Fluoride-salt High-temperature Reactor (FHR) NEA Benchmark Phase I-C: Results and Lessons Learned

Bojan Petrovic[1,*], Jonathon Faulkner[1], Kyle Ramey[2], Zeyun Wu[3], Mohamed Elhareef[3], Cihang Lu[4], Evzen Losa[5], Pauline Benchetrit[5], Kathryn Huff[6], Luke Seifert[6], Oleksander Yardas[6], Gwendolyn Chee[6], Javier Gonzalez[7], David Novog[7], Davor Grgić[8], Radomir Ječmenica[8], Madicken Munk[9]

[1]Georgia Institute of Technology, Atlanta, GA, USA
[2] Argonne National Laboratory, Lemont, IL, USA
[3]Virginia Commonwealth University, Richmond, VA, USA
[4]Brookhaven National Laboratory, Upton, NY, USA
[5]Research Centre Rez, Husinec-Řež, Czech Republic
[6]University of Illinois at Urbana-Champaign, Champaign, IL, USA
[7]McMaster University, Hamilton, ON, Canada
[8]University of Zagreb, Zagreb, Croatia
[9]Oregon State University, Corvallis, OR, USA

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ABSTRACT

This paper summarizes progress and status of the multi-phase Benchmark modelling Fluoride salt High Temperature Reactor (FHR) under the auspices of OECD NEA. Phase I-A and I-B (a “pseudo 2D” slice of infinite lattice of fuel assemblies) had been successfully completed and previously reported. Phase I-C extrudes the model axially to include five regions of finite heights of active fuel, top and bottom fuel element structure, and top and bottom axial reflector, together with vacuum boundary conditions at the top and bottom. Specifications defining the “extruded” geometry, benchmark exercises, and required results are summarized. The exercises included static (no depletion) and depletion cases under various conditions. Nine participating organizations from four countries have participated in exercises and provided their results. This paper summarizes the results, issues identified, resulting modifications to the specifications, and lessons learned from Phase I-C efforts. It contrasts results of the infinite and finite assembly height to elucidate impact of the axial leakage and axial structures/reflector beyond the active core region. Moreover, it points to modeling and simulations challenges for large loosely coupled systems. Finally, lessons learned from Phase I-C have been used to improve definition of the Phase II (full 3D model) specifications.

Keywords: NEA Benchmark, Phase I-C. Fluoride-salt High-temperature Reactor (FHR)

1. INTRODUCTION

1.1. NEA FHR benchmark

The Fluoride salt High Temperature Reactor (FHR) benchmark problem [1] is an OECD-NEA benchmark representing a FLiBe cooled and graphite moderated FHR with a plank type fuel design. It is based on ORNL Advanced High Temperature Reactor (AHTR) [2,3]. TRISO fuel particles embedded in graphite fuel plates present a double heterogeneity; the complex fuel geometry (Fig. 1) makes the modelling even more challenging [4]. These challenging features, however, make it an attractive benchmark problem, as demonstrated by participation of multiple institutions in the benchmark activities.

* bojan.petrovic@gatech.edu

1.2. NEA FHR benchmark, Phase I-A and I-B

Phases I-A (no depletion) and Phase I-B (with depletion) of the NEA FHR benchmark model an infinite array of FHR fuel assemblies by considering a single assembly with periodic radial boundary conditions (Figure 1, left). A fuel assembly slice ("pseudo 2D") with top/bottom reflective boundary conditions represents infinitely tall reactor. A number of Cases (zero and full power, with and without control rods, with and without burnable absorbers) is defined. A detailed description is provided in [1].

