

FHR/AHTR NEA Benchmark



Bojan Petrovic, Kyle Ramey
Georgia Institute of Technology
Atlanta, Georgia, USA
Bojan.Petrovic@gatech.edu

9th SERPENT User Group Meeting
Georgia Tech, Atlanta, Oct. 14-17, 2019

AHTR (FHR with plank fuel) benchmark

OUTLINE

- Background and motivation/rationale for the benchmark
- FHR/AHTR basic info and reactor physics challenges
- Benchmark high-level scope (Phase I, II & III)
- Specific cases by Phase
- Benchmark geometry specifications
- Timeline
- Required results
- Sample templates for results
- Sample results

Rationale for the NEA benchmark

Rationale:

- Attractive features of molten salt cooled reactors (high temperature and efficiency, low operating pressure)
- Over the last 10+ years, renewed interest in USA, for the liquid-salt cooled designs, including with solid fuel (i.e., liquid salt used as coolant only, not as fuel)
- Denoted as FHR (Fluoride-salt-cooled High-temperature Reactor)
- “Plank” fuel (AHTR, developed by ORNL) and pebble-bed (PB-FHR, UCB/Kairos) designs
- Very challenging modeling (reactor physics, and multi-physics in general)
- Need to verify and validate simulation capabilities
- Several participants/groups confirmed interest to participate in this benchmark

NOTE: More recently, in US, renewed interest also in traditional MSR → separate issues

Modelling challenges (in reactor physics):

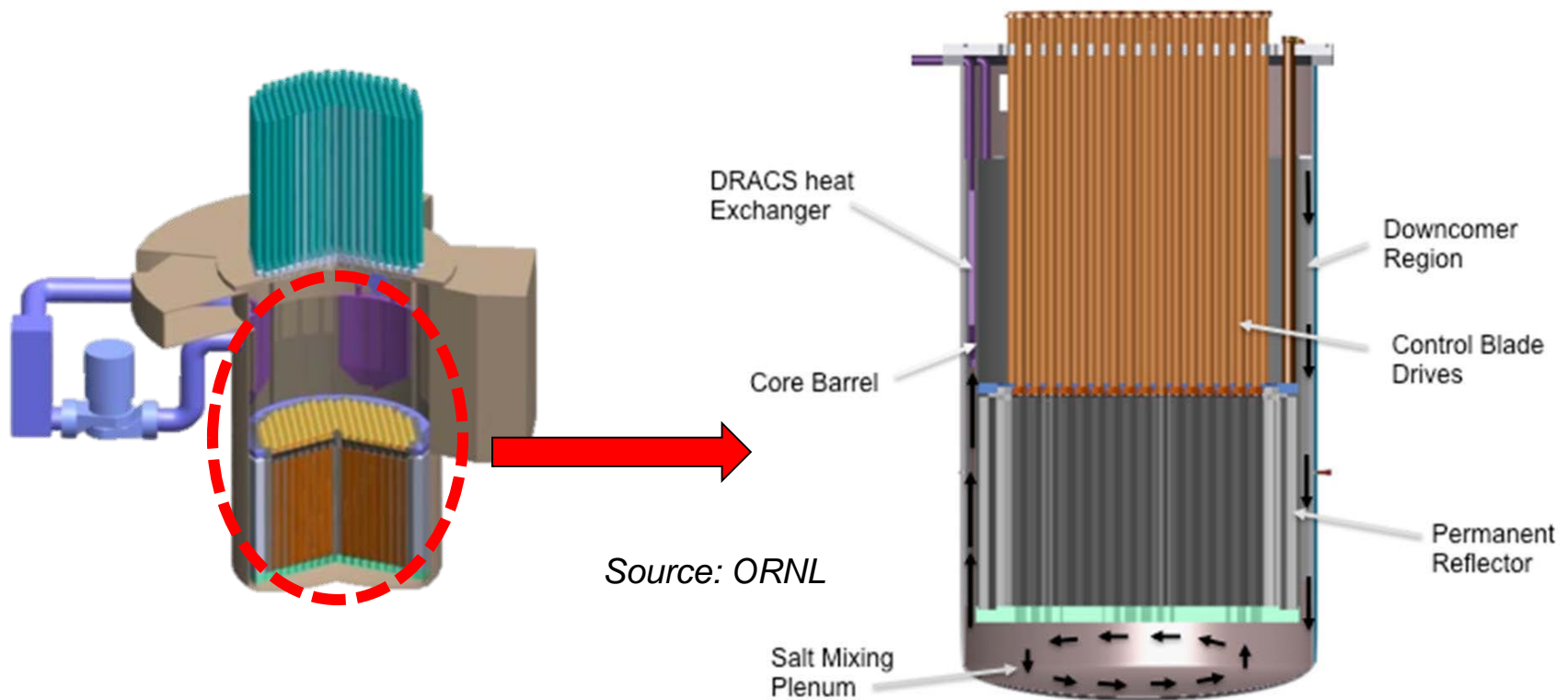
- AHTR plank fuel design has double (triple?) heterogeneity
- Error in reactivity may amount to thousands of pcm's if inadequately modeled

NEA benchmark:

- Multi-phase, start with a fuel element 2D depletion benchmark, develop a sequence to full core 3D with feedback and depletion

FHR design developed at ORNL: Advanced High Temperature Reactor (AHTR)

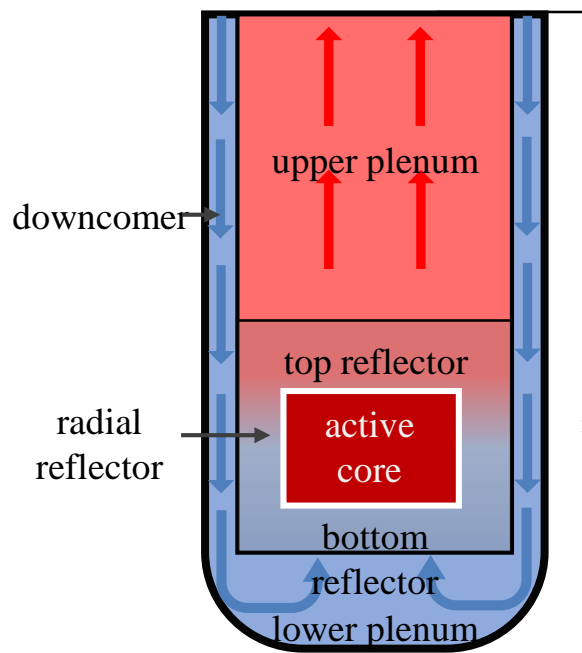
- 3,400 MWth
- Power density $\sim 13 \text{ W/cm}^3$, i.e., higher than in gas-cooled reactors, but lower than in water-cooled reactors (PWR and BWR)
- Large (low pressure) reactor vessel, $\sim 10\text{m}$ O.D.



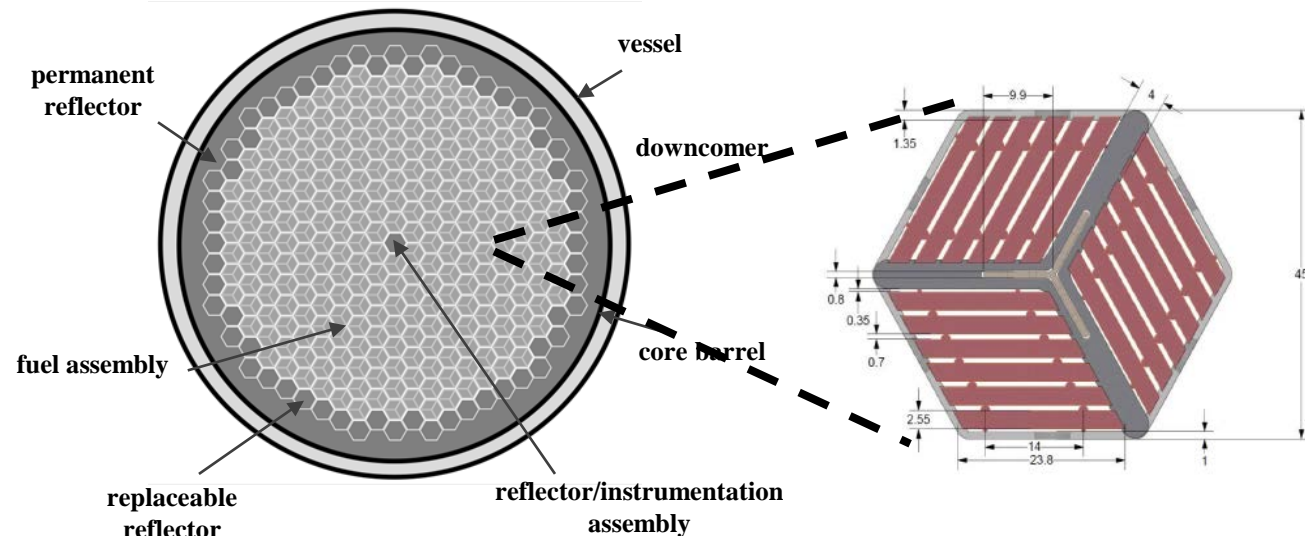
Advanced High Temperature Reactor (AHTR)

