OAK RIDGE National Laboratory

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

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Introduction

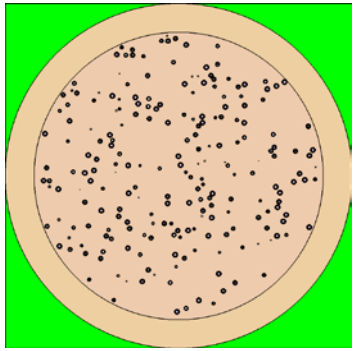
- In the United States, interest is growing in advancing modeling and simulation capabilities for advanced reactor systems
- The SCALE 6.2.3 code package offers a number of neutron transport sequences for criticality and depletion analysis
- SCALE is part of the US Nuclear Regulatory Commission (NRC) 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

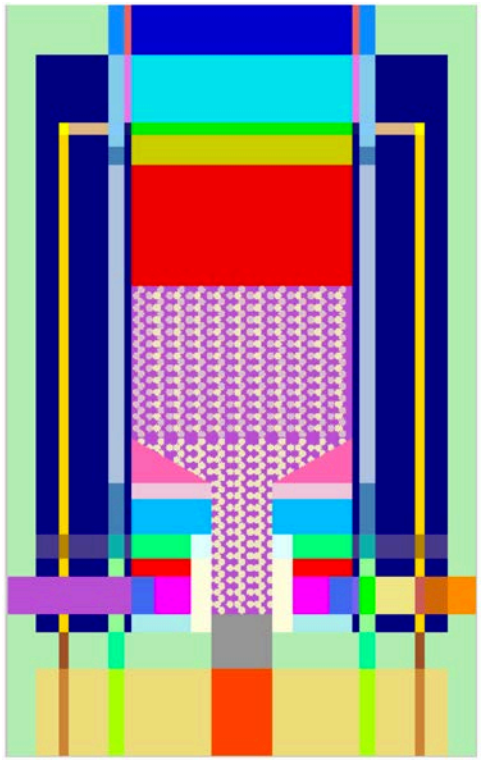
- Method: Monte Carlo (MC)
  - KENO-VI of SCALE 6.2.3 (continuous energy [CE] and multigroup [MG])
  - Shift development version of SCALE 6.3 via CsasShift (CE and MG)
  - MCNP 6.2v2.0 (CE)
  - Serpent 2.1.30 (CE)
- Cross section libraries:
  - Mainly ENDF/B-VII.1
  - Some calculations with ENDF/B-VII.0 and VIII.0

Models

- HTR-10 (High Temperature Gas-cooled Reactor) pebble in infinite square lattice
  - 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-10 fuel pebble