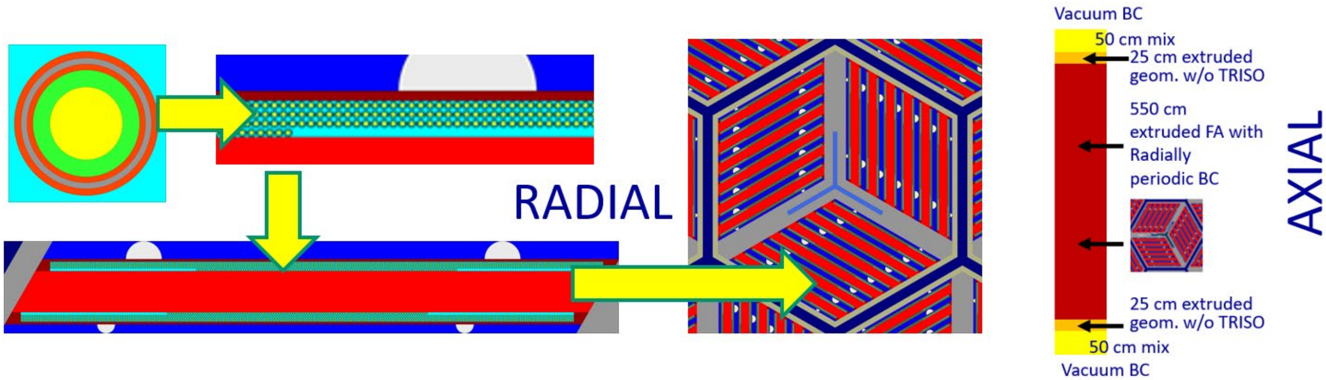

Figure 1. FHR assembly: (a) Left: 2D radial sections depicting double heterogeneity and geometric complexity; (b) Right: axial five-region assembly configuration

1.3. Phase I-C specifications

In Phase I-C [5], fuel assembly geometry is extruded to form a 700 cm tall single-assembly model with top and bottom vacuum boundary conditions, thus accounting for the axial leakage effects. The model (Fig. 1, right) axially consists of five regions:

- Central 550 cm tall active core region (geometry as in Figure 1, left).
- Two regions, 25 cm tall each, extending the fuel assembly geometry structure identical to that of the central region, but without TRISO particles in graphite plates.
- Top and bottom reflector region, 50 cm tall each, assumed to consist of 50%-50% volumetric mix of salt and graphite.

Radial boundary conditions remain periodic, reflecting the 120-degree symmetry of fuel elements.

Six exercises are defined, three without and three with depletion, as follows.

No Depletion Exercises:

- EX-1: Axially symmetric core with uniform temperature
- EX-2: Replica runs of EX-1
- EX-3: EX-1 with stepwise CR insertion

Depletion Exercises, up to a burnup of 70 GWd/MTHM

- EX-4: EX-1 depletion with single axial fuel zone
- EX-5: Modified EX-4 with axial temperature and fission density rate and depletion in 16 fuel zones
- EX-6: Modified EX-5 with discrete Eu poison

Requested quantities and uncertainties include:

- Multiplication factor (k-eff or k), together with uncertainty in pcm
- Axial fission density rate distribution, together with absolute and relative uncertainty

- Axial 3-group flux distribution, together with absolute and relative uncertainty
- Axial offset (optional), together with propagated absolute and relative uncertainty
- Nubar ($\bar{\nu}$), together with absolute uncertainty
- Recoverable energy per fission (Er) used to deplete fuel
- Isotopics (together with uncertainty, if available or otherwise estimated).

1.4. Summary of results presented/published so far

Preliminary results of Phase I-A and I-B were presented in [6] followed by a detailed NEA report with all I-A and I-B results [7]. A variety of related “branch” studies are documented in [8-16]. Of particular interest is the study examining impact of recoverable energy (Er) on depletion analysis [13], and the study analyzing axial xenon-induced oscillations [15].

1.5. Benchmark participants

Results from eight participants from four countries are presented in this paper. Table I lists the participants together with the modelling and simulation (M&S) method, and code(s) [17-19] and library(ies) used. University of Cambridge participated in Phase I-A and I-B, but (for the time being) not in I-C. CIEMAT (Spain) recently joined this Benchmarking effort and generated Phase I-C results, but their results have not yet been incorporated.

Table I. Benchmark participants overview.

