recommended!

The difference in neutron capture in carbon between the two ENDF libraries can lead to significant eigenvalue differences (>1,000 pcm) in graphite-moderated systems.
CSAS6 criticality safety sequence: composition

- There are different ways to define composition via standard composition, atom percent compositions, solutions, etc. Fulcrum’s autocompletion can be used for assistance.

- Here is one example: entering nuclide-wise number densities (atoms/barn-cm):

<table>
<thead>
<tr>
<th>Nuclide</th>
<th>#mix</th>
<th>0</th>
<th>nuclide_density</th>
<th>temperature</th>
<th>end</th>
</tr>
</thead>
<tbody>
<tr>
<td>h</td>
<td>1</td>
<td>0</td>
<td>0.0667531</td>
<td>300.0</td>
<td>end</td>
</tr>
<tr>
<td>pu-238</td>
<td>2</td>
<td>0</td>
<td>4.747e-07</td>
<td>293.0</td>
<td>end</td>
</tr>
<tr>
<td>pu-239</td>
<td>2</td>
<td>0</td>
<td>1.068e-04</td>
<td>293.0</td>
<td>end</td>
</tr>
<tr>
<td>pu-240</td>
<td>2</td>
<td>0</td>
<td>1.577e-05</td>
<td>293.0</td>
<td>end</td>
</tr>
<tr>
<td>pu-241</td>
<td>2</td>
<td>0</td>
<td>5.626e-06</td>
<td>293.0</td>
<td>end</td>
</tr>
<tr>
<td>pu-242</td>
<td>2</td>
<td>0</td>
<td>6.187e-07</td>
<td>293.0</td>
<td>end</td>
</tr>
<tr>
<td>rh-103</td>
<td>2</td>
<td>0</td>
<td>1.104e-05</td>
<td>293.0</td>
<td>end</td>
</tr>
</tbody>
</table>
CSAS6 criticality safety sequence: parameter

• KENO-VI parameters:
  - numbers of particles per generation (npg)
  - number of total generations (gen)
  - number of inactive generations (nsk)
  - optional: desired eigenvalue uncertainty, random number, doppler broadening rejection correction (DBRC), energy group structure for output when using CE mode, etc.

• Ensure fission source convergence: check convergence tests of Shannon entropy in output file

• Remember statistical uncertainty ~ 1/√N
KENO-VI geometry

- Volumes are built in sections called **units**. Each unit is independent of all other units and has its own coordinate system.

- Units are built using **regions**. Regions are made using the KENO-VI geometry shapes. The unit boundary must fully enclose all defined regions in the unit.

- Regions may share boundaries, may intersect, and may be rotated.
KENO-VI geometry (continued)

- A **hole** is used to place a unit within a region of a different unit. The hole must be completely contained within the region and may not intersect other holes or nested arrays.

- An **array** is an ordered stack of units. The touching faces of adjacent units in an array must be the same size.

- A **global unit** that encloses the entire system must be specified. All geometry data used in a problem are correlated by the global unit coordinate system.
KENO-VI array types

Hexagonal (or triangular)

Standard hex

Rotated hex

Rectangular

Dodecahedral
KENO-VI input records

• Three types of records are used to define the volume, position, and material contents of the regions in a unit:
  1. Geometry records
  2. Contents records
  3. Boundary records

```
unit 100
sphere 1 0.0250
sphere 2 0.0340
sphere 3 0.0380
sphere 4 0.0415
sphere 5 0.0455
cuboid 6 6p0.097634150
media 100 1 1
media 101 1 2 -1
media 102 1 3 -2
media 103 1 4 -3
media 104 1 5 -4
media 105 1 6 -5
boundary 6
```
KENO-VI input records

• Three types of records are used to define the volume, position, and material contents of the regions in a unit

1. Geometry records

2. Contents records

3. Boundary records

- Geometry keyword
- Geometry record label
- Geometry boundary definitions
- Geometry modification data

```
unit 100
sphere 1 0.0250
sphere 2 0.0340
sphere 3 0.0380
sphere 4 0.0415
sphere 5 0.0455
cuboid 6 6p0.097634150
media 100 1 1
media 101 1 2 -1
media 102 1 3 -2
media 103 1 4 -3
media 104 1 5 -4
media 105 1 6 -5
boundary 6
```
KENO-VI input records