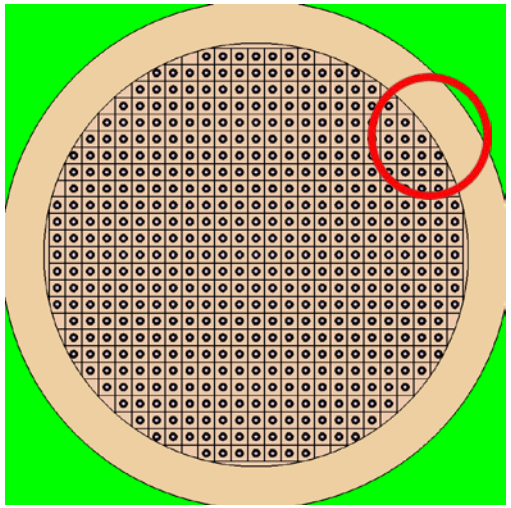


HTR-10

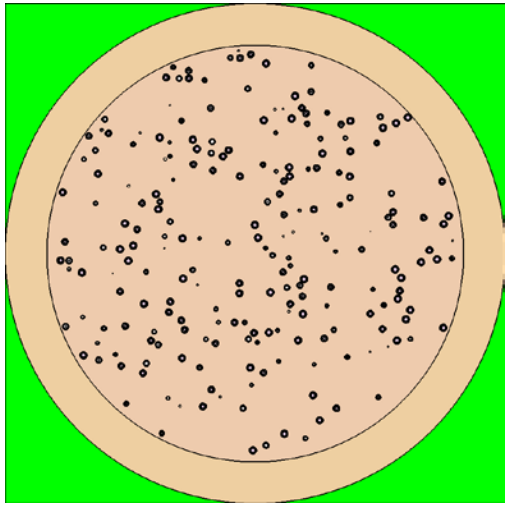
International Handbook of Reactor Physics Experiments, "Evaluation of the Initial Critical Configuration of the HTR-10 Pebble-Bed Reactor," HTR10-GCR-RESR-001, NEA/NSC/DOC(2006)1.

HTR fuel pebble models for CE calculations

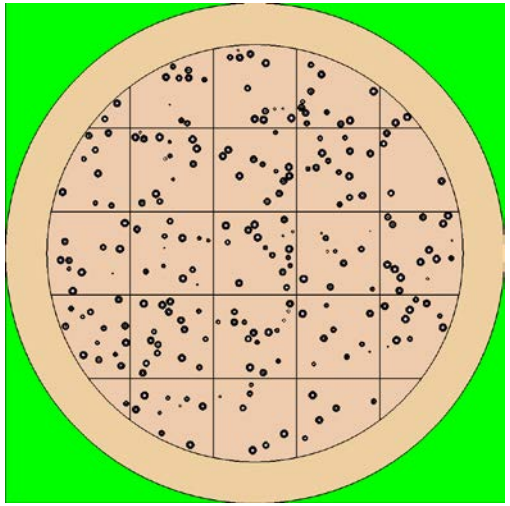
- All MC codes: particle array with particles removed to avoid clipping
- Shift, MCNP, Serpent: explicit placement of randomly dispersed particles
- KENO-VI: random distribution within mesh cells to improve runtime