ID	Organization	Method	Code	Library	Energy structure
GT	Georgia Institute of Technology, USA	MC	SCALE6.2.4 SCALE6.3.1	ENDF/B-VII.1	CE, MG
ANL	Argonne National Laboratory, USA	MC	Serpent 2.x	ENDF/B-VII.1	CE
BNL	Brookhaven National Laboratory, USA	MC	Serpent 2.x	ENDF/B-VII.1 VII.1, VIII.0	CE
CVREZ	Research Centre Rez, Czech Republic	MC	Serpent 2.x	ENDF/B-VII.0	CE
FER	University of Zagreb, Croatia	MC	SCALE6.2.4 Serpent 2.x	ENDF/B-VI.8, VII.1	CE
MAC	McMaster University, Canada	MC	OpenMC	ENDF/B-VII.1	CE
UIUC	University of Illinois, USA	MC	OpenMC	ENDF/B-VII.1	CE
VCU	Virginia Commonwealth University, USA	MC	Serpent 2.x	ENDF/B-VII.0	CE

Selection of the nuclear data library is left to each participant. Most results presented in this paper have been generated using ENDF/B-VII.1 data. However, results obtained using ENDF/B-VI.8 ENDF/B-VII.0, ENDF/B-VII.1, ENDF/B-VIII.0 are also available. Propagation of nuclear data uncertainties into results is not planned as a mandatory benchmark requirement for each participant, but a separate branch-study is foreseen instead.

2. RESULTS AND ANALYSIS

2.1. Multiplication factor

Multiplication factors in each of the exercises are the first comparisons made between participants. Presented in Table II are multiplication factors for the static (no depletion) cases. All multiplication factors for each static exercise are within 250 pcm of the average for that exercise. This agreement, considering past FHR benchmark experience, is acceptable since most results for simpler 2D cases without depletion were within 200 pcm of the average result [7]. Figure 2 shows multiplication factors during depletion as well as the difference between each participant and the "reference" result. Results of one arbitrarily selected participant were chosen to serve as the reference not because of accuracy or precision with the "true" solution but instead to avoid using the average value which might include large outliers and skew the interpretation of the results. Comparing multiplication factors during depletion, most results were within 500 pcm of the reference result – which is significantly higher than multiplication factor differences during static cases. This difference is likely due to a variety of factors including recoverable energy per fission used in each code (in particular when a difference monotonically diverges with increasing burnup), cross section libraries, or discrepancies in depletion schemes used by each participant [13].

Table III. Multiplication factors for static exericses.

	Exercise 1	Ex. 3 – 25%	Ex. 3 – 50%	Ex. 3 – 75%	Ex. 3 – 100%
Participant 1	1.37840 ± 7e-5	1.36867 ± 8e-5	1.34797 ± 9e-5	1.27959 ± 9e-5	1.02203 ± 9e-5
Participant 2	1.37965 ± 9e-5	1.37000 ± 9e-5	1.34931 ± 9e-5	1.28103 ± 9e-5	1.02397 ± 9e-5
Participant 3	1.38164 ± 1e-5	1.37200 ± 1e-5	1.35128 ± 1-5	1.28292 ± 1e-5	1.02243 ± 2e-5
Participant 4	1.38205 ± 11e-5	1.37240 ± 11e-5	1.35164 ± 11e-5	1.28304 ± 10e-5	1.02380 ± 10e-5
Participant 5	1.37912 ± 4e-5	1.36957 ± 4e-5	1.34884 ± 4e-5	1.28036 ± 4e-5	1.02245 ± 4e-5
Participant 6	1.38024 ± 11e-5	1.37082 ± 11-e5	1.34985 ± 10e-5	1.28142 ± 11e-5	1.02272 ± 11e-5
Participant 7	1.37927 ± 7e-5	1.36959 ± 8e-5	1.34851 ± 9e-5	1.28032 ± 10e-5	1.02348 ± 12e-5
Participant 8	1.37901 ± 5e-5	1.36958 ± 5e-5	1.34866 ± 5e-5	1.27978 ± 6e-5	1.02320 ± 8e-5