• Three types of records are used to define the volume, position, and material contents of the regions in a unit

  1. Geometry records
  2. Contents records
  3. Boundary records

• Contents keyword (array, hole, media)
• ID number (array #, unit #, mixture #)
• Bias ID number (media only)
• Region definition vector (array, media)

unit 100
sphere 1 0.0250
sphere 2 0.0340
sphere 3 0.0380
sphere 4 0.0415
sphere 5 0.0455
cuboid 6 6p0.097634150
media 100 1 1
media 101 1 2 -1
media 102 1 3 -2
media 103 1 4 -3
media 104 1 5 -4
media 105 1 6 -5
boundary 6
KENO-VI input records

• Three types of records are used to define the volume, position, and material contents of the regions in a unit

1. Geometry records
2. Contents records
3. Boundary records

Specify the overall volume of a unit:
• **One and only one boundary record** is required for each unit
• Only the volume defined in the region definition vector of the unit’s boundary record is contained within the unit
• Volumes outside the boundary record’s region definition vector are not included in the unit

---

unit 100
sphere 1 0.0250
sphere 2 0.0340
sphere 3 0.0380
sphere 4 0.0415
sphere 5 0.0455
cuboid 6 6p0.097634150
media 100 1 1
media 101 1 2 -1
media 102 1 3 -2
media 103 1 4 -3
media 104 1 5 -4
media 105 1 6 -5
boundary 6
SCALE/KENO-VI double-het CE model
SCALE/KENO-VI double-het CE model

- Continuous-energy modeling:
  - Infinite particle array
  - Particle array with particles removed to avoid clipping
  - Explicit placement of randomly dispersed particles (not covered here)
  - Random distribution within mesh cells to improve runtime (not covered here)
1. **TRISO particle** in its cuboid lattice cell
   - cuboid side length is lattice pitch of particle array

2. Lattice cell filled with graphite only

   unit 100
   sphere 1 0.0250
   sphere 2 0.0340
   sphere 3 0.0380
   sphere 4 0.0415
   sphere 5 0.0455
   cuboid 6 6p0.097634150
   media 100 1 1
   media 101 1 2 -1
   media 102 1 3 -2
   media 103 1 4 -3
   media 104 1 5 -4
   media 105 1 6 -5
   boundary 6
SCALE/KENO-VI double-het CE model: particle array

- **Infinite TRISO particle array definition:**
  ```plaintext
  read array
  ara=1 nux=27 nuy=27 nuz=27 typ=cuboidal
  fill
  100 100 100 100 100 [...] 100 100 100
  end fill
  end array
  ```

- Better fill using fido input “f”:
  ```plaintext
  read array
  ara=1 nux=27 nuy=27 nuz=27 typ=cuboidal
  fill f100 end fill
  end array
  ```

In this way, the particles are clipped by the outer cylinder/pebble/plate in which this array is placed.
SCALE/KENO-VI double-het CE model: particle array

• TRISO particle array without particle clipping:

read array
  ara=1 nux=27 nuy=27 nuz=27 typ=cuboidal
fill
  200 200 200 200 200 [...] 200 200 200
  200 200 200 100 100 [...] 200 200 200
  200 200 100 100 100 [...] 100 200 200
  200 100 100 100 100 [...] 100 100 200
  [...] 200 200 200 100 100 [...] 200 200 200
  200 200 200 200 200 [...] 200 200 200
end fill
end array

Place pure graphite cells in outer area of array

• Better repeat unit numbers

read array
  ara=1 nux=27 nuy=27 nuz=27 typ=cuboidal
fill
  27r200
  3r200 21r100 3r200
  2r200 23r100 2r200
  200 25r100 200
  [...] 3r200 21r100 3r200
  27r200 end fill
end array
SCALE/KENO-VI double-het CE model: particle array

- **Fuel component:**
  - Place fuel particle array into volume
  - Add the other materials
  - Place fuel component into array, declare as global unit, etc.