Lattice without clipping



Truly random

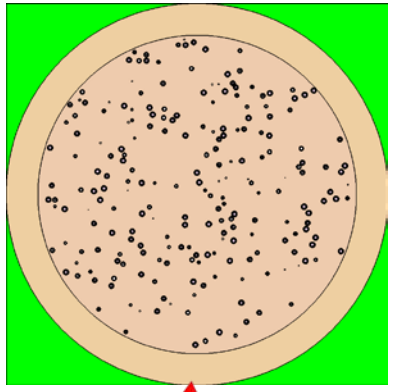


Random-mesh

HTR fuel pebble models for CE calculations

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:**

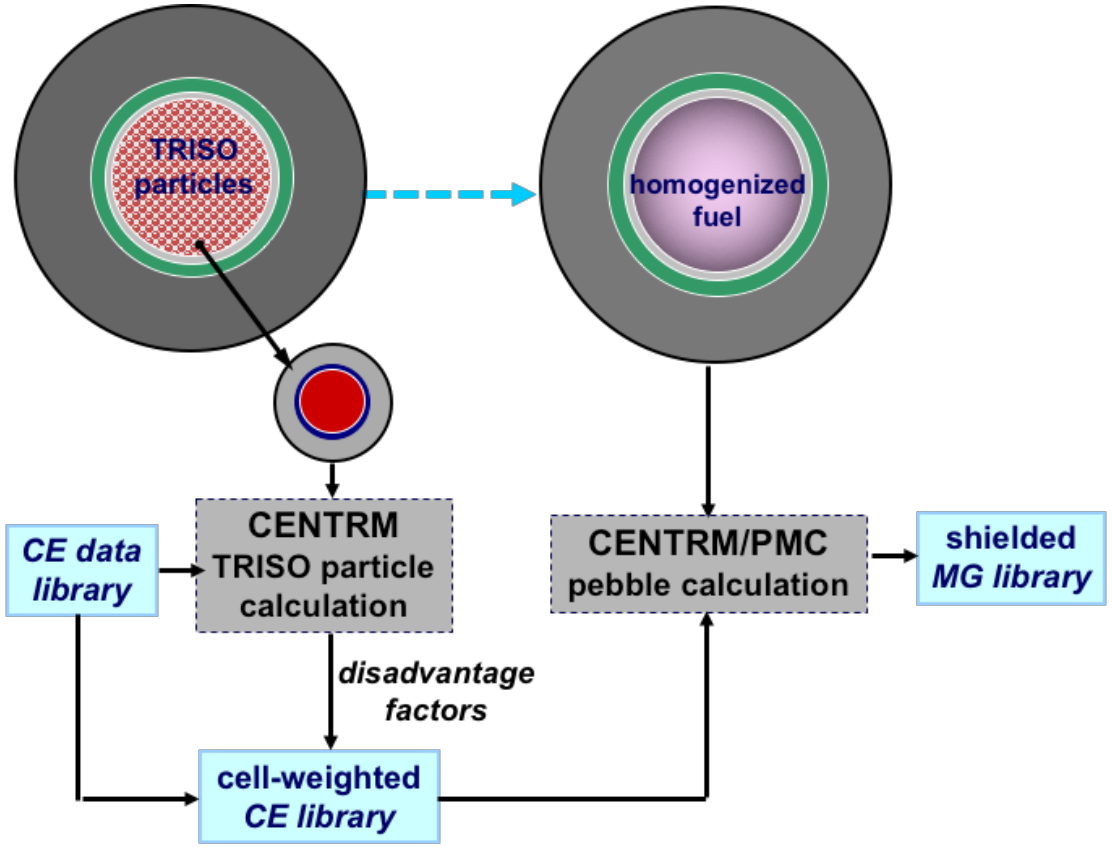


```
TRISO
particle
unit 1
```

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

```
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
```