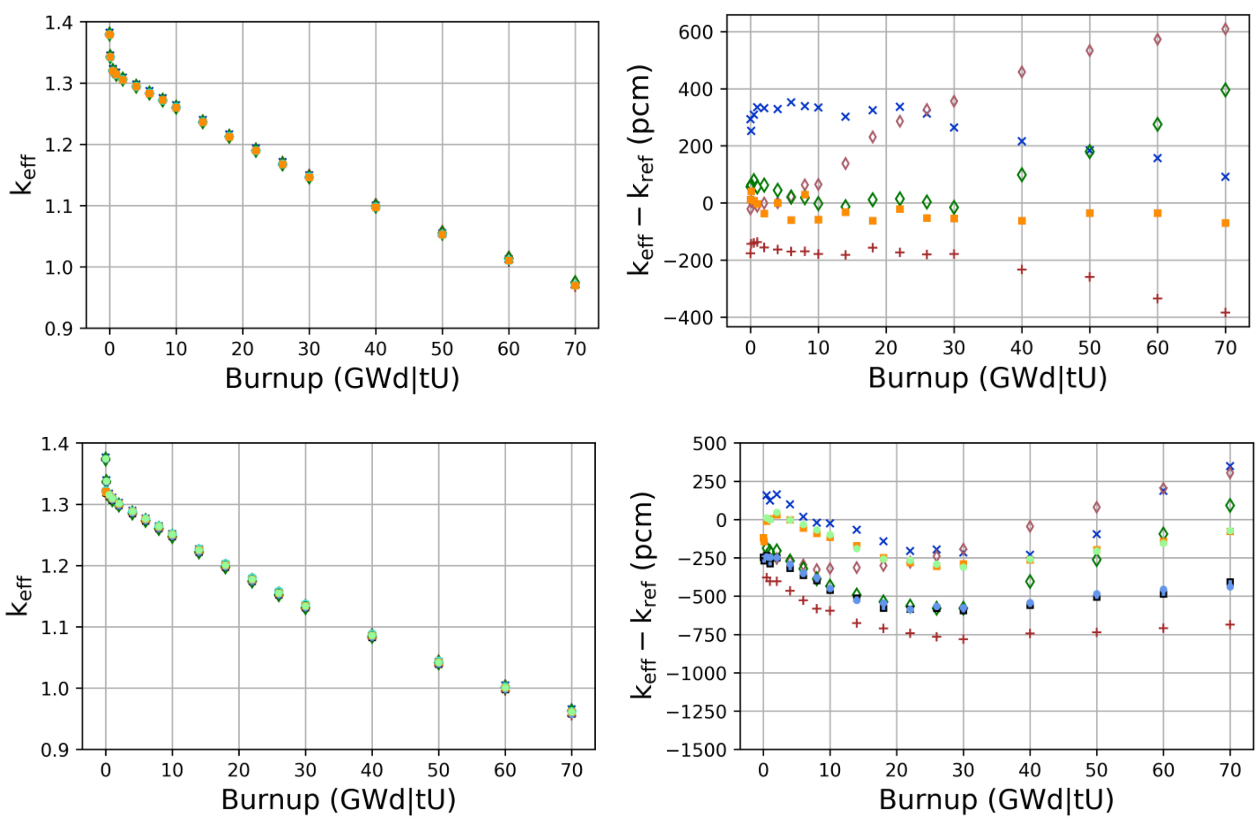

Figure 2. Multiplication factors (left) and multiplication factor differences (right) during depletion in Exercise 4 (top) and Exercise 5 (bottom). Differences shown use one of the participant's results as the reference value.

2.2. Controlled assembly axial fission density

Exercise 3 considered stepwise insertion of the control element into the assembly's active fuel region. In addition to multiplication factors, participants reported normalized spatial fission density distributions for insertions of 25%, 50%, 75%, and 100%. Results are shown in Figure 3; generally, agreement between participants is excellent and there are very few outliers.