Core Design

- 252 hexagonal fuel elements
- 5.5m active core height
- ~8m core radius

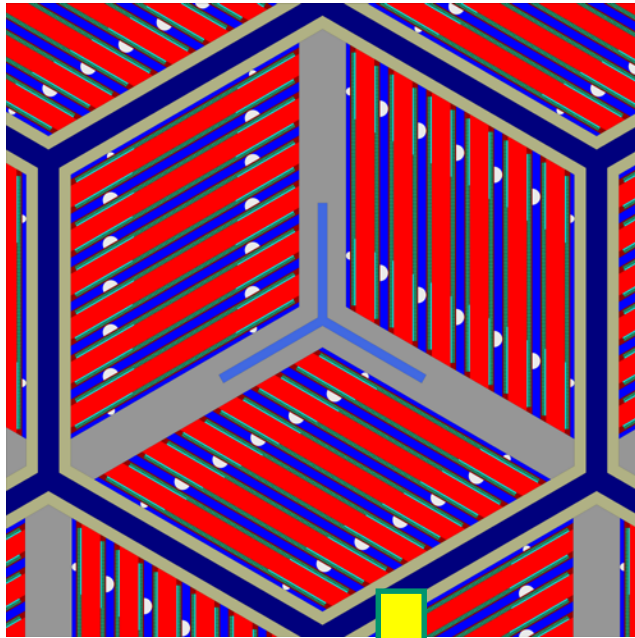


Reactor Vessel



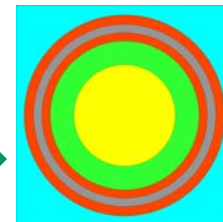
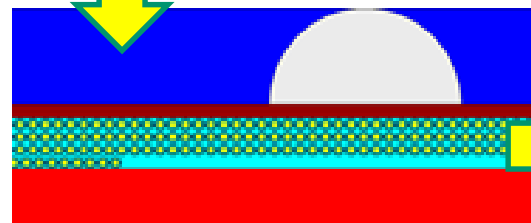
Double (triple?) heterogeneity

Fuel Assembly SERPENT Model



Fuel element

- 3 groups of 6 planks each; 120-deg rotational symmetry
- Fuel plank: two fuel stripes (TRISO particles embedded in matrix), one on each side
- TRISO particles – fuel kernel plus protective layers
- TRISO particles usually assumed in a “lattice”; in reality, randomized
- Central Y-shaped structure and control rod
- Carbonaceous materials (carbon, graphite, mix..?)



Series of incremental benchmarks

AHTR 2D/3D Fuel Assembly, 3D core & Depletion

Phase I – Fuel assembly

- Phase I-A – “2D” (pseudo)-2D, steady state (no depletion)
- Phase I-B – Depletion
- Phase I-C – 3D depletion

Phase II – 3D full core

- Phase II-A – Steady-state (no depletion)
- Phase II-B – Depletion with feedback
- Phase II-C – Multicycle

Overarching objective: Cross-verify codes and methodologies for challenging AHTR geometry, **for accurate and efficient reactor design and analyses**

NOTE: Since FHR uses spherical fuel, it is not “extruded” geometry, there is no true 2D equivalent. In Monte Carlo simulations, modeling a slice with reflective top/bottom is possible. In deterministic codes, a different approach needs to be used.

Complex geometry. 120-deg rotational symmetry. Geometry defined (hopefully unambiguously) in tables and figures

Slide 8

NEA FHR/AHTR Benchmark, Phase I-A

“2D” fuel element, no depletion

CASE 1A: Hot zero power (HZP) with uniform temperature of 923K in all regions, nominal (cold) dimensions, 9 wt% enrichment, no burnable poison (BP), control rods (CR) out.

CASE 2A: **Reference case: Hot full power (HFP)**, with prescribed temperatures for fuel, graphite, and coolant, otherwise same as CASE 1.

Perturbation cases

CASE 3A: CR inserted, otherwise same as CASE 1.

CASE 4A: Discrete europa BP, otherwise same as CASE 1.

CASE 5A: Integral (dispersed) europa BP, otherwise same as CASE 1.

CASE 6A: Increased HM loading (4 to 8 layers of TRISO), hence decreased C/HM (from ~400 to ~200), otherwise same as CASE 1.

CASE 7A: Fuel enrichment 19.75 wt%, otherwise same as CASE 1.

OBJECTIVE: Identify/resolve major/fundamental discrepancies (due to ambiguous specifications, nuclear data, physics,) before proceeding to depletion and 3D

NEA FHR/AHTR Benchmark, Phase I-B

“2D” fuel element, depletion

Downselect 4+3 cases for depletion. Deplete only fuel and burnable poison, i.e., FLiBe isotopics kept fixed except in CASE 2B4. Define what results at what steps.

CASE 2B: Hot full power (HFP), with prescribed temperatures for fuel, graphite, and coolant.

- CASE 2B1 → deplete with critical spectrum
- CASE 2B2 → deplete with “as-is” spectrum
- CASE 2B3 → deplete with reactivity control and near criticality
- CASE 2B4 → with critical spectrum, deplete fuel and FLiBe

CASE 4: Discrete europia BP, otherwise same as CASE 2B1.

CASE 6: Increased HM loading (4 to 8 layers of TRISO), hence decreased C/HM (from ~400 to ~200), otherwise same as CASE 2B1.

CASE 7: Fuel enrichment 19.75 wt%, otherwise same as CASE 2B1.

OBJECTIVE: Identify specific depletion-related effects, that may not be as pronounced in most other reactor types.

[This is a high-LEU enrichment, epithermal spectrum reactor, with high specific power, using non-traditional BP.]

NEA FHR/AHTR Benchmark, Phase I-B

Results requested at
BU steps.

BURNUP [GWd/tU]	k-eff (a)	Fission source distribution (b)	3-group flux (c)	3-group flux distrib. (d)	Neutron spectrum (e)	Isotopics (f)
0	All	All	All	All	All	All
0.1	All		All			All
0.5	All		All			All
1	All	All	All	All	All	All
2	All		All			All
4	All		All			All
6	All		All			All
8	All		All			All
10	All		All			All
14	All		All			All
18	All		All			All
22	All		All			All
26	All		All			All
30	All	All	All	All	All	All
40	All		All			All
50	All		All			All
60	All		All			All
70	All	All	All	All	All	All
80	CASE 7		CASE 7			CASE 7
90	CASE 7		CASE 7			CASE 7
100	CASE 7		CASE 7			CASE 7
120	CASE 7		CASE 7			CASE 7
140	CASE 7		CASE 7			CASE 7
160	CASE 7	CASE 7	CASE 7	CASE 7	CASE 7	CASE 7

NEA FHR/AHTR Benchmark, Phase I-C

3D fuel element, depletion

Same 4 cases as I-B. Add top/bottom reflector regions.

CASE 2C: Hot full power (HFP), with prescribed temperatures for fuel, graphite, and coolant.

- CASE 2C1 → deplete with critical spectrum, uniform axial temp.
- CASE 2C2 → deplete with “as-is” spectrum, uniform axial temp.
- CASE 2C5 → 2C1 with prescribed axial temperature gradient

CASE 4C: Discrete europa BP, otherwise same as CASE 2C4.

CASE 6C: Increased HM loading (4 to 8 layers of TRISO), hence decreased C/HM (from ~400 to ~200), otherwise same as CASE 2C4.

CASE 7C: Fuel enrichment 19.75 wt%, otherwise same as CASE 2C4.

OBJECTIVE: Impact of reflector (expected larger than “usual”, large migration length!) and axial temperature gradient (expected small)

Required Results

2D FUEL ELEMENT (Phase I-A and I-B)

