PRELIMINARY RESULTS OF THE NEA FHR BENCHMARK PHASE I-A AND I-B (FUEL ELEMENT 2-D BENCHMARK)

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Outline

- Motivation
- Molten salt reactors (MSR – FHR – AHTR)
- Preliminary FHR reactor physics studies
- Proposed benchmark
- Phase IA & IB
- Participants
- Results
- Findings
- Next steps

Motivation (general)

- Interest in advanced reactors
- Renewed interest (started ~15 years ago) in molten salt reactors
- Molten salt reactors operate at
  - high working fluid temperature (→ high efficiency)
  - low near-atmospheric pressure (→ enhanced safety)

"Molten Salt Reactors"

- MSR – typically denotes a reactor with molten fuel-containing salt
- FHR – typically denotes a reactor cooled by non-fueled fluoride molten salt that utilizes solid fuel
  - Stationary solid fuel (e.g., ORNL AHTR)
  - Moving/circulating solid fuel (e.g., Kairos PB-FHR)
- Need to V&V analysis methods

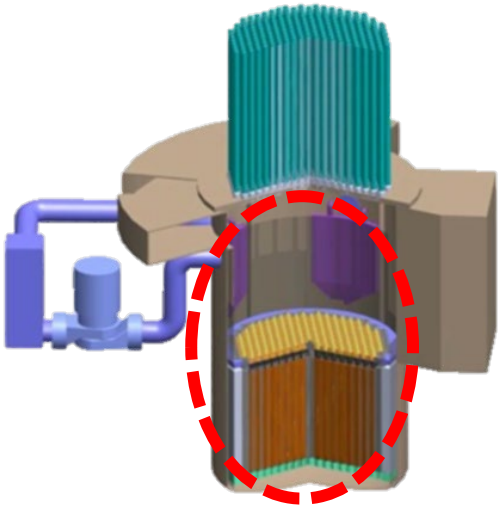
Motivation (more specifically)

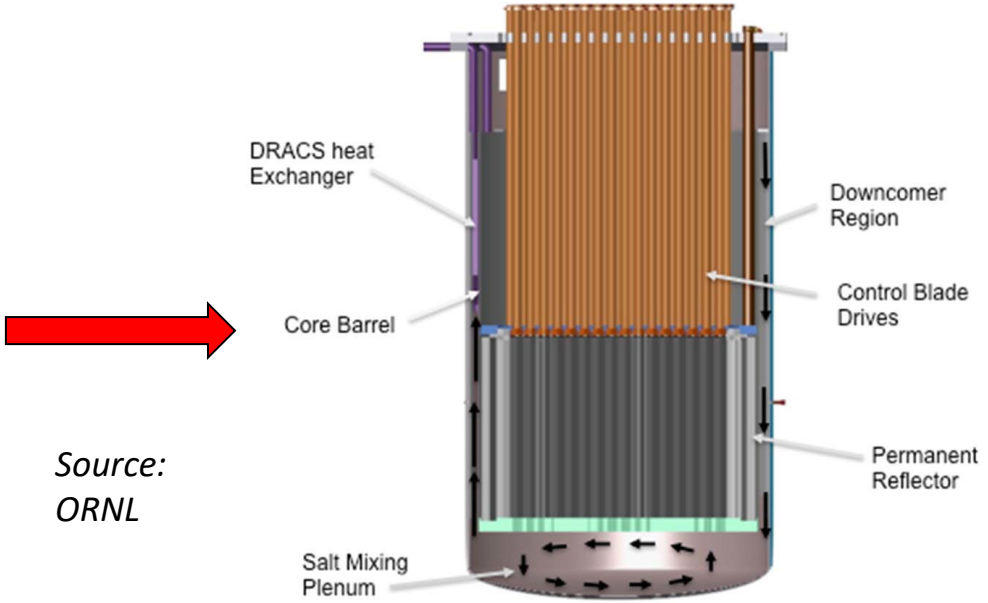
- AHTR fuel utilization and design optimization studies performed at Georgia Tech over the last decade
- Modelling challenges
- No FHR experiments. Performed internal cross-verification

- Developed/proposed computational benchmark for broader international cross-verification
- Performed under the auspices of OECD/NEA
- Subject of this presentation

ORNL Advanced High Temperature Reactor (AHTR)

- In the approximately 2005-2015 period, ORNL developed a concept of a large power (3,400 MW-th) Fluoride salt cooled High temperature Reactor (FHR), Denoted it as Advanced High Temperature Reactor (AHTR)
- Cooled by unfueled salt; fueled by hexagonal fuel elements with plate ("plank") fuel containing TRISO particles
- We focus on AHTR reactor design, refer to it by the more common name FHR, but specifically have in mind FHR with non-movable large hexagonal fuel elements.