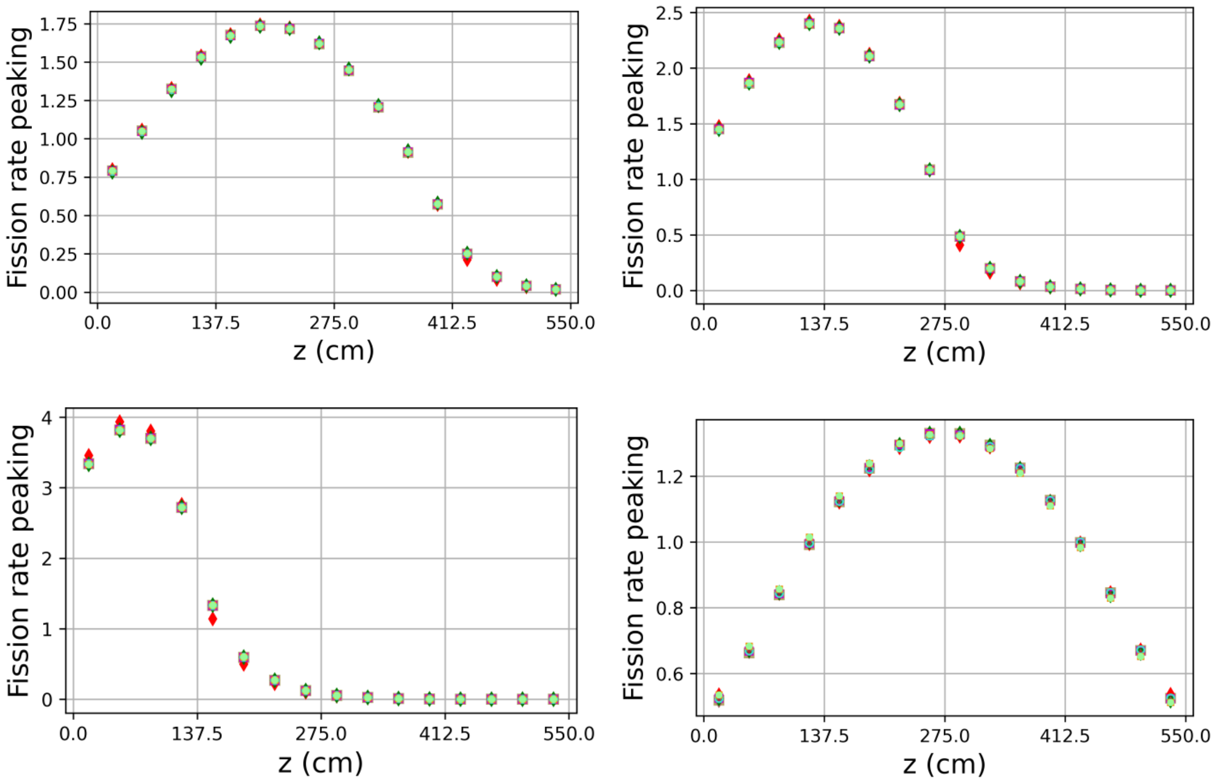

Figure 3. Fission densities during 25% (top left), 50% (top right), 75% (bottom left) and 100% (bottom right) control rod insertion in Exercise 3. Each result is normalized to the fission density averaged over 16 fuel zones.

2.3. Fuel depletion and isotopic evolution

Nuclide number densities after depletion for Exercises 4 and 5 were also analyzed. Absolute values of relative differences compared to results of one arbitrarily selected participant (selected for this exercise as the "reference") at end of life burnup (70 GWd/tU) for various nuclides are shown in Figure 4 (Exercise 4) and Figure 5 (Exercise 5). For Exercise 4, most relative differences are less than 1% of the reference result with the exception of ^{110m}Ag, ^{149}Sm, and ^{151}Sm. For Samarium isotopes, most results are relatively close and it is actually the reference result that is in disagreement with other participants. For Exercise 5, relative differences are generally higher. For example, even the ^{235}U relative differences are higher than 1% for a number of participants while many results for Plutonium isotopes are greater than even 5%. For Exercise 5, Samarium results are in reasonable agreement among most participants and it is again the chosen reference result that is in disagreement.