Multigroup calculation of double-het systems with SCALE

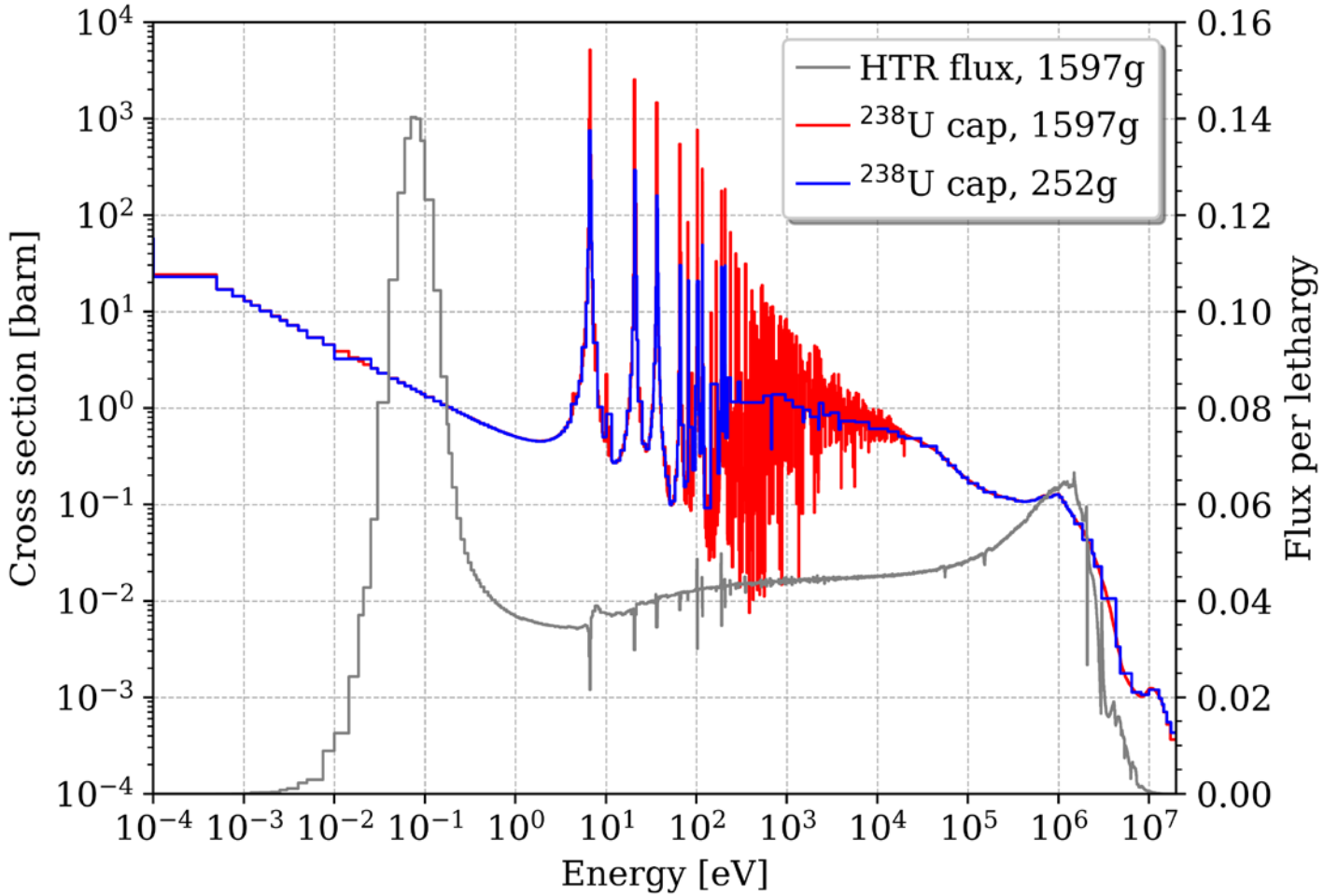


Double-het computational procedure for a pebble fuel component with SCALE

- 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

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



^{238}U capture cross section, HTR neutron flux

HTR-10 pebble: ENDF/B-VII.1 continuous-energy eigenvalue comparison

Code	Random		Array		Array vs. random
	k_∞	Δk [pcm]	k_∞	Δk [pcm]	Δk [pcm]
KENO-VI	1.6770(4)	(ref)	1.6745(1)	(ref)	−250(35)
Shift	1.6764(8)	−62(78)	1.6738(2)	−66(15)	−254(71)
MCNP	1.6765(3)	−47(45)	1.6745(3)	1(32)	−202(42)
Serpent	1.6764(1)	−54 (34)	1.6750(1)	48(10)	−148(4)

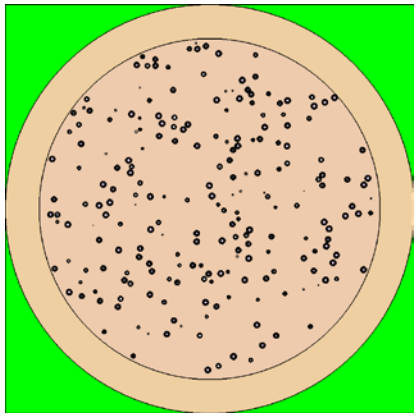
Note: The 1σ statistical uncertainties are given in parentheses.

- 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

Library	Code	XS lib	k_∞	Δk [pcm]
ENDF/B-VII.1	KENO	CE	1.6770(4)	(ref)
	KENO	1,597 g	1.6749(1)	−210(35)
	KENO	252 g	1.6742(1)	−277(35)
	Shift	CE	1.6764(8)	(ref)
	Shift	252 g	1.6748(2)	−158(72)
ENDF/B-VIII.0	KENO	CE	1.6722(4)	(ref)
	KENO	252 g	1.6684(1)	−379(34)

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



HTR-10 fuel pebble

- 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 → ??