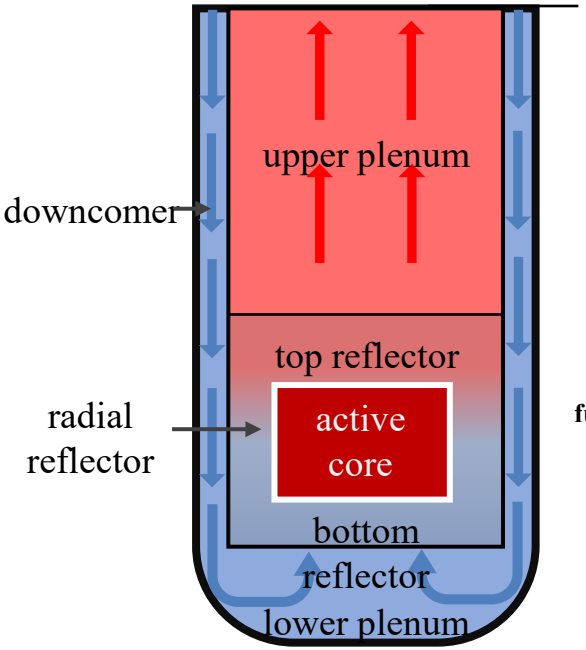




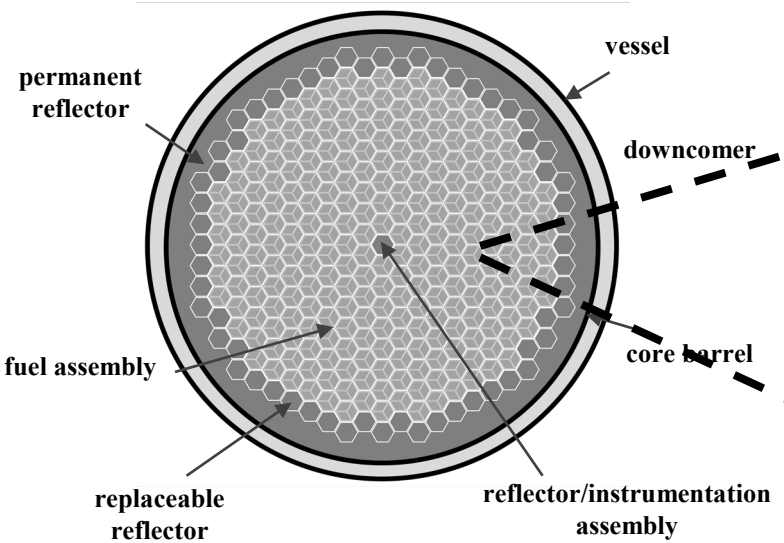
Source: ORNL

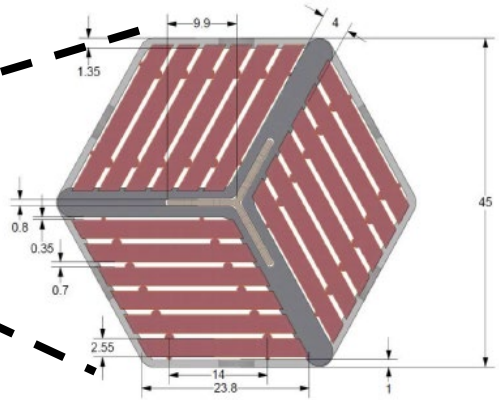
AHTR/FHR Core Design

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



Reactor Vessel



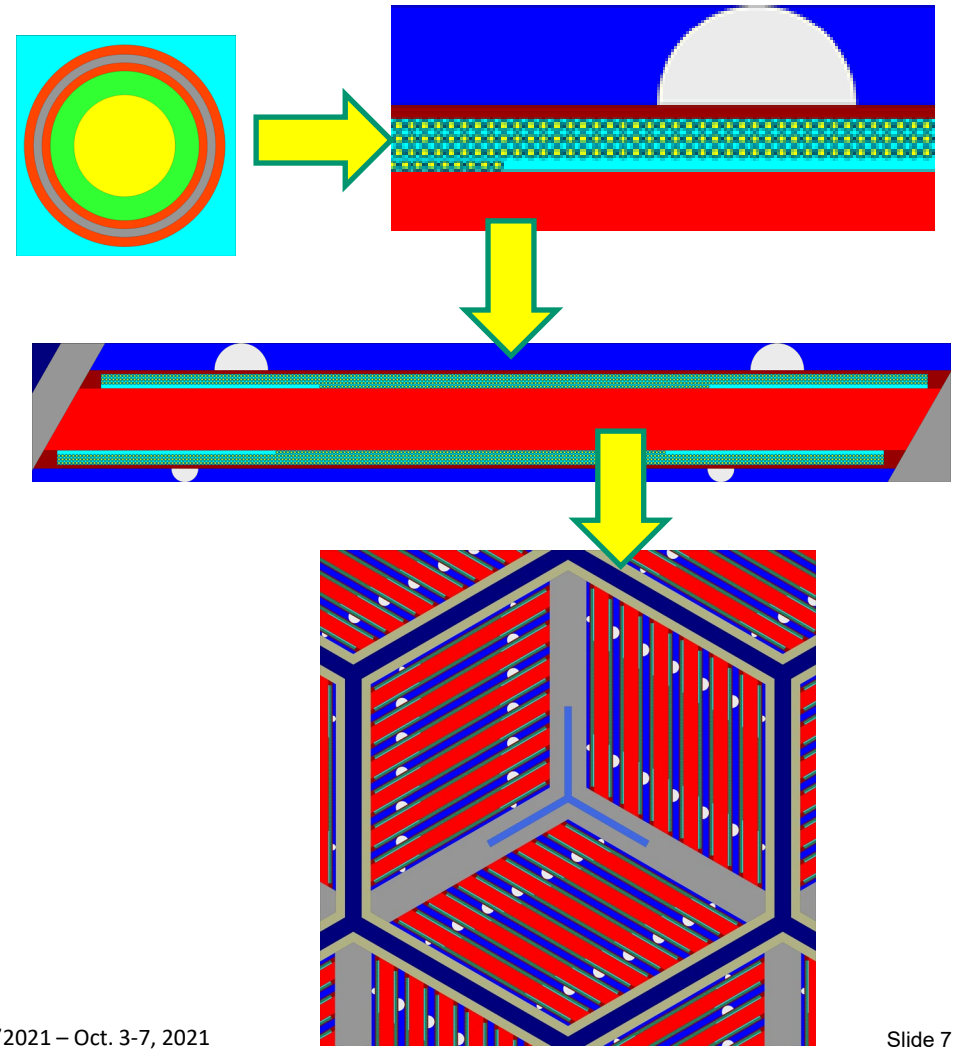


FHR → complex geometry
Challenging modeling and simulation problem

TRISO layers → TRISO → Fuel stripe → Fuel plate → Fuel element → Core

Fuel element – double (or triple?) heterogeneity

- 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..?)



Sample internal Georgia Tech cross-verification results: 3-group flux comparison (fast, intermediate, thermal)

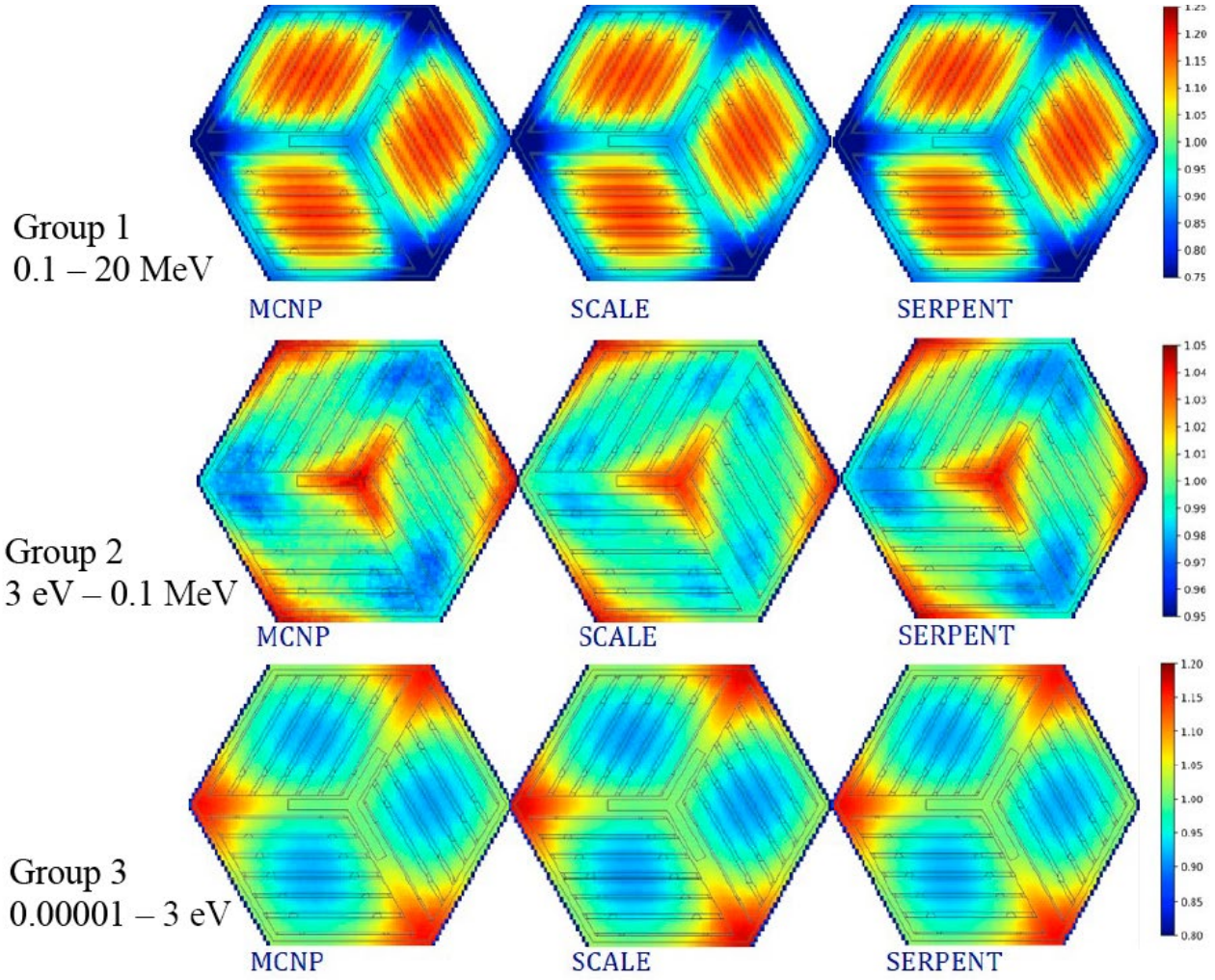


Figure 2. Comparison of neutron flux distribution over FHR fuel element, obtained by 3 codes, visualized in 3 broad energy groups with energy cutoff at 3 eV and 0.1 MeV [8]

FHR international benchmark Under OECD NEA Auspices

- Proposed to OECD NEA in 2018
- Accepted in 2019
- Specification prepared; published as OECD NEA Report NEA/NSC/R(2020)5