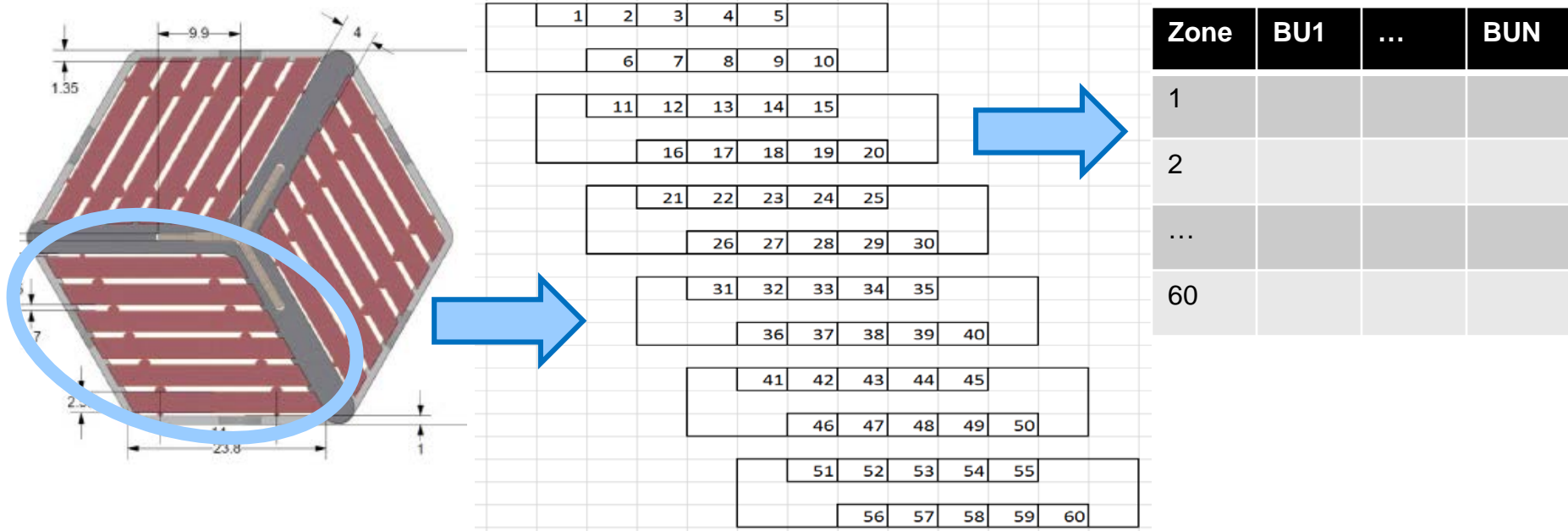
- a) Effective multiplication factor, and its change with depletion.
- b) Tabulated fission source distribution, at several levels of granularity (~~by fuel plate~~, by fuel stripe, by 1/5-th fuel stripe), and its change with depletion, at selected burnups.
Optional: visualized fission density distribution.
- c) Neutron flux, averaged over the whole model, tabulated in 3 coarse energy groups (upper energy boundaries 3 eV for thermal group and 0.1 MeV for intermediate group), and its change with depletion, at selected burnups.
- d) Visualized distribution of the neutron flux distribution, in 3 coarse energy groups, and its change with depletion, at selected burnups.
- e) Neutron spectrum, fuel assembly average. Optional: by region
- f) Fuel (and burnable poison, when applicable) isotopic change with depletion. [Details, i.e., which isotopes at what burnup – specify.]
- g) FLiBe isotopic change and tritium production (one case only)

3D FUEL ELEMENT (Phase I-C), at prescribed burnups:

- a) Effective multiplication factor
- b) Axial fission density distribution
- c) Axial 3-group flux distribution
- d) Axial burnup distribution

Templates for Results – fission source

- a) Tabulated fission source distribution, by fuel stripe and by 1/5-th fuel stripe, and its change with depletion, at selected burnups. [180 per assembly. Similar granularity to fuel pins per LWR assembly.]
Optional: visualized fission density distribution.



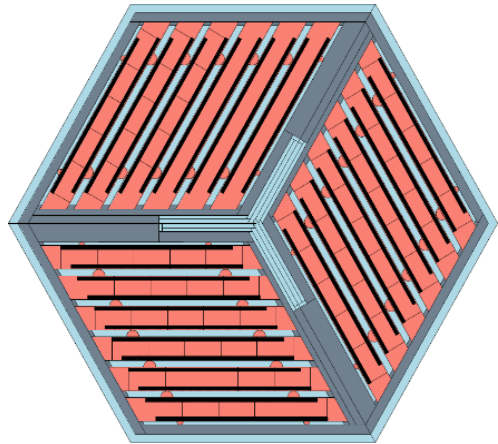
Preliminary Models and Results

Developed SERPENT, SCALE and MCNP models, very similar to benchmark

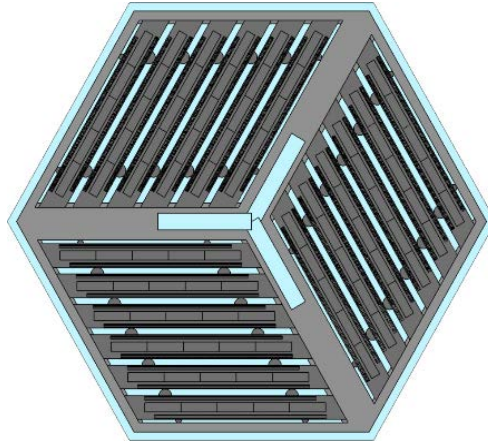
- To identify issues with benchmark specifications
- To get some feel for results, times, sensitivities,
- These preliminary results, while not providing results exactly corresponding to the benchmark cases, should help the participants to identify early misinterpretation of specifications or other errors (the unique and complex AHTR core design being more likely to such modeling issues)

Sample Fuel Element Models/Results

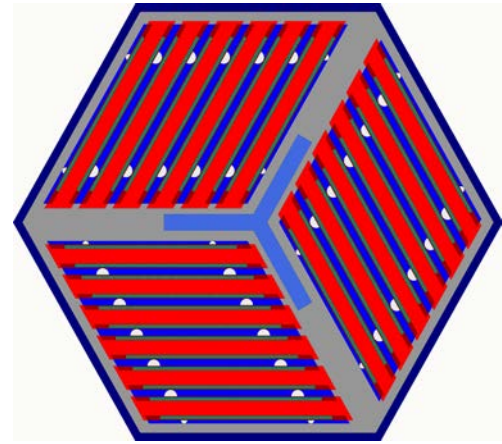
MCNP, SCALE and SERPENT models



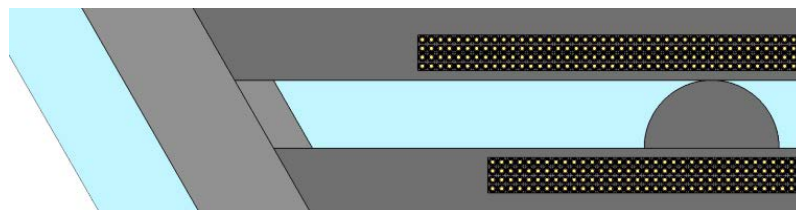
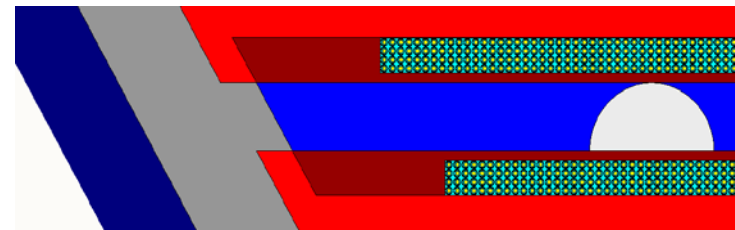
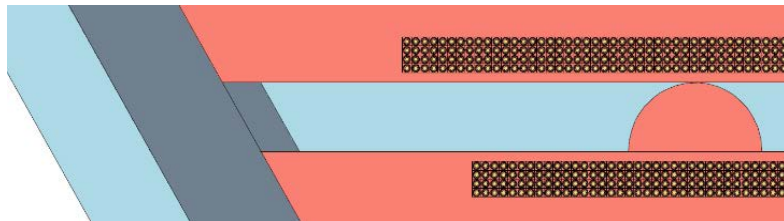
MCNP



SCALE



SERPENT

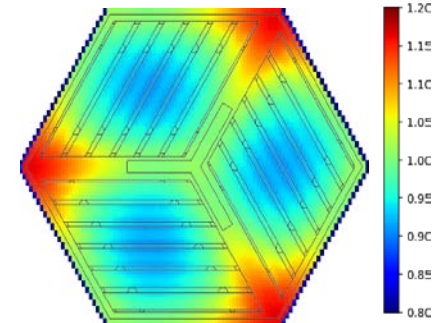
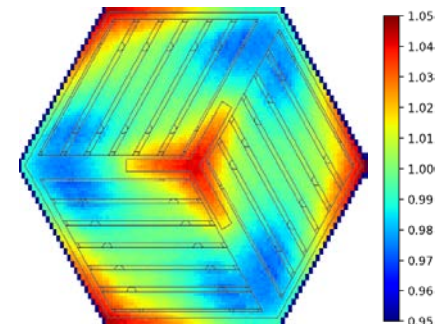
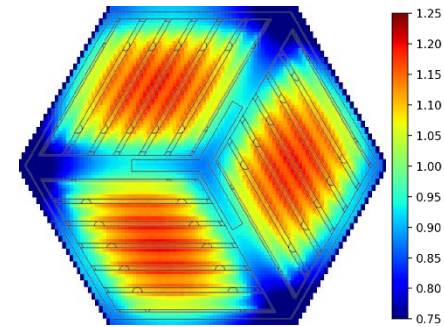
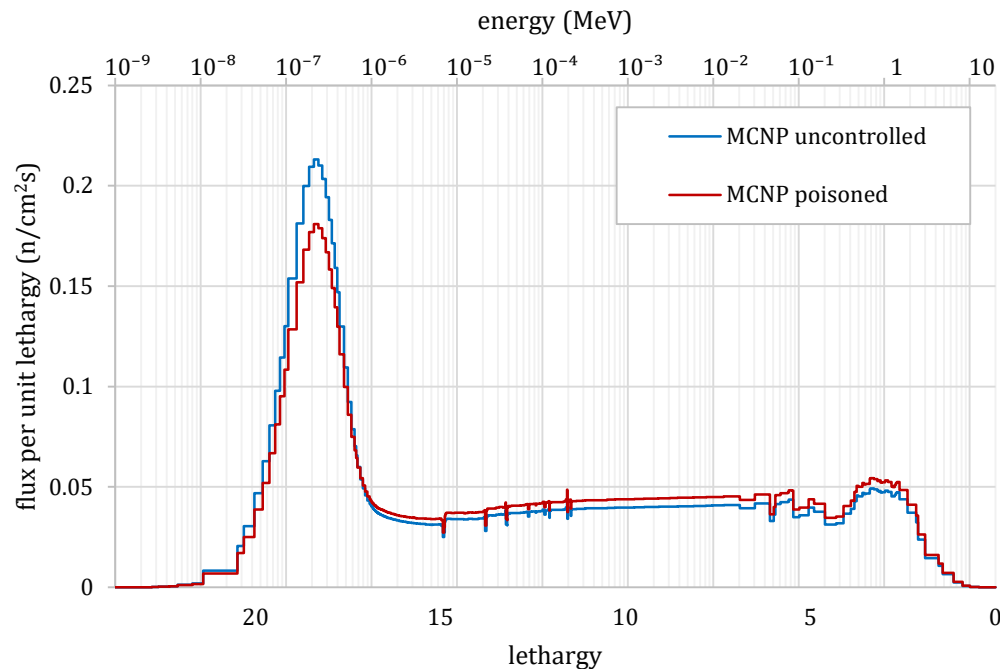