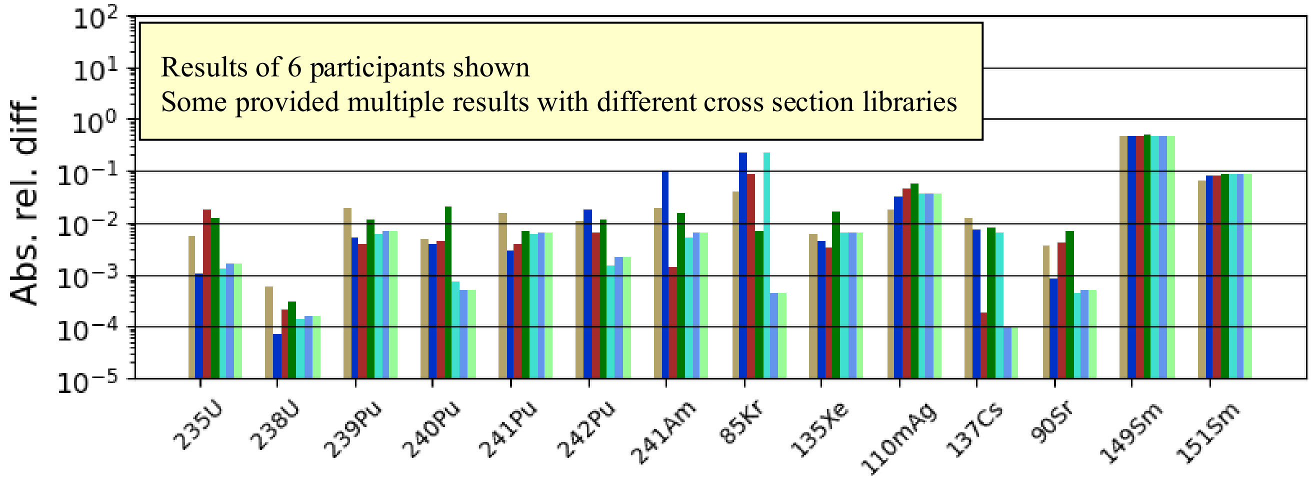

Figure 4. Absolute relative difference for select isotopes at EOL (70 GWd/tU) for single zone depletion in Exericse 4. Results of one arbitrarily selected participant are taken as the reference values.

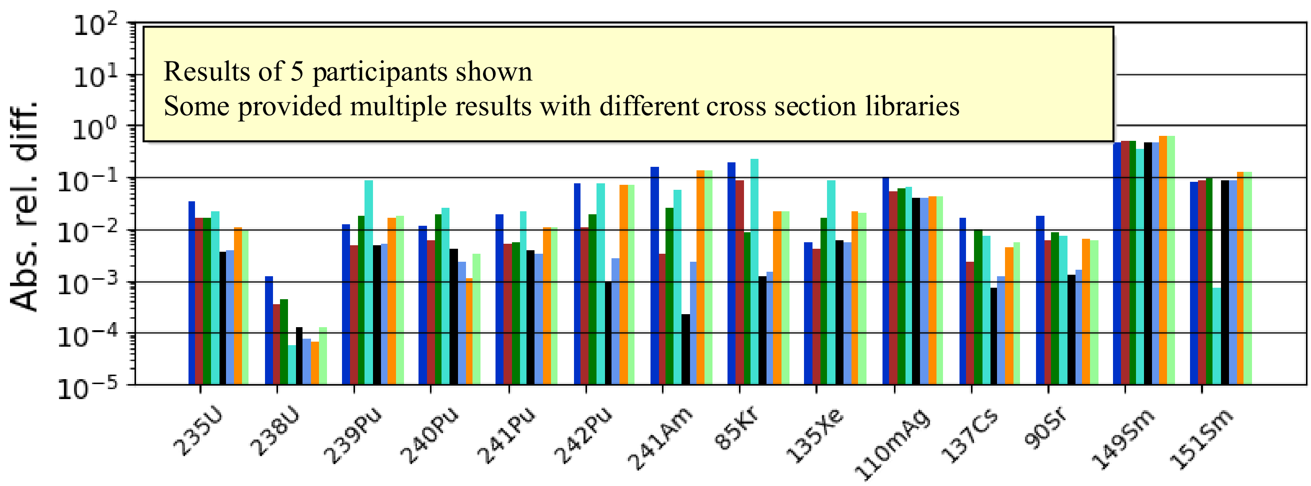

Figure 5. Absolute relative difference for select isotopes at EOL (70 GWd/tU) for multizone depletion in Exercise 5. Isotope number densities are averaged across all depletion zones Results of one arbitrarily selected participant are taken as the reference values.