  NEA, "Benchmark Specifications for the Fluoride-salt High-temperature Reactor (FHR) Reactor Physics Calculations: Phase 1-A and I-B: Fuel Element 2D Benchmark," (Prepared by B. Petrovic, K. M. Ramey and I. Hill), Nuclear Science, OECD Publishing, Paris, France, 2021.
- Tremendous support of Mr. Ian Hill, OECD/NEA

Phase I – Fuel assembly (2D/3D with depletion)

- Phase I-A – "2D" (pseudo-2D) model, steady state (no depletion) }
- Phase I-B – 2D model depletion
- Phase I-C – 3D model depletion

Phase II – 3D full core with depletion

- Phase II-A – Steady-state (no depletion)
- Phase II-B – Depletion

Phase III – 3D full core with feedback and multicycle analysis

- Phase III-A – Full core depletion with feedback
- Phase III-B – Multicycle analysis

FHR benchmark Phase I-A & I-B participants

7 participating organizations from 4 countries.
(individual participants listed as co-authors)

- Stochastic **and deterministic methods**
- Two different MC codes
- Different participants (4, 2) using the same MC code
- CE and MG energy discretization
- Three cross section libraries

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ID	Organization	Method	Code	Library	Energy structure
CVREZ	Research Centre Rez, Czech Republic	MC	SERPENT2	ENDF/B-VII.0	CE
GT	Georgia Institute of Technology, USA	MC	SERPENT2	ENDF/B-VII.0	CE
PNNL	Pacific Northwest Nat'l Lab (PNNL), USA	MC	SERPENT2	ENDF/B-VII.0	CE
VCU	Virginia Commonwealth University, USA	MC	SERPENT2	ENDF/B-VII.0	CE
MAC	McMaster University, Canada	MC	OpenMC	ENDF/B-VII.1	CE
UIUC	University of Illinois at Urbana-Champaign, USA	MC	OpenMC	ENDF/B-VII.1	CE
CAM	University of Cambridge, UK	DET	WIMS	JEFF-3.1.2	MG 172

MC = Monte Carlo; DET = deterministic; CE = continuous energy; MG = multigroup

FHR benchmark Phase I-A & I-B
9 cases

Reference/baseline:

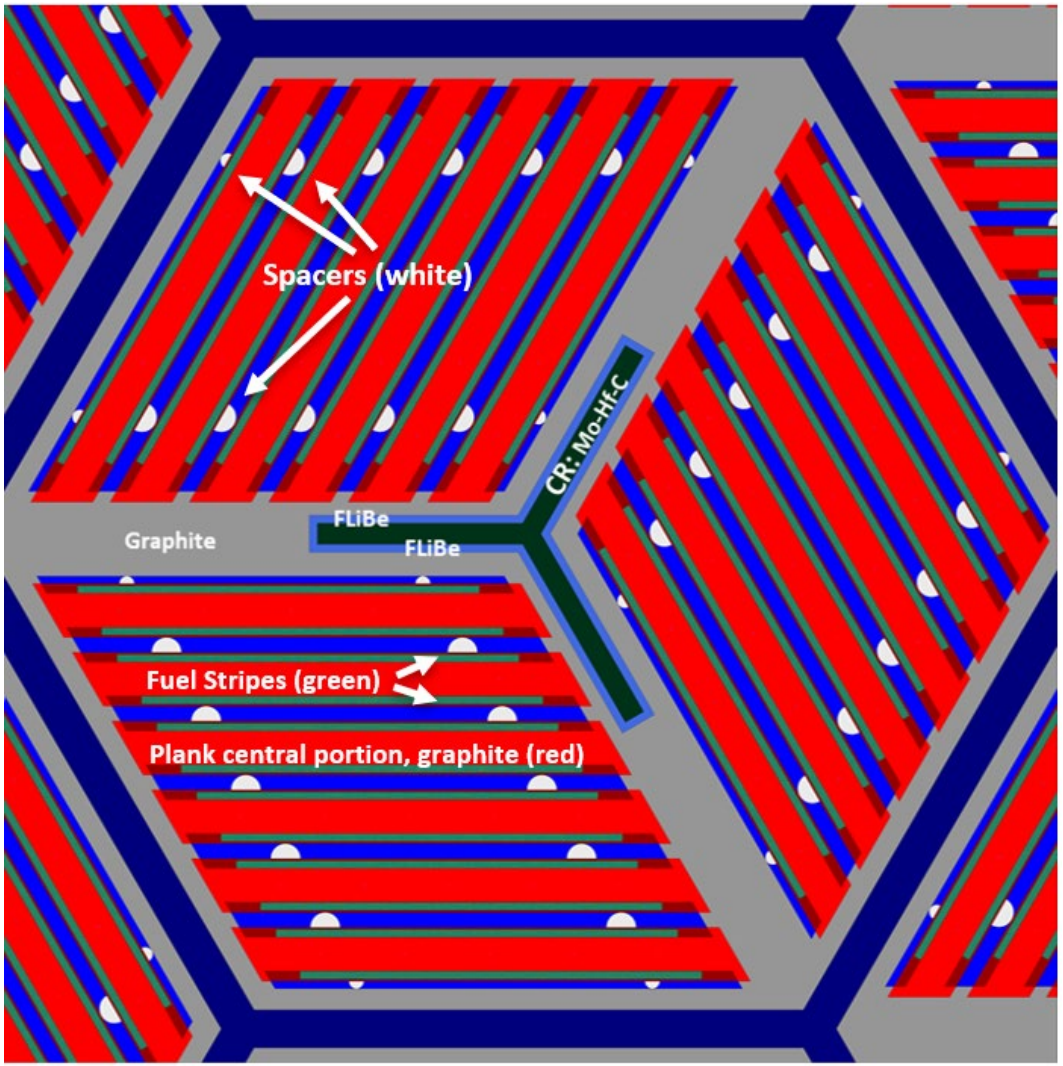
- A representative FHR hexagonal fuel element design
- 9 wt% fuel enrichment
- no burnable poison (BP)
- control rods (CR) out

The following nine cases are to be analyzed:

CASE 1:	Reference case at hot full power (HFP)
CASE 2H:	Reference case at hot zero power (HZP)
CASE 2C:	Reference case at cold zero power (CZP)
CASE 3:	CR inserted, otherwise same as CASE 1.
CASE 4:	Discrete europia BP used, otherwise same as CASE 1.
CASE 4R:	Discrete europia BP, and CR inserted, otherwise same as CASE 1.
CASE 5:	Integral (dispersed) europia BP, otherwise same as CASE 1.
CASE 6:	Twice increased HM loading (4 to 8 layers of TRISO).
CASE 7:	Fuel enrichment increased to 19.75 wt%, otherwise same as CASE 1.

FHR benchmark Phase I-A & I-B
Pseudo-2D Fuel Element

- Reflective (i.e., periodic) boundary conditions radially
- Finite height with reflective boundary conditions axially
- Note that 2D case is not possible due to spherical TRISO particles



Phase I-A and I-B results requested

Fairly extensive set of results requested (~10^6 values per participant)
Selected high-level results presented here

	INFORMATION REQUESTED
I-A a Multiplication Factor	9 cases
I-A b Reactivity Coefficients	(9 cases)*(4 values) Beta-eff + 3 reactivity coefficients
I-A c Fission Distribution	(9 cases)*(60 values) 60 fuel stripes with 10 sub-regions each
I-A d Neutron Flux	(9 cases)*(3 values) 3 groups average for the whole problem
I-A e Neutron Flux Distribution	(9 cases)*(3 groups)*(100x100 distribution)
I-A f Neutron Spectrum	(9 cases)*(252 values) 252 groups, average for the whole problem
I-B a Depletion	(3 cases)*(up to 24) k for prescribed Bus
1-B c Fission Distribution	(3 cases)*(60 regions)*(4 or 5 prescribed BUs)
I-B d Neutron Flux	(3 cases)*(3 groups)*(~20 Bus) average for the whole problem
1-B e Neutron Flux Distribution	Five worksheets for each of the 5 BUs (0-1-30-70-160) (5 worksheets/BUs)*(3 cases)*(3 groups)*(100x100)
I-B f Neutron Spectrum	(3 cases)*(252 values)*(5 BU steps) 252 groups, problem average, for prescribed Bus 0-1-30-70-160
I-B g Isotopic Change	3 worksheets for 3 cases: (3 cases)*(18-24 BU steps)*(#isotopes)