Sample BOC results:

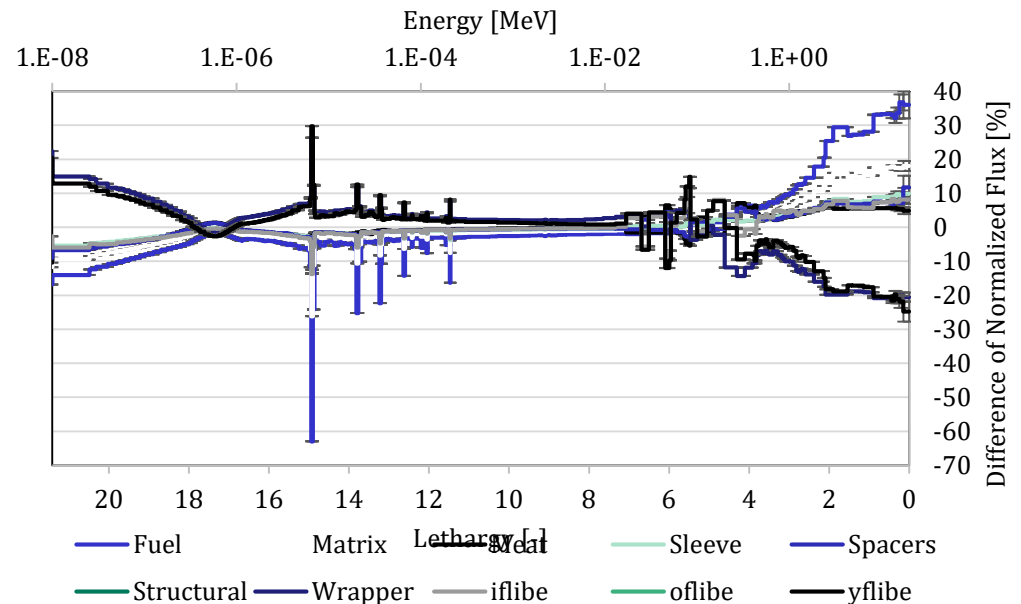
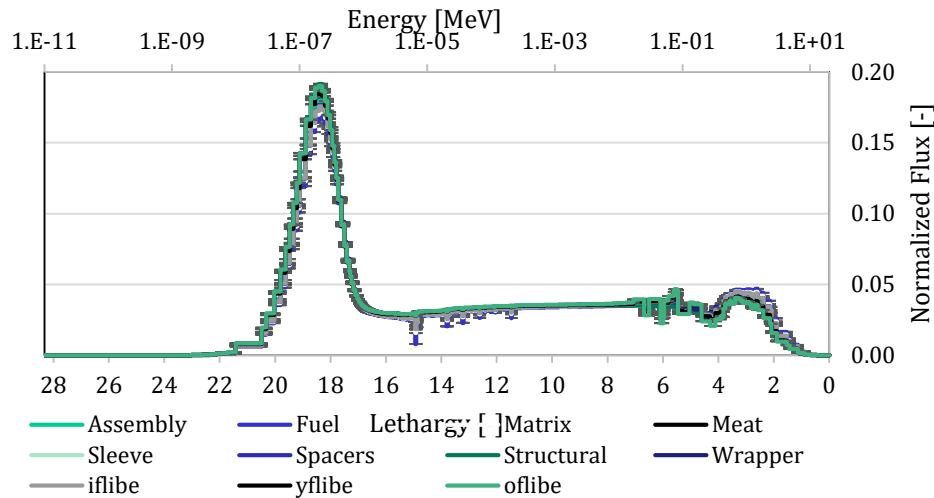
Neutron spectrum and 3-group flux distribution

Energy groups boundaries:
 10^{-5} eV, 3 eV, 0.1 MeV, 20 MeV

Neutron spectrum:
Unpoisoned and poisoned assembly

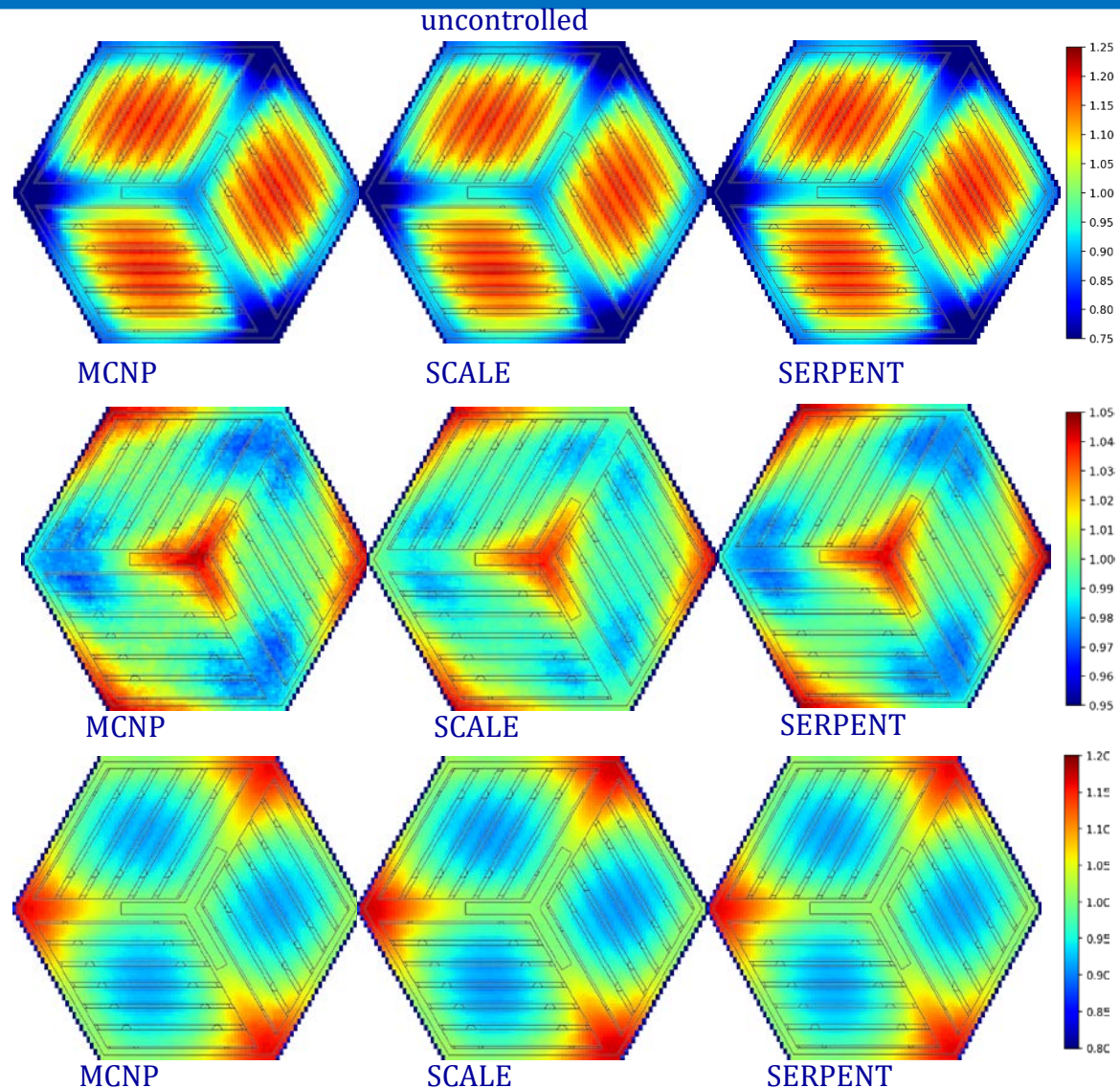


Sample results: Fuel element neutron spectrum and region-wise spectra differences