- **Fuel pebble:**

  ```
  global unit 1
  sphere 1 2.5
  sphere 2 3.0
  cuboid 3 6p3.0
  array 1 1 place 14 14 14 0 0 0
  media 106 1 2 -1
  media 300 1 3 -2
  boundary 3
  ```
SCALE/KEO-VI double-het *multigroup* model
SCALE/KENO-VI double-het multigroup model

• Addition of cell data block:
  - Double heterogeneous self-shielding cell
  - Basically two self-shielding calculations
  - Simple user input in cell block for self-shielding
  - Creates one mixture to be placed in geometry model

Double-het computational procedure for a pebble fuel component with SCALE

MG HTR fuel pebble model

TRISO particles

CENTRM
TRISO particle calculation

CENTRM/PMC pebble calculation

homogenized fuel

disadvantage factors

cell-weighted CE library

shieldsed MG library

Double-het mix

Double-het mix
Unit cell geometries for MG double-het fuel components

- **Particle**
  - Unit cell for (annular) cylindrical rods in a square pitch or spherical pellets in a cubic lattice

- **Unit cell for (annular) cylindrical rods in a triangular pitch or spherical pellets in a bi-centered or face-centered hexagonal close-packed lattice**
Unit cell geometries for MG double-het fuel components

Symmetric array of slabs

Periodic but asymmetric array of slabs

Note: Plate-fuel double-het cells are not yet extensively tested
Cell data for MG double-het fuel component

- **gfr/gfd**: fuel grain radius/diameter
- **coatt/coatr/coatd**: coating thickness, radius, diameter
- **numpar**: number of particles
- **vf**: packing fraction

**Don’t fall into the d/r/t-trap:**

- **d**: diameter
- **r**: radius
- **t**: thickness

Often both **d** and **r** are possible, and for coating, additionally **t**

doublehet
right_bdy=white
fuelmix=10 end
gfr=0.1 1
coatt=0.2 2
coatt=0.3 3
coatt=0.4 4
coatt=0.5 5
matrix=6
numpar=15000
vf=0.1
end grain

rod
triangpitch
right_bdy=white
left_bdy=reflected
hpitch=5.0 7
fuelr=1.0
cladr=2.0 8
fuelh=3.0
end
Cell data for MG double-het fuel component

- **pitch**: (half) pitch of fuel component infinite lattice
- **fuelr**: fuel component radius/diameter
- **cladr**: cladding radius/diameter
- **fuelh**: fuel component height
- Others: gaps, central hole

```
doublehet
right_bdy=white
fuelmix=10 end

gfr=0.1 1
coatt=0.2 2
coatt=0.3 3
coatt=0.4 4
coatt=0.5 5
matrix=6
numpar=15000
vf=0.1
doublehet
right_bdy=white
fuelmix=10 end

rod
triangpitch
right_bdy=white
left_bdy=reflected
hpitch=5.0 7
fuelr=1.0
cladr=2.0 8
fuelh=3.0
end
```

particle (grain)

rod/plate/pebble
SCALE/KENO-VI double-het multigroup model

• **Steps**
  1. Create double-het cell block
  2. Place fuel mix into volume that includes the particles

• **Fuel pebble**
  
  ```
  global unit 1
  sphere 1 2.5
  sphere 2 3.0
  cuboid 3 6p3.0
  media 10 1 1
  media 106 1 2 -1
  media 300 1 3 -2
  boundary 3
  ```
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• Outlook to SCALE 6.3
High-temperature gas-cooled reactor (HTGR) prismatic pin cell in infinite lattice

1. Multigroup model using the double-het cell
2. Continuous-energy model using an infinite array of particles

Use provided SCALE composition block
→ htgr-prismatic-pin-cell-composition.txt

Use Fulcrum’s auto-completion!