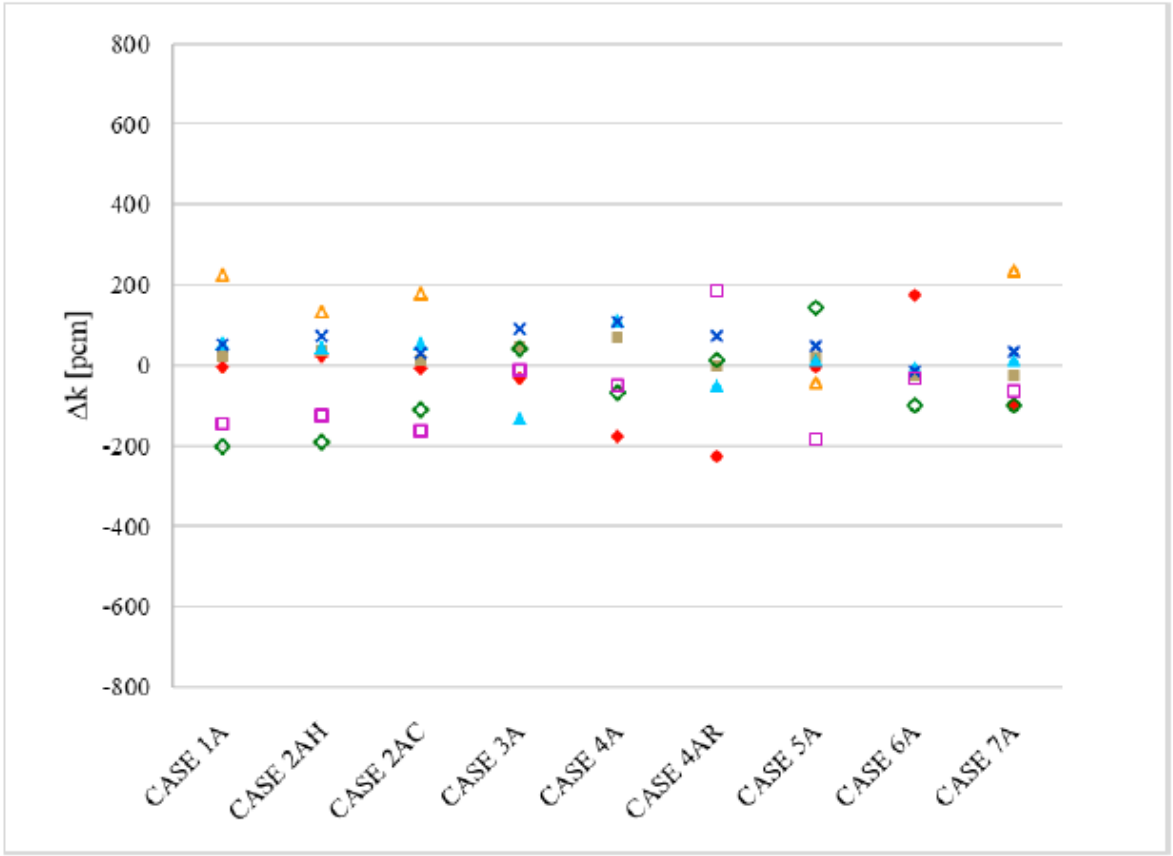
FHR benchmark conduct

- Desire to perform blind benchmark, as far as meaningful
- First iteration – fully blind benchmark
- Results compared
- Generally reasonable agreement
- Some k differences were larger than desired (1-2%)
- Traced to ambiguous specifications and in some cases input errors
- Errors or inconsistent assumptions were corrected, but no other “tweaking” was allowed

- Second iteration, presented here – denoted as “semi-blind” benchmark

FHR benchmark, Phase I-A
Multiplication factor

- Generally very good agreement
- One case by one participant excluded



Graphic comparison of obtained multiplication factors (k) for nine cases considered

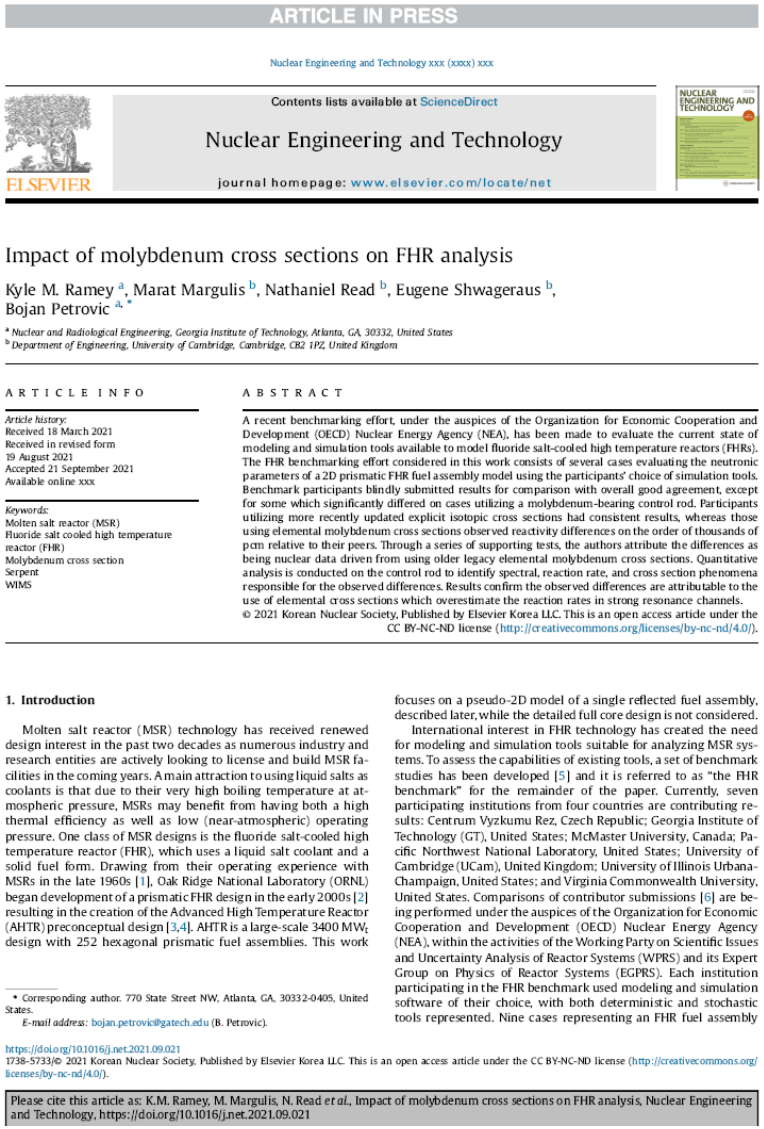
FHR benchmark, Phase I-A
Multiplication factor

CASE	1	2	3	4	5	6	7	Average	σ_k(pcm)
CASE 1	1.39559	1.39530	1.39590	1.39587	1.39333	1.39762	1.39389	1.39536	141
CASE 2H	1.40557	1.40540	1.40561	1.40590	1.40328	1.40650	1.40395	1.40517	114
CASE 2C	1.42065	1.42044	1.42107	1.42084	1.41944	1.42232	1.41891	1.42052	111
CASE 3	1.03205	1.03127	1.03029	1.03251	1.03200	See [10]	1.03147	1.03160	78
CASE 4	1.09886	1.09638	1.09927	1.09922	1.09748	n/a	1.09766	1.09814	116
CASE 4R	0.83969	0.83745	0.83922	0.84045	0.83982	n/a	0.84158	0.83970	137
CASE 5	0.80041	0.80016	0.80032	0.80068	0.80163	0.79975	0.79837	0.80019	99
CASE 6	1.26301	1.26502	1.26324	1.26313	1.26228	n/a	1.26294	1.26327	92
CASE 7	1.50567	1.50496	1.50604	1.50625	1.50493	1.50828	1.50526	1.50591	116
Max 1σ	0.00003	0.00004	0.00015	0.00023	0.00008	n/a	0.00011		78-141