Sample results: 3-group flux distribution comparison (fast, intermediate, thermal)

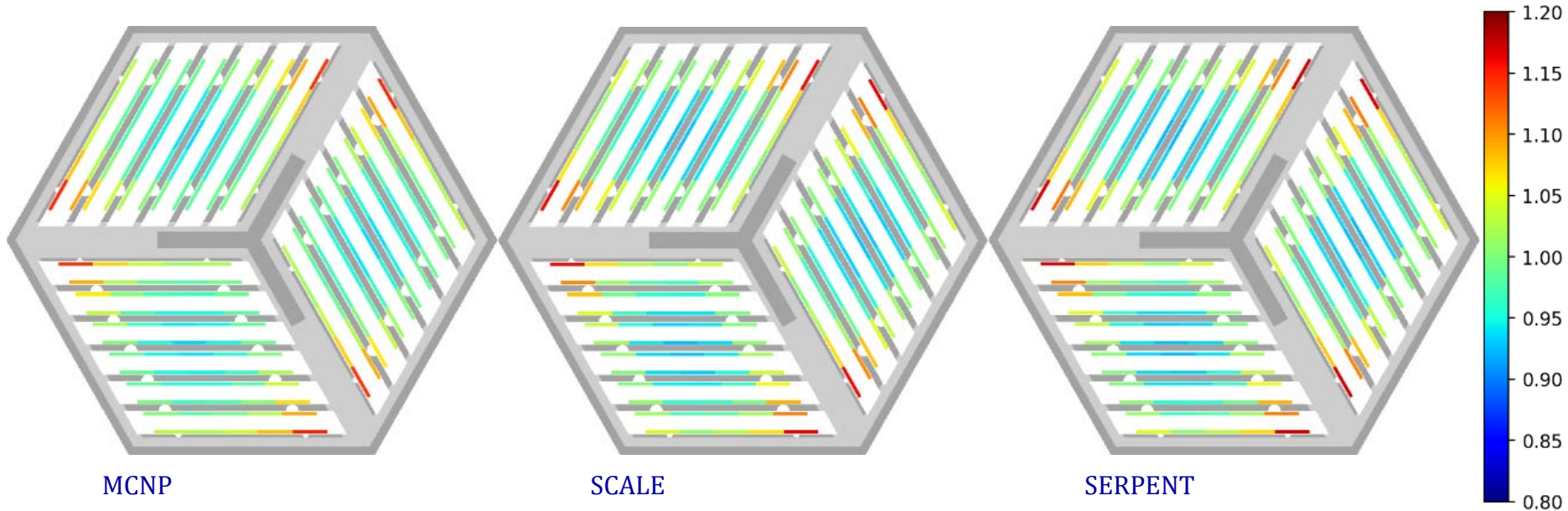
Consistent results
Obtained for
Consistent models



Sample results: fission rate distribution (180 regions per assembly)

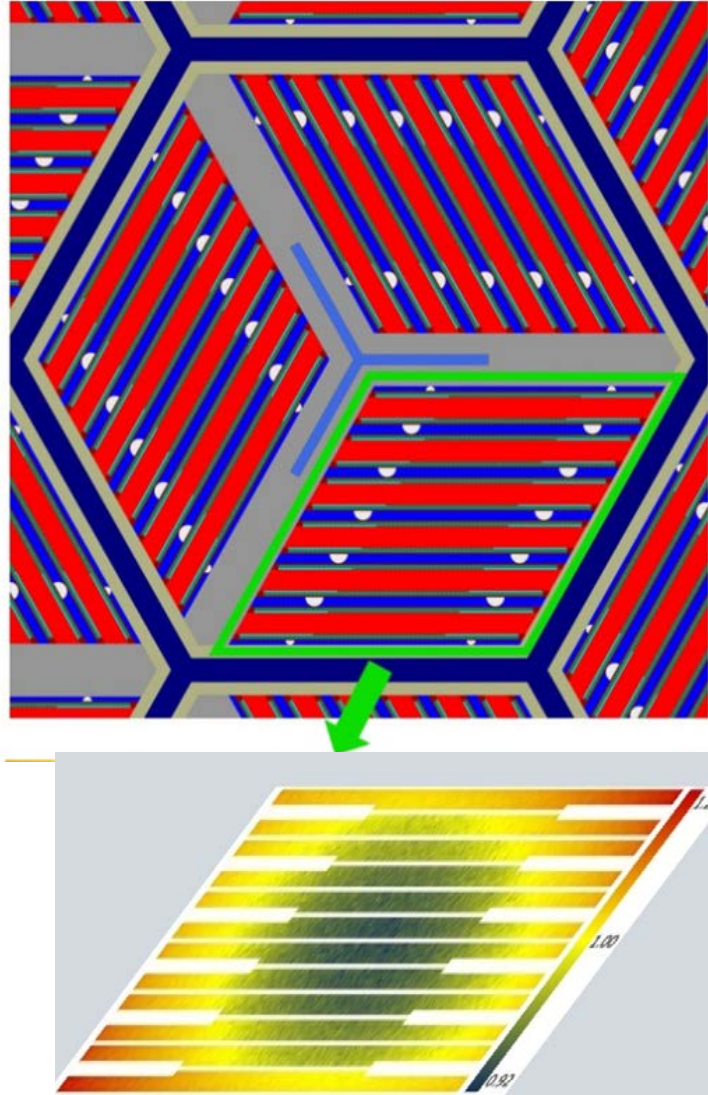
5 regions lengthwise per fuel stripe
2 fuel stripes per fuel plank
18 fuel planks per fuel assembly

180 power (fission) regions for depletion
(similar granularity as pin-powers in PWR FA)



Sample results: optional fission rate distribution per individual TRISO particle

At fuel element level feasible to obtain TRISO-particle-wise fission density with acceptable statistics



Sample results:

Comparison of peaking factors

Case		Plank Peaking Factor (18)	Stripe Peaking Factor (36)	Fifth-Stripe Peaking Factor (180)
unpoisoned				
MCNP		1.042	1.064	1.148
SCALE		1.041	1.063	1.146
SERPENT		1.042	1.067	1.155
poisoned				
MCNP		1.050	1.075	1.172
SCALE		1.048	1.074	1.174
SERPENT		1.050	1.079	1.183

NOTE: Cross-sections used in simulations are not fully consistent between codes

Benchmark Specs and Participation

Benchmark accepted/approved by OECD/NEA
[Expert Group on Reactor Physics and Advanced Nuclear
Systems (EGRPANS) under the Working Party on
Scientific Issues of Reactor Systems (WPRS)]

Benchmark homepage at OECD/NEA:

<https://www.oecd-neo.org/science/wprs/fhr/index.html>

Access to working area and full specifications granted to
participants

If interested:

- **Download and complete/sign the participation conditions form (available at benchmark homepage)**
- **Email the form with participation request to wprs@oecd-neo.org (and cc-me)**

The image shows the cover page of a document titled "Benchmark Specifications for the Fluoride-salt High-temperature Reactor (FHR) Reactor Physics Calculations". The document is published by the Nuclear Energy Agency (NEA) and the Nuclear Science Committee. It is identified as "Phase I-A and I-B: Fuel Element 2D Benchmark". The authors are listed as B. Petrovic* and K. Ramey, from the Georgia Institute of Technology, USA. The document is identified as "Rev. 0" and dated "July 2019". The page number is "Page 1 of 34" and the revision date is "Rev. 0, 2019-07-17".

