Assessment of SCALE Capabilities for High-Temperature Reactor Modeling and Simulation

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Introduction

• In the United States, interest is growing in advancing modeling and simulation capabilities for advanced reactor systems.

• The SCALE 6.2.3 code package offers a number of neutron transport sequences for criticality and depletion analysis.

• SCALE is part of the US Nuclear Regulatory Commission (NRC) licensing path that will soon be confronted with advanced reactor systems.

• Calculations of various double heterogeneous systems are performed to assess SCALE’s capabilities to model and simulate these systems.
Methods

• Method: Monte Carlo (MC)
  - KENO-VI of SCALE 6.2.3 (continuous energy [CE] and multigroup [MG])
  - Shift development version of SCALE 6.3 via CsasShift (CE and MG)
  - MCNP 6.2v2.0 (CE)
  - Serpent 2.1.30 (CE)

• Cross section libraries:
  - Mainly ENDF/B-VII.1
  - Some calculations with ENDF/B-VII.0 and VIII.0
Models

• HTR-10 (High Temperature Gas-cooled Reactor) pebble in infinite square lattice
  - $\text{UO}_2$ fuel density: 10.4 g/cm$^3$
  - Uranium enrichment: 17 wt%
  - Number of particles in pebble: 8,385
  - Pebble radius: 3 cm (fuel zone: 2.5 cm)

• HTR-10 initial criticality
  - 9,627 fuel pebbles
  - 7,263 dummy pebbles
  - 61% packing fraction
  - Room temperature, ambient air

HTR fuel pebble models for CE calculations

- All MC codes: particle array with particles removed to avoid clipping
- Shift, MCNP, Serpent: explicit placement of randomly dispersed particles
- KENO-VI: random distribution within mesh cells to improve runtime

Lattice without clipping
Truly random
Random-mesh
New randomgeom block in CsasShift

- **New MC code Shift**
  - MG and CE calculations
  - Use of KENO-VI input via CsasShift sequence
  - Other supported input formats: own format and MCNP input

**New block to simplify random placement of particles in CE mode:**

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

```plaintext
global unit 10
com='fuel pebble'
sphere 1 2.5
sphere 2 3.0
cuboid 3 6p5.0
media 105 1 1
media 106 1 2 -1
media 300 1 3 -2
boundary 3
```
Multigroup calculation of double-het systems with SCALE

- 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

- This results in simple modeling and fast computation time

Double-het computational procedure for a pebble fuel component with SCALE
New very fine group library in SCALE 6.3

- Available MG library in SCALE: 252 groups
- New data libraries to be distributed with SCALE 6.3:
  - 1,597-group cross section library
  - ENDF/B-VIII.0 data
HTR-10 pebble: ENDF/B-VII.1 continuous-energy eigenvalue comparison

<table>
<thead>
<tr>
<th>Code</th>
<th>Random</th>
<th>Array</th>
<th>Array vs. random</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>k&lt;sub&gt;o&lt;/sub&gt;, Δk [pcm]</td>
<td>k&lt;sub&gt;o&lt;/sub&gt;, Δk [pcm]</td>
<td>Δk [pcm]</td>
</tr>
<tr>
<td><strong>KENO-VI</strong></td>
<td>1.6770(4) (ref)</td>
<td>1.6745(1) (ref)</td>
<td>−250(35)</td>
</tr>
<tr>
<td><strong>Shift</strong></td>
<td>1.6764(8) −62(78)</td>
<td>1.6738(2) −66(15) −254(71)</td>
<td></td>
</tr>
<tr>
<td><strong>MCNP</strong></td>
<td>1.6765(3) −47(45)</td>
<td>1.6745(3) 1(32) −202(42)</td>
<td></td>
</tr>
<tr>
<td><strong>Serpent</strong></td>
<td>1.6764(1) −54 (34)</td>
<td>1.6750(1) 48(10) −148(4)</td>
<td></td>
</tr>
</tbody>
</table>

Note: The 1σ statistical uncertainties are given in parentheses.

- Good agreement between the four MC codes
- Modeling bias of particle array vs. random distribution of 150–250 pcm
HTR-10 pebble: KENO-VI and Shift eigenvalue comparison

<table>
<thead>
<tr>
<th>Library</th>
<th>Code</th>
<th>XS lib</th>
<th>$k_\infty$</th>
<th>$\Delta k$ [pcm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>ENDF/B-VII.1</td>
<td>KENO</td>
<td>CE</td>
<td>1.6770(4)</td>
<td>(ref)</td>
</tr>
<tr>
<td></td>
<td>KENO</td>
<td>1,597 g</td>
<td>1.6749(1)</td>
<td>-210(35)</td>
</tr>
<tr>
<td></td>
<td>KENO</td>
<td>252 g</td>
<td>1.6742(1)</td>
<td>-277(35)</td>
</tr>
<tr>
<td></td>
<td>Shift</td>
<td>CE</td>
<td>1.6764(8)</td>
<td>(ref)</td>
</tr>
<tr>
<td></td>
<td>Shift</td>
<td>252 g</td>
<td>1.6748(2)</td>
<td>-158(72)</td>
</tr>
<tr>
<td>ENDF/B-VIII.0</td>
<td>KENO</td>
<td>CE</td>
<td>1.6722(4)</td>
<td>(ref)</td>
</tr>
<tr>
<td></td>
<td>KENO</td>
<td>252 g</td>
<td>1.6684(1)</td>
<td>-379(34)</td>
</tr>
</tbody>
</table>

Note: The 1σ statistical uncertainties are given in parentheses.