- For all cases the standard deviation is in the range of 78-141 pcm
- Maximum spread in the $\pm$200 pcm range
- Considering the complicated nature of this non-water moderated multiplying system with double heterogeneity, and recognizing that 3 different codes were used employing continuous energy and multigroup data coming from 3 different nuclear libraries, the overall agreement is noteworthy

FHR benchmark, Phase I-A
Multiplication factor

- Generally very good agreement
- One case by one participant excluded
- Traced to difference in Mo XS, separate paper in NET, just published



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Impact of molybdenum cross sections on FHR analysis

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ABSTRACT

A recent benchmarking effort, under the auspices of the Organization for Economic Cooperation and Development (OECD) Nuclear Energy Agency (NEA), has been made to evaluate the current state of modeling and simulation tools available to model fluoride salt-cooled high temperature reactors (FHRs). The FHR benchmarking effort considered in this work consists of several cases evaluating the neutronic parameters of a 2D prismatic FHR fuel assembly model using the participants' choice of simulation tools. Benchmark participants blindly submitted results for comparison with overall good agreement, except for some which significantly differed on cases utilizing a molybdenum-bearing control rod. Participants utilizing more recently updated explicit isotopic cross sections had consistent results, whereas those using elemental molybdenum cross sections observed reactivity differences on the order of thousands of pcm relative to their peers. Through a series of supporting tests, the authors attribute the differences as being nuclear data driven from using older legacy elemental molybdenum cross sections. Quantitative analysis is conducted on the control rod to identify spectral, reaction rate, and cross section phenomena responsible for the observed differences. Results confirm the observed differences are attributable to the use of elemental cross sections which overestimate the reaction rates in strong resonance channels.

1. Introduction

Molten salt reactor (MSR) technology has received renewed design interest in the past two decades as numerous industry and research entities are actively looking to license and build MSR facilities in the coming years. A main attraction to using liquid salts as coolants is that due to their very high boiling temperature at atmospheric pressure, MSRs may benefit from having both a high thermal efficiency as well as low (near-atmospheric) operating pressure. One class of MSR designs is the fluoride salt-cooled high temperature reactor (FHR), which uses a liquid salt coolant and a solid fuel form. Drawing from their operating experience with MSRs in the late 1960s [1], Oak Ridge National Laboratory (ORNL) began development of a prismatic FHR design in the early 2000s [2] resulting in the creation of the Advanced High Temperature Reactor (AHTR) preconceptual design [3,4]. AHTR is a large-scale 3400 MW_t design with 252 hexagonal prismatic fuel assemblies. This work focuses on a pseudo-2D model of a single reflected fuel assembly, described later, while the detailed full core design is not considered.

International interest in FHR technology has created the need for modeling and simulation tools suitable for analyzing MSR systems. To assess the capabilities of existing tools, a set of benchmark studies has been developed [5] and it is referred to as "the FHR benchmark" for the remainder of the paper. Currently, seven participating institutions from four countries are contributing results: Centrum Vyzkumu Rez, Czech Republic; Georgia Institute of Technology (GT), United States; McMaster University, Canada; Pacific Northwest National Laboratory, United States; University of Cambridge (UCam), United Kingdom; University of Illinois Urbana-Champaign, United States; and Virginia Commonwealth University, United States. Comparisons of contributor submissions [6] are being performed under the auspices of the Organization for Economic Cooperation and Development (OECD) Nuclear Energy Agency (NEA), within the activities of the Working Party on Scientific Issues and Uncertainty Analysis of Reactor Systems (WPRS) and its Expert Group on Physics of Reactor Systems (EGPRS). Each institution participating in the FHR benchmark used modeling and simulation software of their choice, with both deterministic and stochastic tools represented. Nine cases representing an FHR fuel assembly

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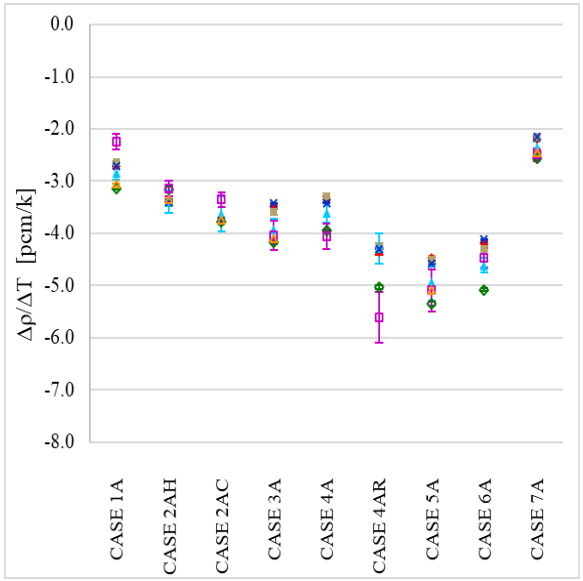
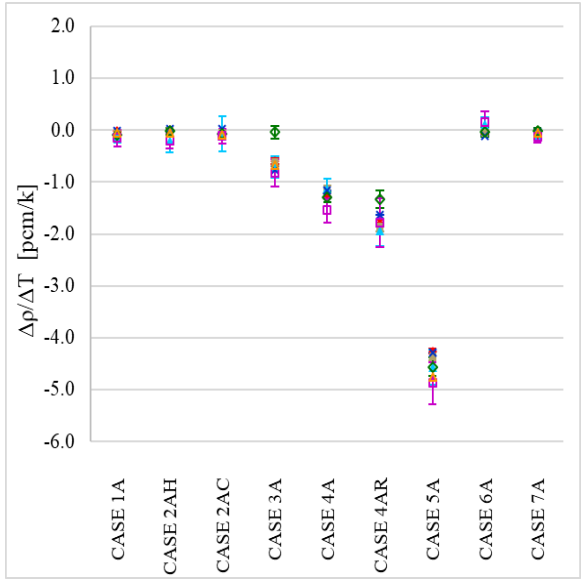
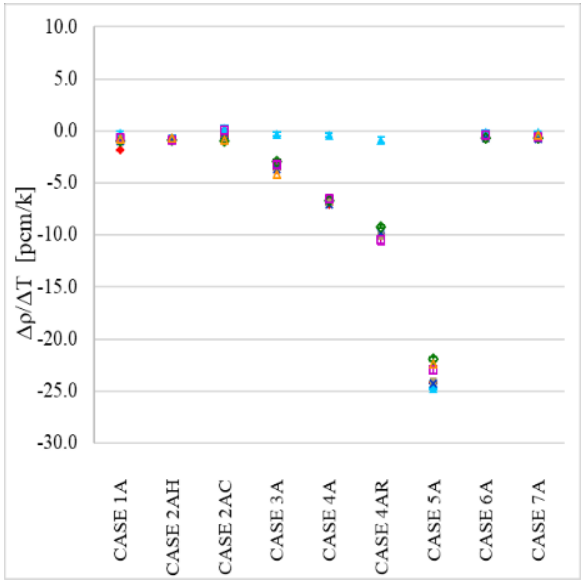
FHR benchmark, Phase I-A
Reactivity Temperature Coefficients

- Separately perturbed the temperature of fuel, coolant (FLiBe) and graphite, by ±50K
- Associated statistical uncertainties were propagated.
- With exception of several isolated points, the results agree fairly well, among themselves and with the expected values.