NEA/NSC/X(2019)X

Nuclear Science NEA/NSC/X(2019)X

Nuclear Energy Agency
Nuclear Science Committee

Benchmark Specifications for the
Fluoride-salt High-temperature Reactor (FHR)
Reactor Physics Calculations

Phase I-A and I-B: Fuel Element 2D Benchmark

B. Petrovic*, K. Ramey
Georgia Institute of Technology, USA

(* Email: bojan.petrovic@gatech.edu)

Rev. 0
July 2019

Page 1 of 34 Rev. 0, 2019-07-17

Benchmark Status and Timeline

- Benchmark released 7/30
- First group of participants approved (7 in August/September)

Tentative schedule

- Conference-call end-October or early November (informal kick-off, initial feedback/issues)
- Will introduce the benchmark at the ANS RPD meeting in D.C. in November
- Finalize (first batch) of participants by end-November
- Conference-call end-November (formally initiate)
- Preliminary results (Phase I-A) at the 2020 WPRS/EGRPANS meeting (NEA, Feb. 2020). Discuss, resolve inconsistencies.
- Phase I-A final results due by 4/30/2020.
- Phase I-B and I-C specifications – in 2020
- Phase I-B and I-C results, present/discuss, 2021 WPRS
- Phase-II specifications

•

Benchmark Participants/Codes

We are participating with SERPENT (Kyle Ramey)
[with some additional spot-comparisons to MCNP and SCALE]
Other participants using SERPENT are expected

Benefits of multiple participation with the same code:

- Complex geometry, neutronics may be modeled in different ways, but core physics without feedback is expected to provide near-identical results for MC codes
- Comparison to deterministic results (if there are participants) will be very interesting; limited experience for this type of reactor
- May need to develop new options/interfaces (e.g., triangular mesh)
- There are many possible interesting sensitivity studies, that are outside of the benchmark scope, but important for FHR and even MSR (level of graphitization of carbonaceous materials, dimensional changes, material properties change with irradiation, etc.). The benchmark will provide a framework.
- For analyses with feedback, differences in approach and results are expected; it will be useful to quantify
- Efficiency and practicality issues (memory, parallel performance) for 3D full core cycle depletion analysis with feedback

Sample further studies at GT

Sensitivity studies

Introduction

BACKGROUND: Advanced High Temperature Reactor (AHTR^{1,2}) is a type of Fluoride salt-cooled High-temperature Reactor (FHR) which features TRISO fuel kernels in fuel planks. The coolant is a fluoride salt (LiF-BeF₂, or simply FLiBe).

OBJECTIVE: Analyze the sensitivity of reactor physics parameters to perturbations in the AHTR design features. Create the reference model in SERPENT³ based on the 2012 Oak Ridge National Laboratory design⁴. Sensitivity results provide information on the impact of design modifications and uncertainties.

SCOPE: Create a 2D model of the AHTR fuel assembly in SERPENT. Allow for tailoring of very detailed (TRISO-wise) fission rates, construction of multigroup flux meshes, use of thermal scattering data for carbonaceous moderating materials, depletion of fuel kernels in the TRISO particles, and changing the compositions of the materials. Summarize the results of the sensitivity studies where appropriate and provide estimates for future design implementations.

APPROACH: 2D assembly model developed in SERPENT using highly-detailed geometry with periodic, radial, boundary conditions and mirrored axial boundaries. Model is 100 TRISO particles high with fuel stripes distributed in four layers of TRISO particles. Average operating conditions were assumed where applicable for temperatures and densities.

Note: results shown here come from published work⁵.

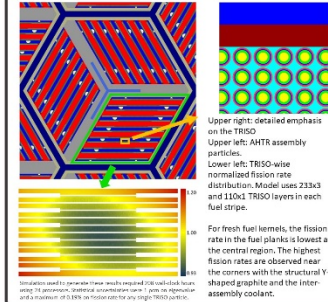
Base Case Parameters

Material	Density [g/cc]	Temperature [K]	Modeled As
Fuel ^a	10.9	1110	9 wt% UO ₂ /SiC _{0.15}
Buffer	1	1110	Carbon
PyC	1.9	1110	Graphite using 1200 K Si(a,b)
SiC	3.2	1110	Graphite using 1200 K Si(a,b)
DPVC	1.87	1110	Graphite using 1200 K Si(a,b)
Matrix	1.75	1110	Graphite using 1200 K Si(a,b)
Meat	1.75	1110	Graphite using 1200 K Si(a,b)
Sleeve	1.95	948	Graphite using 1000 K Si(a,b)
Spacer	1.75	1029	Graphite using 1000 K Si(a,b)
Structural	1.75	948	Graphite using 1000 K Si(a,b)
FLiBe	1.957888	948	Li ₂ BeF ₄

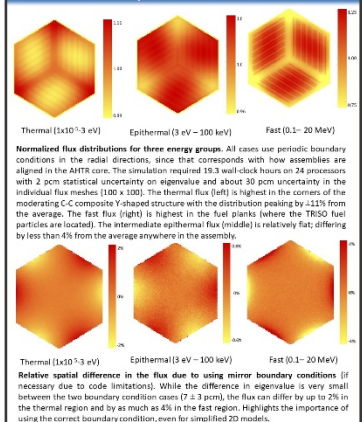
^aTRISO fuel kernels are assumed to be 0.24 UO₂

The sensitivity studies presented in this poster all use a base model of an AHTR assembly with fuel stripes consisting of 23343 and 13043 TRISO particles in four fuel layers (809 total particles per layer) with a cubic lattice. Note that these results will differ from those assuming a 2024 (809 total particles per layer) TRISO particle distribution (due to geometric effects). The densities, temperatures, and other parameters of select materials are summarized in the table above. Most of the temperatures correspond to the core-average value since this model aims to be representative of the whole core (which would obviously have variation in the axial and radial dimensions). Thermal scattering data for graphite is used for both graphite and C-C composite materials, as is shown to be acceptable in "Thermal Scattering in Graphite".

TRISO-Wise Fission Rate Distribution



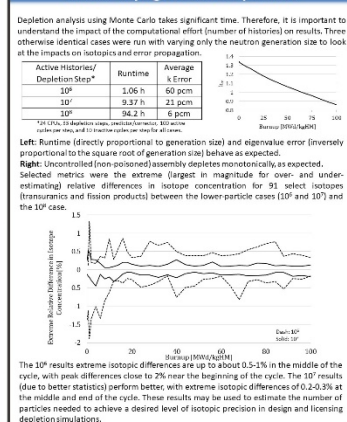
3-Group Flux Distributions



Thermal Scattering in Graphite



Error Propagation in Depletion

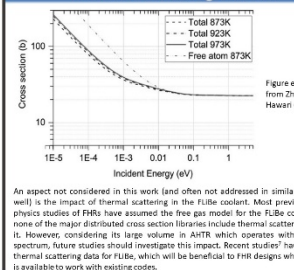


Graphite Density

Modified Material	k(-10%) ^a	Normal ^b	k(+10%) ^a	Δk(-10%) [pcm]	Δk(+10%) [pcm]
Fuel Matrix	1.39174	1.39327	1.39484	-153 ± 7	167 ± 7
Plank Meats	1.38468	1.39327	1.4018	-879 ± 7	853 ± 7
Plank Sleeve	1.39213	1.39327	1.39457	-114 ± 7	130 ± 7
Spacer	1.39301	1.39327	1.39367	-26 ± 7	40 ± 7
Structural Y	1.38819	1.39327	1.39176	-503 ± 7	357 ± 7
Assembly Wrapper	1.39084	1.39327	1.39577	-243 ± 7	250 ± 7
All (sum Δ)	1.3727	1.39286	1.41037	-1867 ± 17	1889 ± 17
All (simulated)	1.3727	1.39286	1.41037	-2016 ± 7	1751 ± 7

The AHTR design uses carbonaceous material (including graphite) for many in-core components. While the reference design provides nominal densities for these materials, deviations are expected when it comes to manufacturing physical components. Historically, graphite densities can vary by 10% based on fabrication methods⁶. Several carbonaceous assembly components listed above had their densities perturbed by ±10% to investigate the impact on eigenvalue. As expected, more carbon improved moderation and raised the eigenvalue, while less carbon lowered it. The largest perturbation was observed in changing the density of the graphite between the fuel stripes in a fuel plank (plank meats). The sum of the individually considered perturbations (all sum Δ) differed somewhat from the explicit modeling of those perturbations in the same simulation (All simulated) by about 140 pcm (about 7.5% error from expected). Thus, estimating perturbations on k are likely appropriate for limited density variation of individual components, but large changes such as changing all the carbonaceous material densities by 10% or more would require repeating the simulation for the new case.

Thermal Scattering in FLiBe



Conclusions

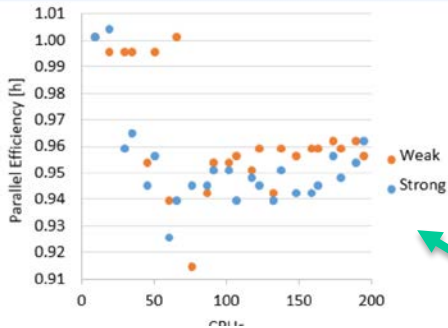
- 2D model of AHTR assembly was created in SERPENT to allow for sensitivity studies to be conducted. Analyses completed for various parameters.
- TRISO-wise fission rate distribution tracking is feasible and allows for very detailed results on power production in an assembly.
- Flux distributions show that the thermal flux is highest in large carbonaceous components while the fast flux is highest in the fuel planks.
- A comparison of periodic and mirrored boundary conditions shows that while the difference in eigenvalue is very small (0.1%), spatial group fluxes can be off by a few percent.
- Thermal scattering is important for a thermal reactor design like AHTR. Use of Si(a,b) scattering matrices can impact results by a few hundred pcm.
- Depletion studies with error propagation analysis completed for three different generation sizes with 10⁶ active particles being the largest. Eigenvalue uncertainty, eigenvalue over cycle, and runtime performed as expected. When tracking 91 isotopes, peak isotope differences were about 0.2-0.3% for 10-times fewer particles and 0.5-1% for 100-times fewer particles.
- Graphite density sensitivities computed for various carbonaceous components. Collectively sensitivity for all components was about 188 pcm/% density change.
- Future studies should evaluate the impact of thermal scattering in FLiBe.