- Consistent results between KENO and Shift
- Extremely long computation time for CE calculations
- MG bias between 150 and 280 pcm for ENDF/B-VII.1 data
- Larger MG bias when using ENDF/B-VIII.0 data → ??
HTR-10 pebble: KENO-VI and Shift eigenvalue comparison

<table>
<thead>
<tr>
<th>Library</th>
<th>Code</th>
<th>XS lib</th>
<th>$k_\infty$</th>
<th>$\Delta k$ (pcm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>ENDF/B-VII.1</td>
<td>KENO</td>
<td>CE</td>
<td>1.6770(4)</td>
<td>(ref)</td>
</tr>
<tr>
<td>ENDF/B-VIII.0</td>
<td>KENO</td>
<td>CE</td>
<td>1.6722(4)</td>
<td>$-438(57)$</td>
</tr>
</tbody>
</table>

Note: The 1σ statistical uncertainties are given in parentheses.

Replace individual nuclides in ENDF/B-VII.1 calculation by ENDF/B-VIII.0 data:

<table>
<thead>
<tr>
<th>Basis: ENDF 7.1</th>
<th>$\Delta k$ to all ENDF 7.1 (pcm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>But: graphite</td>
<td>$-7$</td>
</tr>
<tr>
<td>But: $^{235}U$</td>
<td>$-702$</td>
</tr>
<tr>
<td>But: $^{238}U$</td>
<td>$239$</td>
</tr>
<tr>
<td>All ENDF 8.0</td>
<td>$-438$</td>
</tr>
</tbody>
</table>

- Differences between ENDF/B-VII.0 and VII.1: carbon capture
- Differences between ENDF/B-VII.1 and VIII.0: $^{235}U$ and $^{238}U$
HTR-10: KENO-VI eigenvalue comparison

<table>
<thead>
<tr>
<th>Library</th>
<th>$k_{\text{eff}}$</th>
<th>$\Delta k$ (pcm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>ENDF/B-VII.0</td>
<td>CE 1.0138(1)</td>
<td>1,108(14)</td>
</tr>
<tr>
<td></td>
<td>CE 1.0027(1)</td>
<td>(ref)</td>
</tr>
<tr>
<td>ENDF/B-VII.1</td>
<td>252 g 1.0029(1)</td>
<td>20(14)</td>
</tr>
<tr>
<td></td>
<td>1,597 g 1.0029(1)</td>
<td>27(14)</td>
</tr>
<tr>
<td>ENDF/B-VIII.0</td>
<td>CE 1.0058(1)</td>
<td>315(13)</td>
</tr>
<tr>
<td></td>
<td>252 g 1.0045(1)</td>
<td>180(14)</td>
</tr>
<tr>
<td>Benchmark value</td>
<td></td>
<td>1.0000(37)</td>
</tr>
</tbody>
</table>

Note: The 1σ statistical uncertainties are given in parentheses.

- Influence of ENDF library: 1,100 and >300 pcm between ENDF/B-VII.0 and VIII.0 vs. VII.1, respectively
- No MG bias for the eigenvalue when using ENDF/B-VII.1 data
- Small bias of 180 pcm when using ENDF/B-VIII.0 data
- Agreement of calculations with experiment when using ENDF/B-VII.1 and VIII.0 data
If we always want our porosity? In each area?

ENDF/B-VIII.0: graphite with different porosities

With ENDF/B-VIII.0, graphite data with different porosities are available: perfect crystal, 10% porosity, and 30% porosity

<table>
<thead>
<tr>
<th>Applied graphite data</th>
<th>k-inf</th>
<th>Δk (pcm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>All c-graphite</td>
<td>1.00582(8)</td>
<td>(ref)</td>
</tr>
<tr>
<td>c-10_graph in reflector (but not in pebbles)</td>
<td>1.00583(48)</td>
<td>1(49)</td>
</tr>
<tr>
<td>c-30_graph in reflector (but not in pebbles)</td>
<td>1.00415(54)</td>
<td>-167(55)</td>
</tr>
<tr>
<td>All c-10_graph</td>
<td>1.00929(27)</td>
<td>347(28)</td>
</tr>
<tr>
<td>All c-30_graph</td>
<td>1.01259(25)</td>
<td>677(26)</td>
</tr>
</tbody>
</table>

Note: The 1σ statistical uncertainties are given in parentheses.

Conclusions

• KENO-VI and Shift show consistent results in CE calculation comparisons with MCNP and Shift

• KENO-VI MG calculations show an eigenvalue bias of <300 pcm compared with CE for a fuel pebble, small or no bias for full core

• Eigenvalue difference between ENDF/B-VII.1 and VIII.0 of a few hundred pcm, mainly due to updates in $^{235}$U and $^{238}$U; these differences should be better understood

• SCALE 6.3: 1,597-group library, ENDF/B-VIII.0 data libraries including new graphite evaluations (perfect crystal and porous graphite)
  - A change in graphite porosity can have a large impact on eigenvalue
  - Do we know the porosity to appropriately model our system?
Outlook

• More extensive testing (e.g., with prismatic HTTR)
• Fuel pebble depletion calculation
• Uncertainty quantification using SAMPLER
• Extension of this assessment to other reactor types (e.g., molten salt-cooled reactors)