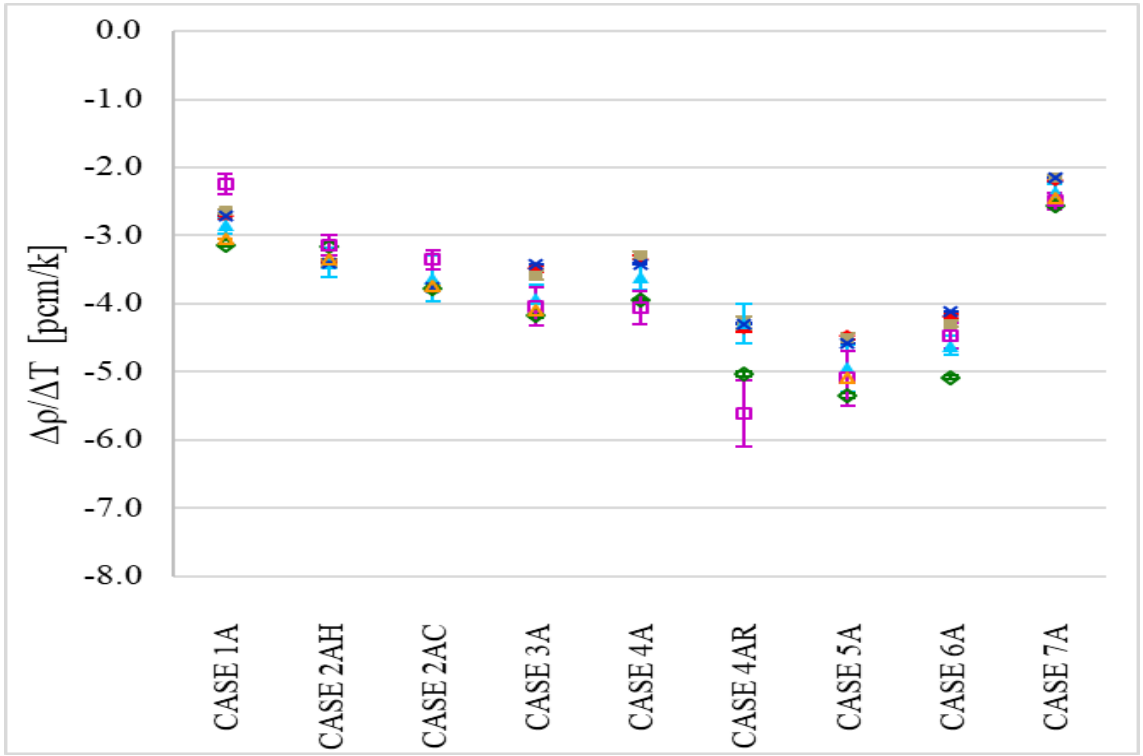






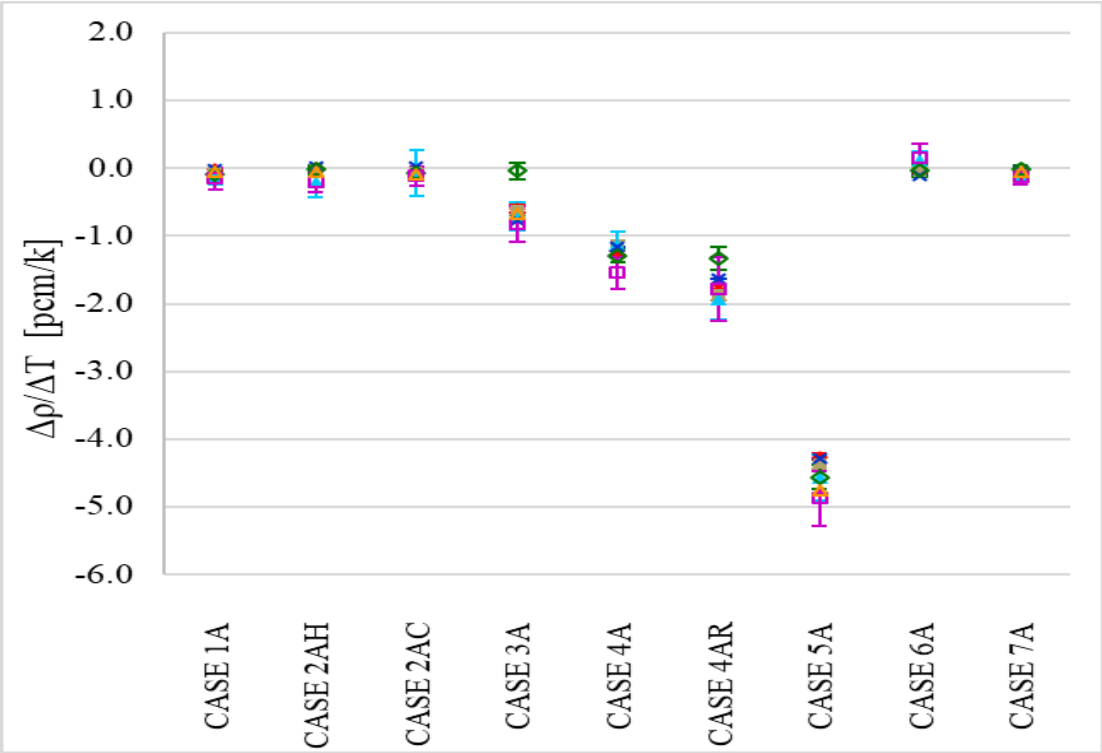
Reactivity Temperature Coefficients: fuel (left), FLiBe coolant (middle), graphite (right)

FHR benchmark, Phase I-A
Reactivity Temperature Coefficient – Fuel



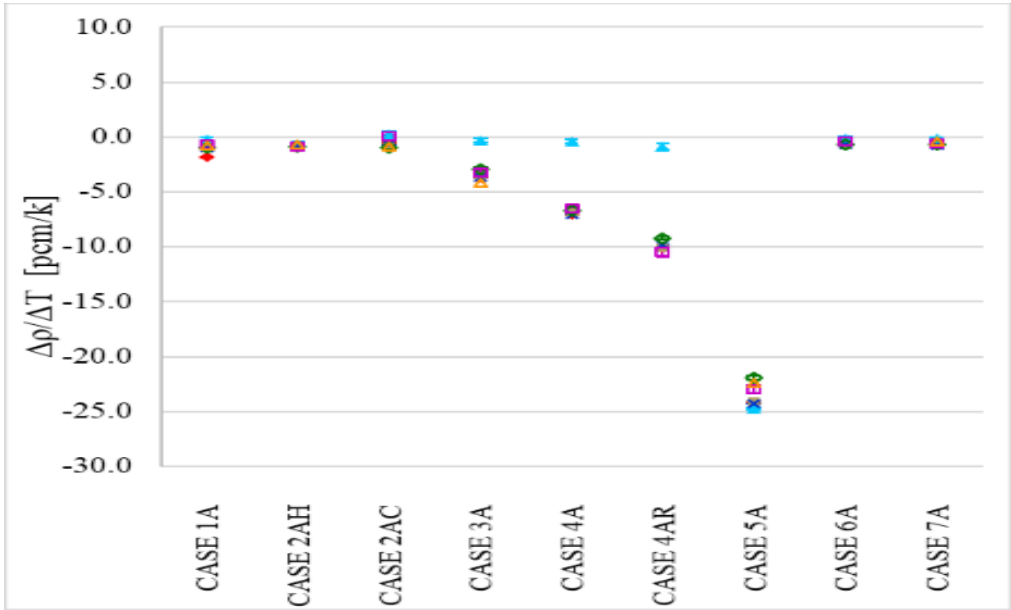
- Values for the reference Case 1A are in the -2.2 to -3.1 pcm/K range, with all values within ±0.5 pcm/K from the average.
- A similar and acceptable spread is observed in all Cases.
- With a significant hardening of spectrum in Cases 4AR (discrete BP and CR inserted), 5A (dispersed BP) and 6A (twice reduced carbon-to-HM ratio), the fuel temperature coefficient becomes more negative.

FHR benchmark, Phase I-A
Reactivity Temperature Coefficient – Coolant (FLiBe)



- For the FLiBe coolant temperature coefficient, previous studies reported values around zero, and similar values are also observed here.
- More negative values are again obtained for Cases 4AR, 5A and 6A, and the spread of values in each case is again approximately ±0.5 pcm/K from the average.