References

- ¹K. Varga, et al. *AHTR Mechanical Structure*, and *Neutronic Performance* Design. Oak Ridge National Laboratory (2013).
- ²B. Petrovic, C. L. Mader, *Fuel and Core Design Options to Overcome the Heavy Metal Loading Limit and Improve Performance and Safety of Liquid Salt Cooled Reactors*. Georgia Institute of Technology and University of Tennessee (2016).
- ³Leppanen, *Serpent - A Continuous-Energy Monte Carlo Reactor Physics Burnup Calculation Code V1.1*. Technical Report, Centre of Nuclear Energy (2013).
- ⁴C. Haines, B. Petrovic, *Monte Carlo Modeling and Simulation of AHTR Fuel Assembly by Support Tools of MCNP Code*. Annual of Nuclear Energy **118**, 272-282 (2018).
- ⁵C. Haines, et al. *Fabrication of Uranium Oxide Kernels for HTR Fuel*. Proceedings of ITR 2010, Prague, Czech Republic, October 18-20 (2010).
- ⁶J. L. Lathrop, *Thermal Neutron Cross Sections*. Academic Press, New York (1970).
- ⁷D. L. Lathrop, *Thermal Neutron Cross Sections of Liquid FLiBe*. Progress in Nuclear Energy **101**, 168-175 (2017).

Sample further studies at GT

Parallel Efficiency



Prototypical Cycle Analysis

- Problem considered:** AHTR core with 252 fuel assemblies, one cycle depletion, and simplified feedback and criticality search.
- Modeling assumptions:** 4,032 depletion regions, 5 burnup steps with predictor-corrector methodology, and thermal-hydraulic feedback and criticality resolved together with 3 iterations.
- Monte Carlo simulation parameters:** 106 neutrons per cycle, 150 inactive and 850 active generations, and tallying over depletion materials using either the materials tally currently available in SERPENT or an efficient mesh tally (currently in development).
- Computational resources:** parallel cluster with ~200 cores (Xeon E5 2.4 GHz or similar)
- Estimated simulation time:**

	Current material tallies	Efficient mesh tally
Static simulation (no depletion) on a single core	48,000 h	2,400 h
Single burnup step predictor/corrector with thermal hydraulic feedback and criticality search on a cluster	1,440 h (~2 months)	72 h (3 days)
Cycle depletion (5 steps)	7,200 h (~10 months)	360 h (~2 weeks)

Feasibility and Practicality of 3D Monte Carlo AHTR Simulations

Kyle M. Ramey (kmramey@gatech.edu)
 Tim Flaspoepler (timothy.flaspoepler@gatech.edu)
 Advisor: Bojan Petrovic (bojan.petrovic@gatech.edu)

Georgia Institute of Technology - Nuclear and Radiological Engineering - Group for Sustainable Nuclear Power

Introduction

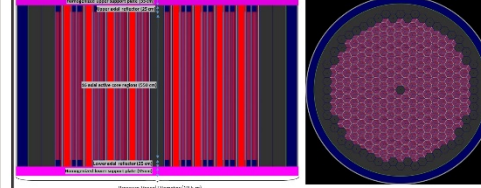
BACKGROUND: Advanced High Temperature Reactor (AHTR)^{1,2} is a type of Fluoride-salt-cooled High-temperature Reactor (FHR) which features TRISO fuel kernels in fuel planks. The coolant is a fluoride salt (ZrF₄-BeF₂ or simply FLiBe).

OBJECTIVE: Evaluate the feasibility, practicality, and required resources for conducting AHTR design and licensing analyses with widely-used Monte Carlo codes.

SCOPE: Create a prototypical 3D model of the AHTR core in SCALE³, SERPENT⁴, and MCNP⁵. Base the reference model on the 2012 Oak Ridge National Laboratory design¹ with assumptions similar to those prescribed in the stylized AHTR benchmark problem². Allow for: 1/3 assembly-wise depletion tracking, 1/16 axial active core partitioning, using a fine Cartesian mesh tally over the hexagonal space to obtain flux distributions, cycle-wise data collection, several separate tallying options in replica runs, parallelizing simulations over several nodes with multiple cores using MPI, and capabilities for conducting a fuel cycle analysis, investigate the practicality of using certain features under the computational burden of using Monte Carlo. Provide estimates and recommendations for future design and licensing simulations.

APPROACH: 3D model developed SCALE, SERPENT, and MCNP using highly-detailed geometry. Model is 670 cm high (550 cm high active core) and 1050 cm wide. 16 axial partitions are used for the active core, which consists of 252 fuel assemblies in a hexagonal lattice.

3D Model



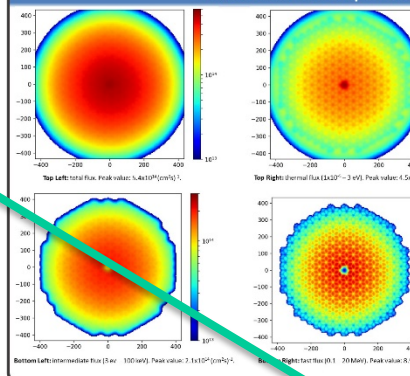
- Left:** Axial cross section of 3D AHTR model from SERPENT. Model is 1050 cm in the radial direction and 670 cm in the axial direction. There are five principal axial partitions: homogenized upper/lower support plates composed of FLiBe and either SiC (upper) or graphite (lower); upper/lower axial reflectors modeled the same as the active core geometry just without fuel (i.e., no TRISO particles in the fuel strips, just entirely graphite planks); and the active core which is modeled as 16 axial sections for depletion analysis capabilities.
- Right:** Radial cross section of 3D AHTR model from SERPENT. Model includes 252 fuel assemblies with removable reflector assemblies on the periphery and at the central position. Beyond the removable reflector assemblies are a permanent reflector, a boron carbide layer, the core barrel, the downcomer region, a thin vessel liner composed of Hastelloy N alloy, and the reactor pressure vessel creating the problem boundary.
- Consistent SCALE, SERPENT, and MCNP models.

Model Description

AHTR core model emphasize the 1/3 assembly resolution with 1/3 periodic core symmetry. Contains 252 uniquely-tracked regions per axial partition.

- 252 fuel assemblies, 16 fuel planks per assembly, 2 fuel strips per fuel plank, and 808 (4x202) TRISO particles in a fuel strip per TRISO layer over 43 billion TRISO particles in model.
- 16 active fuel axial partitions, 371 TRISO layers per axial partition, and 1/3 assembly radial partitioning while also using 1/3 core symmetry.
- Input file size: 430,000 lines (SERPENT) and 320,000 lines (SCALE).
- Difference is actually small. Likely driven by white space, use of comments, and conventional syntax inherent to each code.
- Continuous energy cross sections used (i.e., not multigroup).
- 4032 uniquely-tracked fuel and burnable absorber (Eu/pu) regions.

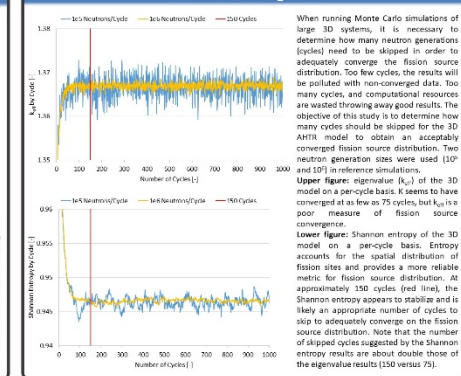
Total and Three-Group Fluxes



The four figures provided here show axially-integrated radial neutron flux distributions within the core. All figures have units of (cm⁻³) for the heat map and radial dimensions in cm from -433 cm. A visualization of this region can be seen below.

The top-left results are for the total flux. As a reference, 2D assembly models² had an average flux of 3.7x10¹⁴ (cm⁻³). This type of distribution is expected from a fresh core with uniform enrichment. The thermal flux peaks in the central moderating assembly and the fast flux peaks in fuel regions in the center of the core. The intermediate flux does not vary much through geometric features of the core (lathes) are evident from the thermal and fast flux distributions.

Source Convergence



When running Monte Carlo simulations of large 3D systems, it is necessary to determine how many neutron generations (cycles) need to be skipped in order to adequately converge the fission source distribution. Too few cycles, the results will be polluted with non-converged data. Too many cycles, and computational resources are wasted throwing away good results. The objective of this study is to determine how many cycles should be skipped for the 3D AHTR model to obtain an acceptably converged fission source distribution. Two neutron generation sizes were used (10⁶ and 10⁷) in reference simulations.