## Dimensions for MHTGR pin cell

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Dimension (cm)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>TRISO fuel particle</strong></td>
<td></td>
</tr>
<tr>
<td>UC$<em>{0.5}$O$</em>{1.5}$ kernel radius</td>
<td>2.125E-02</td>
</tr>
<tr>
<td>Porous carbon buffer layer outer radius</td>
<td>3.125E-02</td>
</tr>
<tr>
<td>Inner PyC outer radius</td>
<td>3.525E-02</td>
</tr>
<tr>
<td>SiC outer radius</td>
<td>3.875E-02</td>
</tr>
<tr>
<td>Outer PyC outer radius</td>
<td>4.275E-02</td>
</tr>
<tr>
<td><strong>Average TRISO packing fraction</strong></td>
<td>0.35</td>
</tr>
<tr>
<td><strong>Fuel compact outer radius</strong></td>
<td>0.6225</td>
</tr>
<tr>
<td><strong>Fuel/helium gap outer radius</strong></td>
<td>0.6350</td>
</tr>
<tr>
<td><strong>Large helium coolant channel radius</strong></td>
<td>0.7940</td>
</tr>
<tr>
<td><strong>Unit cell pitch</strong></td>
<td>1.8796</td>
</tr>
<tr>
<td><strong>Fuel compact height</strong></td>
<td>4.9280</td>
</tr>
</tbody>
</table>
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1. MG model using the double-het cell
2. CE model using an infinite array of particles

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>UO₂ fuel density (g/cm³)</td>
<td>10.4</td>
</tr>
<tr>
<td>Uranium enrichment</td>
<td>17 wt.%</td>
</tr>
<tr>
<td>Fuel kernel radius (cm)</td>
<td>0.025</td>
</tr>
<tr>
<td>Fuel particle coating layer materials (starting from kernel)</td>
<td>Buffer/PyC/SiC/PyC</td>
</tr>
<tr>
<td>Fuel particle coating layer thicknesses (cm)</td>
<td>0.009/0.004/0.0035/0.004</td>
</tr>
<tr>
<td>Fuel particle coating layer densities (g/cm³)</td>
<td>1.1/1.9/3.18/1.9</td>
</tr>
<tr>
<td>Number of particles in pebble</td>
<td>8,385</td>
</tr>
<tr>
<td>Diameter of fuel pebble (cm)</td>
<td>3.0</td>
</tr>
<tr>
<td>Diameter of fuel zone in pebble (cm)</td>
<td>2.5</td>
</tr>
<tr>
<td>Graphite matrix and fuel pebble outer shell density (g/cm³)</td>
<td>1.73</td>
</tr>
</tbody>
</table>

Use provided SCALE composition block
→ htgr-fuel-pebble-composition.txt
3. Modification of CE model of prismatic pin to avoid particle clipping
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What else can we do with double-het systems in SCALE?

- 2D deterministic code calculations using NEWT
- Depletion calculations using Triton in combination with NEWT and KENO-VI (both MG and CE)
- Uncertainty and sensitivity analysis:
  - Perturbation theory: CETUNAMI (using KENO-VI CE as transport code)
  - Random sampling: Sampler (using either NEWT or KENO-VI MG)
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Outlook to SCALE 6.3

- New data libraries:
  - 1597-group cross section library
  - ENDF/B-VIII.0 data, offering graphite as perfect crystal, with 10% and 30% porosity (→ cf. presentation about SCALE double-het capabilities)
Outlook to SCALE 6.3

- New Monte Carlo code Shift
  - MG and CE calculations
  - Use of KENO-VI input via CsasShift sequence (csas6-shift)
  - Other supported input formats: own format and MCNP input
  - **New block to simplify random placement of particles in CE mode:**

```
unit 1
com='TRISO particle'
sphere 1 2.50e-02
sphere 2 3.40e-02
sphere 3 3.80e-02
sphere 4 4.15e-02
sphere 5 4.55e-02
media 100 1 1
media 101 1 2 -1
media 102 1 3 -2
media 103 1 4 -3
media 104 1 5 -4
boundary 5
```

```
global unit 10
com='fuel pebble'
sphere 1 2.5
sphere 2 3.0
cuboid 3 6p5.0
media 105 1 1
randommix='trisos'
media 106 1 2 -1
media 300 1 3 -2
boundary 3
```

read randomgeom
randommix = 'trisos'
type=random
units=1 end
pfs=0.05054954 end
clip=no
seed=1111
end randommix
end randomgeom