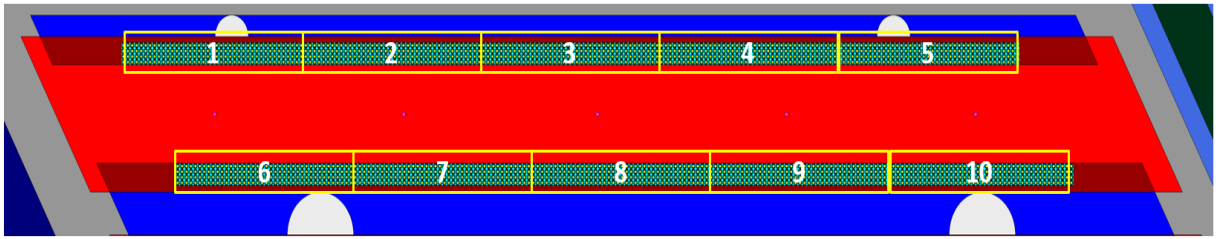
FHR benchmark, Phase I-A
Reactivity Temperature Coefficients – Graphite



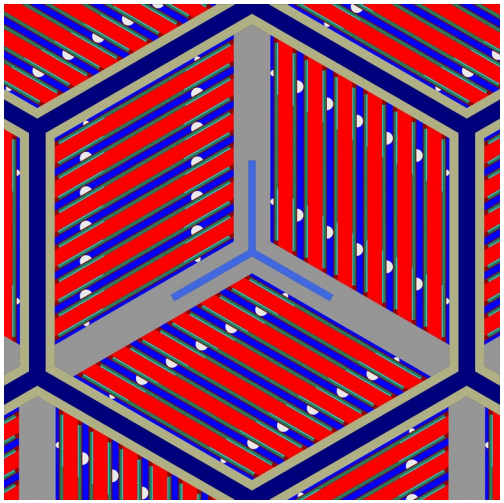
- In most Cases the agreement is good and the spread is similar as for fuel and FLiBe.
- However, several values differ from the rest more than expected; specifically, the blue triangle for Cases 3A, 4A and 4AR.
- These cases will be further examined aiming to identify the source of the differences. Since there are multiple carbonaceous structures (some carbon and some graphite with corresponding S(α,β) matrices) in the complicated geometrical model, the most likely culprit is inconsistencies in the modelling of these regions.

FHR benchmark, Phase I-A
Fission density distribution

- Each fuel stripe with TRISO particles is divided longitudinally into five sections
- There are two fuel stripes per fuel plank, and eighteen fuel planks per fuel element (Fig. 1 and Fig. 3), which defines 180 distinct regions for fuel density distribution. This is a similar granularity to a PWR 17x17 fuel element with 264 fuel pins. Considering the one-third the 120-degree periodic symmetry in FHR and quarter symmetry in PWR, we have almost the same number of regions, 60 vs 64.
- In the ensuing figures, fission density values are plotted against the position index, which in each case goes from 1 to 60 (for each symmetric third of fuel element), even though the actual locations are not linearly arranged.
- Fuel plate 1: Regions 1-10
  Fuel plate 2: Regions 11-20
- Etc.

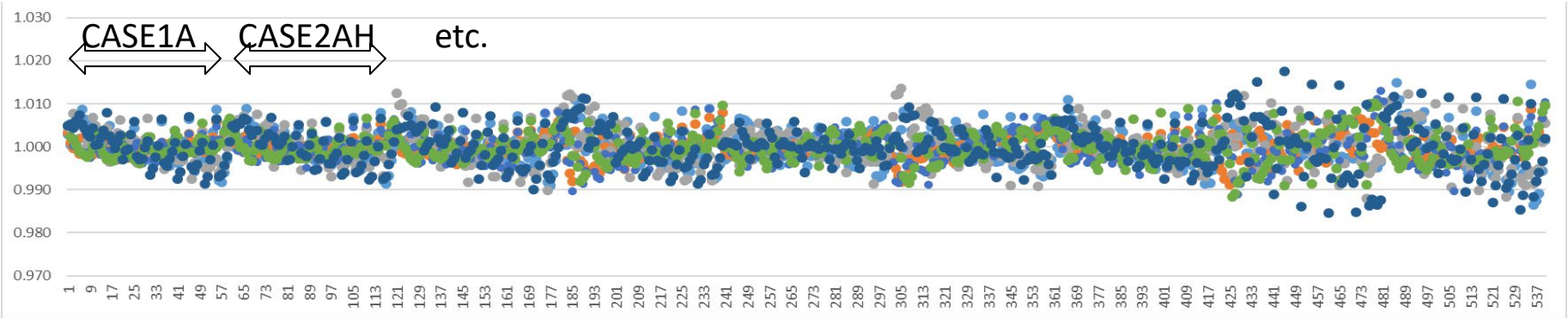


Definition of 10 fission density regions in each fuel plank



FHR benchmark, Phase I-A
Fission density distribution

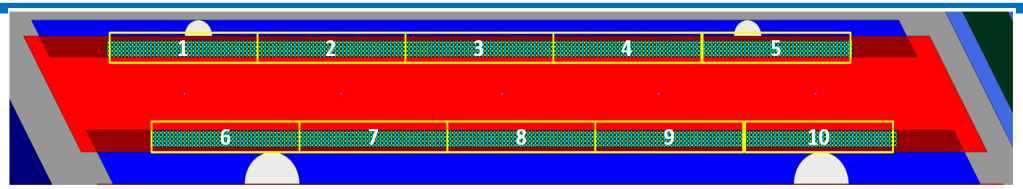
- To enable compact presentation, we combine and present together all 9 cases into a sequence of 540 values (9 times (6x10)). The objective is to visually depict the range of differences rather than to point to specific locations or specific differences.



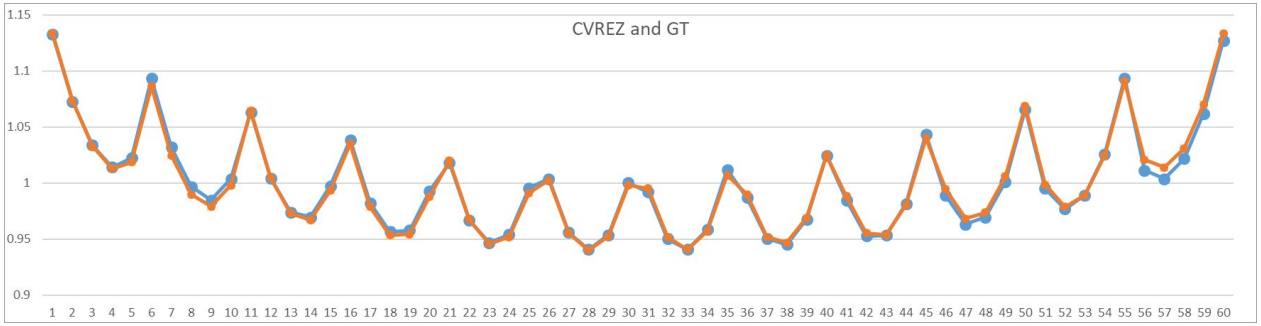
Differences (ratio to average) of each Monte Carlo results against the average

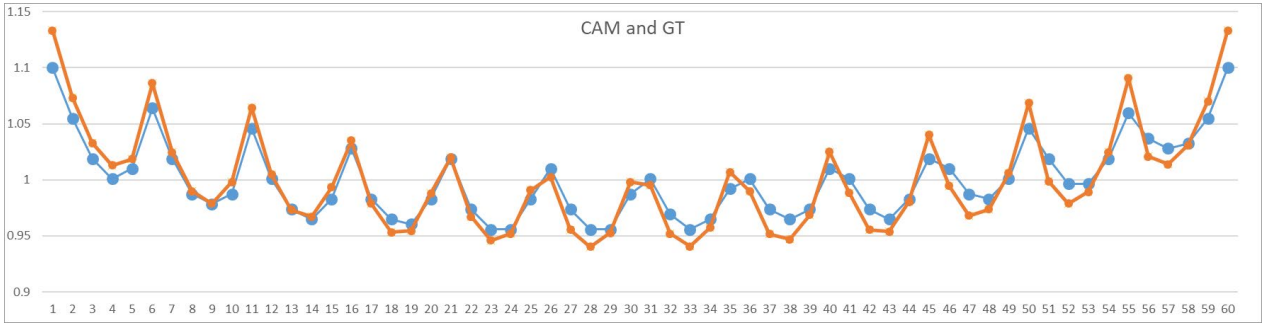
- For the first seven cases (index 1 through 420), the minimum and maximum ratio of all values is 0.990 and 1.013, i.e., practically within ±1%.
- The differences are somewhat higher for the last two cases (Case 6A and 7A), with the minimum and maximum ratio being 0.985 and 1.018, but the large majority is still within ±1%, and all are well within ±2%, quite impressive overall agreement.
- The associated statistical uncertainties on Monte Carlo simulations range—depending on the participant—from 0.0003 to 0.002 (i.e., 0.03% to 0.2%).
- Fission density distribution obtained by deterministic calculations exhibits slightly higher differences, but the minimum and maximum difference to the average remains within ±3% for all cases analyzed (five out of nine defined Cases). This agreement is at least as impressive considering all the differences between continuous-energy Monte Carlo simulations and a multigroup deterministic calculation.