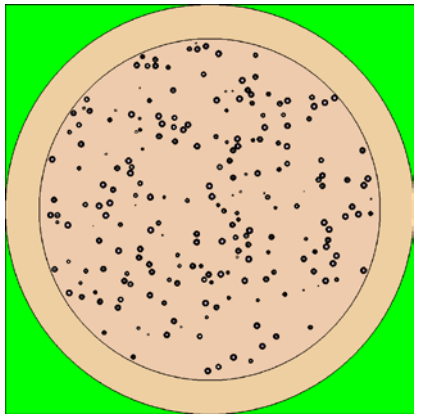
HTR-10 pebble: KENO-VI and Shift eigenvalue comparison

Library	Code	XS lib	k_∞	Δk (pcm)
ENDF/B-VII.1	KENO	CE	1.6770(4)	(ref)
ENDF/B-VIII.0	KENO	CE	1.6722(4)	−438(57)

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

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

Basis: ENDF 7.1	Δk to all ENDF 7.1 (pcm)
But: graphite from ENDF 8.0	−7
But: ^{235}U from ENDF 8.0	−702
But: ^{238}U from ENDF 8.0	239
All ENDF 8.0	−438



HTR-10 fuel pebble

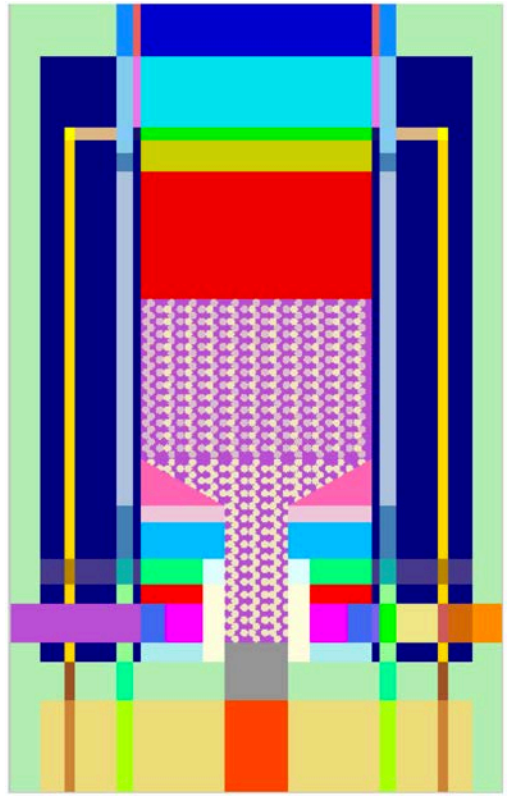
- Differences between ENDF/B-VII.0 and VII.1: carbon capture
- Differences between ENDF/B-VII.1 and VIII.0: ^{235}U and ^{238}U

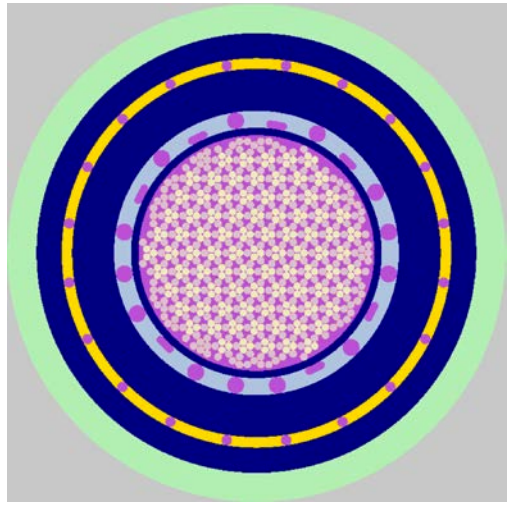
HTR-10: KENO-VI eigenvalue comparison

Library		k_{eff}	Δk (pcm)
ENDF/B-VII.0	CE	1.0138(1)	1,108(14)
ENDF/B-VII.1	CE	1.0027(1)	(ref)
	252 g	1.0029(1)	20(14)
	1,597 g	1.0029(1)	27(14)
ENDF/B-VIII.0	CE	1.0058(1)	315(13)
	252 g	1.0045(1)	180(14)
Benchmark value		1.0000(37)	