Upper figure: eigenvalue (k_{eff}) of the 3D model on a per-cycle basis. k_{eff} seems to have converged at as low as 75 cycles, but k_{eff} is a poor measure of fission source convergence. Lower figure: Shannon entropy of the 3D model on a per-cycle basis. Entropy accounts for the spatial distribution of fission sites and provides a more reliable metric for fission source convergence. At approximately 150 cycles (red line), the Shannon entropy appears to stabilize and is likely an appropriate number of cycles to skip to adequately converge on the fission source distribution. Note that the number of skipped cycles suggested by the Shannon entropy results are about double those of the eigenvalue results (150 versus 75).

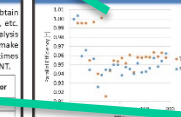
Tallying Computational Resources

When running full core simulations, it is important to use tallies to obtain information for local power, activation of components, spectra, fluxes, etc. While this data is critical for obtaining results and conducting proper analysis of Monte Carlo simulations, the user needs to do so efficiently to make optimal use of computational resources. Below is a summary of runtimes needed for different types of tallies in otherwise identical runs in SERPENT.

Tally Type	Number of Tally	CPU Time to Simulate	Slowdown Factor
Material	252	2.5h	1.01
Cartesian Mesh	7000 (250x280x10)	2.5h	1.01
Hexagonal Mesh	5776 (190x280x10)	2.5h	1.01
Material	8032 (25x25x16)	47.5	18.9
Cell	8032 (25x25x16)	35.4	21.9
Volume	4032 (25x16x16)	21.9	20.4

While all simulations above were run in parallel on multiple cores, the results of the third column are the expected runtimes on a single core. Note that the two spatial meshes (Cartesian and hexagonal) had virtually no impact to runtime on top of reference transport calculation. The material, cell, and universe tallies each slowed-down the simulation by a factor of about 20. This is very significant and would likely limit their use in future simulations. It is important to take the impact of tallies into account because in standard fuel cycle analyses other factors will be relevant: depletion using predictor/corrector (>400), thermal hydraulic feedback with criticality iteration (>40), etc. will collectively increase the required runtime by at least 100x from that of a single statepoint. If computational resources are wasted on inefficient tallies, runtimes will either balloon to become infeasible or results will be poor due to high statistical uncertainty from sampling too few particles.

Parallel Efficiency



- Orange:** weak scaling simulations, which use the same number of particles per core (CPU). Cores used 4x10⁶ neutrons/cycle/core with 20 inactive and 100 active cycles.
- Blue:** strong scaling simulations, which use the same number of particles per simulation. Cores used 10⁶ neutrons/cycle with 20 inactive and 100 active cycles.
- Both the weak and strong scaling results show favorable parallel efficiency with both performing at 94% or better for most cases. Neither show signs of efficiency degradation below 160 or 192 cores, but further testing would be necessary on a larger machine to investigate parallel efficiency at higher parallelism.

Prototypical Cycle Analysis

- Problem considered:** AHTR core with 252 fuel assemblies, one cycle depletion, and simplified feedback and criticality search.
- Modeling assumptions:** 4,032 depletion regions, 5 burnup steps with predictor-corrector methodology, and thermal-hydraulic feedback and criticality resolved together with 3 iterations.
- Monte Carlo simulation parameters:** 106 neutrons per cycle, 150 inactive and 850 active generations, and tallying over depletion materials using either the materials tally currently available in SERPENT or an efficient mesh tally (currently in development).

	Current material tallies	Efficient mesh tallies
Static simulation (no depletion) on a single core	48,000h	2,400h
Single burnup step predictor/corrector with thermal hydraulic feedback and criticality search on a cluster	1,440h (~2 months)	72h (3 days)
Cycle depletion (5 steps)	7,200h (~10 months)	360h (~2 weeks)

References

- K. Varma, et al. *AHTR Mechanical, Structural, and Neutronic Preconceptual Design*. Oak Ridge National Laboratory (2012).
- B. Petrovic, G. J. Maldonado, *Fuel and Core Design Options to Overcome the Heavy Metal Loading Limit and Improve Performance and Safety of Liquid Salt Cooled Reactors*. Georgia Institute of Technology and University of Tennessee (2016).
- H. Zhang, F. Rahmeh, *A Stylized Advanced High Temperature Reactor (AHTR) Benchmark Problem*. Annals of Nuclear Energy **120**, 178-185 (2018).
- T. Bearden, M. A. Josse, Eds. *SCALE Code System, ORO/TM-2005/05, Version 6.2*. Oak Ridge National Laboratory (2016).
- J. Leppanen, *Serpent - A Continuous Energy Monte Carlo Reactor Physics Burnup Calculation Code*. VTT Technical Research Centre of Finland (2013).
- C. J. Werner, et al. *MCNP 2.2 Release Notes*. Los Alamos National Laboratory, Report LA-UR-18-28068 (2018).
- K. Ramey, B. Petrovic, *Monte Carlo Modeling and Simulations of AHTR Fuel Assembly to Support V&V of FHR Core Physics Methods*. Annals of Nuclear Energy **118**, 272-282 (2018).

Conclusions

- V&V for FHR simulation methodologies is needed
- Reactor physics is challenging for AHTR “plank” fuel, due to double (triple?) heterogeneity
- Complex problem, challenges code capabilities
- Short of measured data, benchmark provides cross-verification
- Benchmark provides framework for various sensitivity and efficiency/feasibility studies

Benchmark Status:

- Developed a multi-phase benchmark (2D assembly to 3D full core with depletion & feedback)
- Approved by OECD/NEA WPRS/EGRPANS
- Released; several groups/participants registered
- Preliminary Phase I-A results aimed at by Feb 2020
- Phase I-A full results and evaluation complete by 2021 WPRS
- Phase I-B, I-C, II, ... to follow

Let me know if interested to participate (and contact NEA)

Thank you for your attention!

Questions?

Molten Salt Reactors (MSR) and Fluoride-salt-cooled High-temperature Reactors (FHR)

FHR - Use liquid salt as coolant

Several attractive features:

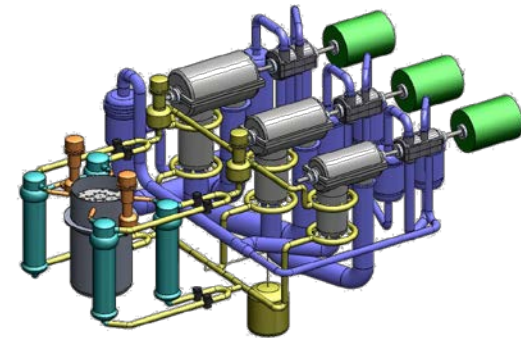
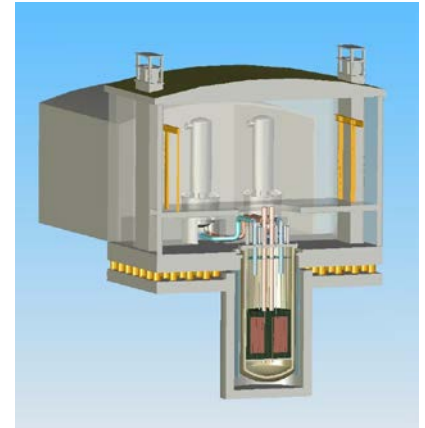
- Near-atmospheric pressure
- Large thermal margin
- High temperature → high efficiency, reduced reject heat
- Possible use for process heat

Fuel

- Molten Salt Reactors (MSR) with fuel dissolved in salt
- FHR reactors, with liquid salt used as coolant only –
focus of the NEA bFHR/AHTR benchmark

Several FHR concepts currently under development

- ORNL: Advanced High Temperature Reactor (AHTR), large power plant 3,400MW_{th}, **focus of the benchmark**
- Pebble Bed - AHTR; medium (410 MW_e) power plant at University of California Berkeley & Kairos
- SmAHTR; deliberately small (125 MW_{th}) process heat & electric system at ORNL
- Chinese test/demo reactors FHR (FHR-SF1, FHR-LF1)
- Other....



Source: ORNL

AHTR Main Parameters

Assembly Model Dimensions and Compositions at 40% PF	
Reactor Power	3400 MWt
Thermal Efficiency	~45%
Number of Fuel Assemblies	253
Assembly Half Pitch	23.375 cm
Plate Thickness	2.753 cm
Thickness of Fuel Regions	0.649 cm
Plate Sleeve Thickness	1 mm
TRISO Pitch	926 μ m
Fuel Kernal Radius	213.5 μ m
Fuel Material	Uranium Oxycarbide
Moderator Material	Graphite/Amorphous Carbon
Coolant	Li_2BeF_4 (Flibe)
Fuel Density	10.9 g/cc
Fuel Enrichment	< 20%
Average Coolant Temperature	948.15 K
Coolant Pressure	atmospheric
Core Volume	263.38 m ³
Core Power Density	12.91 MW/m ³
Mass Flow Rate	28408.1 kg/s
Average Coolant Velocity	1.93 m/s

Varma, V.K., Holcomb, D.E., Peretz, F.J., Bradley, E.C., Ilas, D., Qualls, A.L., Zaharia, N.M., 2012. AHTR mechanical, structural, and neutronic preconceptual design. Oak Ridge National Laboratory, ORNL/TM-2012/320.