FHR benchmark, Phase I-A
Fission density distribution

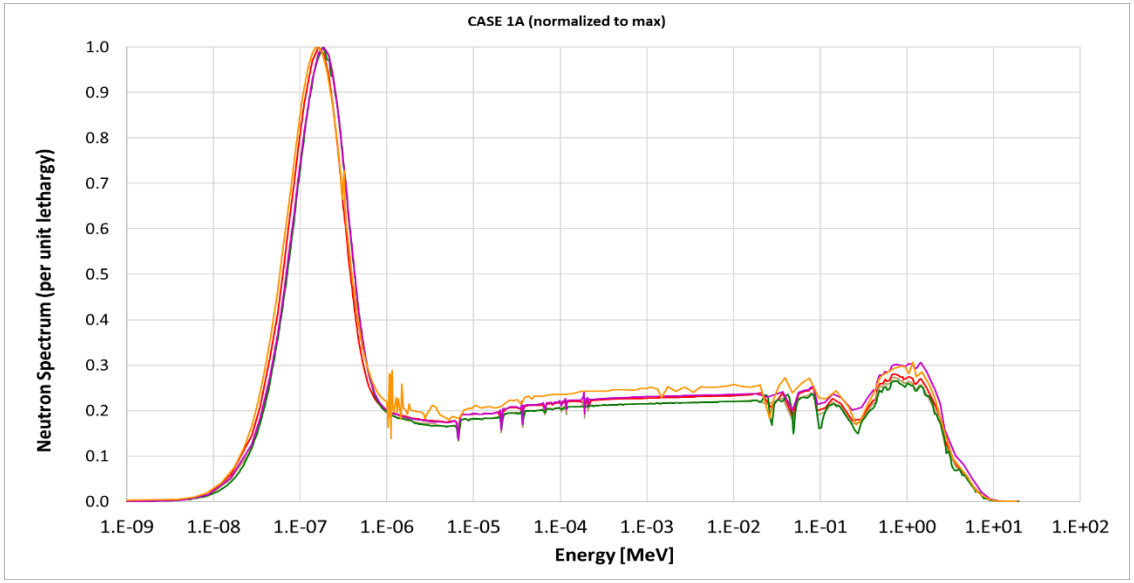


Representative detailed comparisons
For a single case, results (5 points each) for 12 fuel stripes “stitched” together





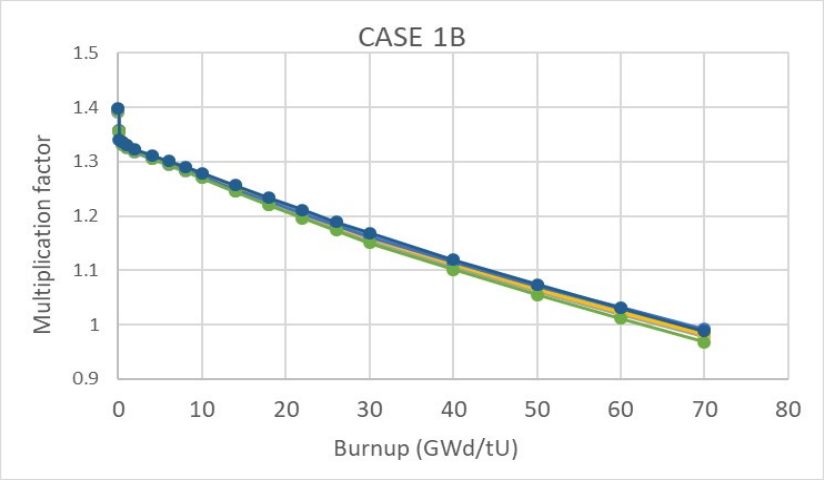
FHR benchmark, Phase I-A
Neutron Spectra (per lethargy)



Comparison of normalized neutron spectra for Case 1A

- Benchmark specifications requested multigroup fluxes, preferably in the SCALE 252-group structure; used in all MC codes
- For deterministic calculations, the multigroup library itself dictated the energy structure.
- Normalized to the maximum value in each case.
- Statistical error bars are not show since they would been indiscernible.
- A good agreement is observed with spectral features corresponding to the materials present in the problem definition.
- Small blips are artifact of processing the results
- Similar agreement is observed in other Cases.

FHR benchmark, Phase I-B
Depletion



Comparison of multiplication factor vs. burnup for Case 1B

- Cases 1B and 4B were depleted to 70 GWd/tU; Case 7B with higher enriched fuel to 160 GWd/tU.
- Compared criticality, fission distribution, flux distribution, and neutron spectrum at selected burnups.
- Due to the space limitations, only the comparison of multiplication factors is presented here.
- Statistical uncertainty, not shown in the Figure, was less than 50 pcm in all cases.
- The agreement is generally good; however, there is a slight divergence with burnup. Main suspects for this divergence are the recoverable energy per fission and possibly different models available in different codes (e.g., depletion with and without critical spectrum). This will be further examined.

FHR benchmark, Phase I-A
Next Steps

Phase I – Fuel assembly (2D/3D with depletion)

- Phase I-A – "2D" (pseudo-2D) model, steady state (no depletion)
- Phase I-B – 2D model depletion

Completed

Next, soon/brief

- Phase I-C – 3D radially reflected but axially finite fuel assembly model depletion
  Much reduced amount of results. Objective to confirm impact of axial leakage/power

Next

Phase II – 3D full core with depletion

- Phase II-A – Steady-state (no depletion)
- Phase II-B – Depletion

Next

Phase III – 3D full core with feedback and multicycle analysis

- Phase III-A – Full core depletion with feedback
- Phase III-B – Multicycle analysis

FHR benchmark, Phase I-A
Conclusions

- There is commercial interest in developing and deploying MSRs, including FHRs, but applicable reactor physics experiments that may be used for validation of codes are scarce
- Under auspices of OECD NEA, a numerical benchmark has been established to enable cross-verification of reactor physics codes considered for simulation of FHRs
- 7 participating organizations from 4 countries
- Phase I-A & IB completed (single reflected hexagonal fuel element). Extension to full 3D core analysis with depletion (Phase II) and feedback (Phase III) is foreseen.
- Very good agreement in most cases, in particular considering that FHR fuel elements include a challenging complex geometry and double heterogeneity.
- Larger differences initially observed in a limited number of cases were in most cases traced to ambiguous specifications and inconsistent assumptions
- Valuable cross-verification opportunity to commercial efforts aimed at designing and licensing FHRs; it also provides a challenging problem that may be used to test the capabilities of modern reactor physics codes and validity of modeling methodologies.
- This benchmark will allow the community to assess the impact of new models and nuclear data libraries on FHR systems, for a variety of neutronics parameters.
- **There are many benchmarks for low (<5%) and high (>90%) enrichments, and for well thermalized and fast systems. FHR is a thermal/epithermal system, using HALEU (9%-20% enrichment) and thus can contribute to expand the database of cross-verifications**

FHR benchmark, Phase I-A

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Thank you for your attention!

Questions