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





SCALE HTR-10 model

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

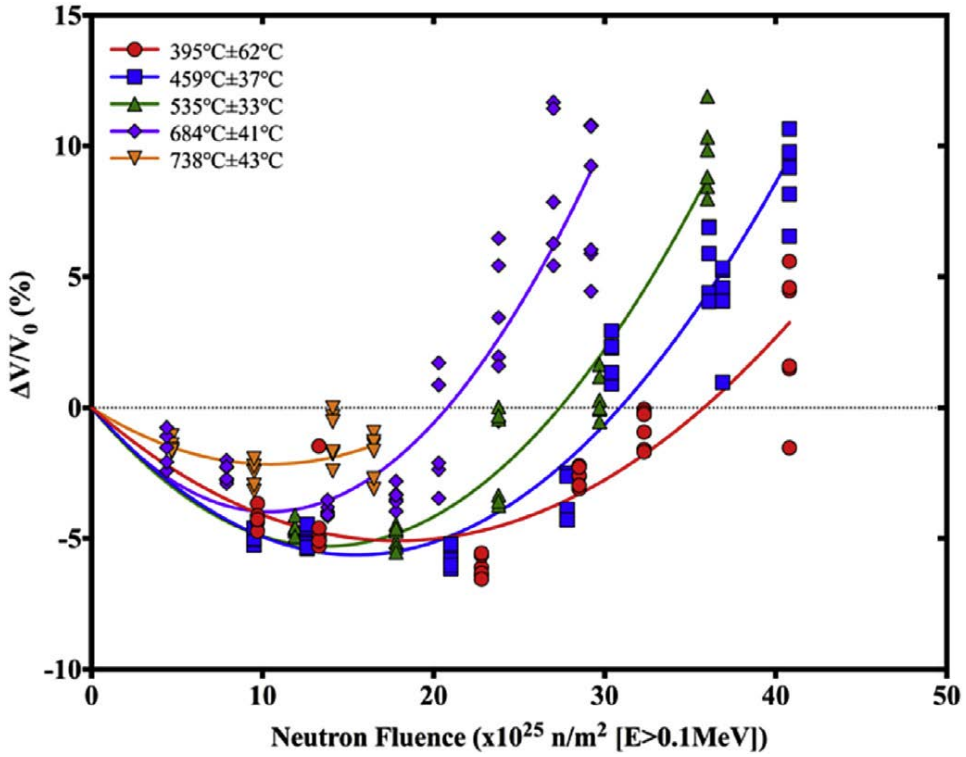
With ENDF/B-VIII.0, graphite data with different porosities are available: perfect crystal, 10% porosity, and 30% porosity

HTR-10: ENDF/B-VIII.0 data, array model

Applied graphite data	k-inf	Δk (pcm)
All c-graphite	1.00582(8)	(ref)
c-10_graph in reflector (but not in pebbles)	1.00583(48)	**1(49)**
c-30_graph in reflector (but not in pebbles)	1.00415(54)	**−167(55)**
All c-10_graph	1.00929(27)	**347(28)**
All c-30_graph	1.01259(25)	**677(26)**

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

Do we always know our porosity? In each area?



Specimen volume change versus neutron fluence for specimens irradiated at different temperatures (courtesy of A. A. Campbell)

Anne A. Campbell, et al., "Property Changes of G347A Graphite Due to Neutron Irradiation," *Carbon* 109, pp. 860–873, 2016.

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)