2.4. Axial offset and resulting modifications to I-C specifications

During examination of the initial depletion results from Exercise 5, it was found that unphysical xenon oscillations occurred during depletion for a number of participants. These oscillations typically occur in Monte Carlo simulations due to statistical uncertainties in the power density of problems with relatively high dominance ratios. The axial offset for the initial depletion results of Exercise 5 as reported by participants is shown in Figure 6. It is observed that results from several participants are affected by these oscillations as the axial offset is seen to oscillate between positive and negative value at every depletion step, and in some cases the magnitude is amplified with depletion. For some participants, the oscillation between positive and negative axial offset can be obfuscated by the choice of predictor-corrector scheme and is instead seen to be only positive or only negative. Larger oscillations were observed, as expected, in runs performed with fewer histories. Finally, it is interesting to note that the large axial offsets do not necessarily imply a large disagreement in eigenvalue results. For example, the axial offset reported by one participant was as large as 10% at the final depletion step while the eigenvalue difference at the same step had a discrepancy of less than 250 pcm with the reference result. This can make interpretation of results from various participants difficult as the problem eigenvalue is often the first (and simplest) indicator of agreement or disagreement. Informed by these issues in early results, improved repeat simulations produced significantly more consistent results.

Unphysical xenon oscillations for the FHR single assembly problem have been examined in [15]; they can be resolved by increasing the fidelity of the simulation through adding more depletion steps and/or by simulating more particles. As a result of the reported oscillations and to keep the problem tractable, future specifications for the FHR benchmark include shortening the active fuel height from 550 cm to 400 cm. This still allows for a very similar problem to the originally envisioned benchmark while also reducing the severity of the xenon oscillations during depletion in both the single assembly calculations and future full core calculations.

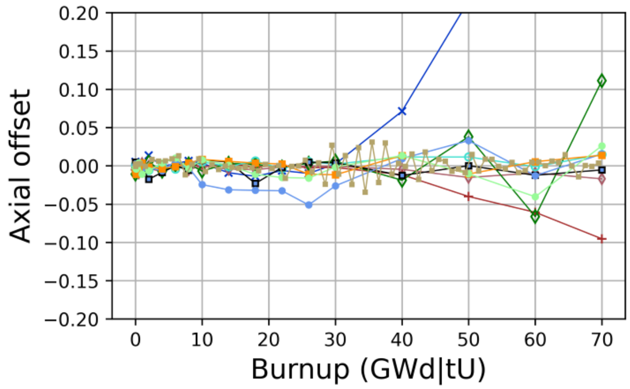

Figure 6. Illustrative axial offset oscillations in initial results during burnup for Exercise 5.

3. CONCLUSIONS AND LESSONS LEARNED

Phase I-C of the OECD-NEA Fluoride-salt High-temperature Reactor benchmark exercise was performed among participants using various Monte Carlo codes; both static cases and cases with depletion were analyzed. Static cases revealed generally good agreement – with most multiplication factor results being within 250 pcm of the average and nearly all fission density results having excellent agreement amongst participants. While relatively large, this range in eigenvalue discrepancy is similar to that observed in previous benchmark phases. Eigenvalue discrepancy observed in depletion cases was larger but typically within the range of 500 pcm of the reference value chosen.

Examination of axial power density distribution during the depletion benchmark exercises revealed large xenon and power oscillations triggered by statistical uncertainties. To keep the problem tractable, future benchmark specifications will use a shortened assembly with an active fuel height reduced from 550 cm to 400 cm. Previous benchmark findings [13] also identified significant discrepancies between codes amplified with depletion, due primarily to the recoverable energy per fission values used during depletion. Specifications will continue to include recommendations on how to handle or set recoverable energy per fission values in the various Monte Carlo and deterministic codes used by participants.

Future work will examine a shortened version of the FHR single assembly problem. The next benchmark Phases II-A and II-B will include a full core description without thermal hydraulic feedback, followed by coupled simulations with thermal hydraulic feedback.

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