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BENCHMARKING OF COBAYA3 PIN-BY-PIN FOR VVER

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ABSTRACT

This paper presents results of the benchmarking of COBAYA3 pin-by-pin for VVER-1000 obtained in the frame of the EU NURISP project. The 3D lattice solver in COBAYA3 uses transport corrected multi-group diffusion approximation with side-dependent interface discontinuity factors of GET or Selengut Black Box type. The objective of this study is to test the few-group calculation scheme when using structured and unstructured spatial meshes. Unstructured mesh is necessary to model the water gaps between the hexagonal assemblies. The benchmark problems include pin-by-pin calculations of 2D subsets of the core and comparison with APOLLO2 and TRIPOLI4 transport reference solutions. COBAYA3 solutions in 2, 4 and 8 energy groups have been tested. The results show excellent agreement with the reference ones when using side-dependent interface discontinuity factors.

1. INTRODUCTION

COBAYA3 [1]-[7] is a 3D core simulator code for Cartesian and hexagonal geometry, developed by UPM. It includes a nodal solver based on the ACMFD method [1], [5] and a pin-by-pin solver using the fine-mesh finite-difference (FMFD) method. [2], [3], [7]. The current pin-by-pin version [2], [7] solves the time-dependent multi-group diffusion equation corrected by interface discontinuity factors. A nodal acceleration can be used to speed up the full core pin-by-pin solution process.

In the frame of the EU NURESIM [8] and NURISP [9] projects, it has evolved to include capabilities of using multi-parameter cross-section (XS) libraries and interface discontinuity factors (IDF) in table-interpolation and functional-fitting format. The code has been coupled with core thermal-hydraulics [3], [4], [5], [6] for reactor safety analysis. Neighborhood-dependent IDF [10] of GET [11] and Selengut Black Box homogenization (BBH) [12] type can be applied. Parallelized coupled pin-by-pin calculations [3], [4], [6] using alternate dissections have been implemented in Cartesian geometry.

The numerical validation base at the pin level includes a series of computational benchmarks for PWR [13], [14], [15], VVER [16] and BWR [17]. This work presents COBAYA3 calculations of the NURISP VVER lattice benchmark [16] performed by INRNE and UPM. The aim is to test the pin-by-pin solver for homogenized cells in structured and unstructured meshes. A specific objective is to test the APOLLO2.8 [18] generated pin-by-pin XS and IDF, and to assess the impact of the number of broad energy groups.

In this paper, the benchmark problems are described in Section 2. The utilized pin-by-pin XS calculation schemes [16] are based on the Method of Characteristics (MOC) in APOLLO2 and are summarized in Section 3. Results and conclusions are given in Sections 4 and 5 respectively.

2. TEST PROBLEMS

The considered geometries are 2D subsets of a VVER-1000 core (19-pin clusters, fuel assembly and assembly cluster), as illustrated in Figures 1 and 2.

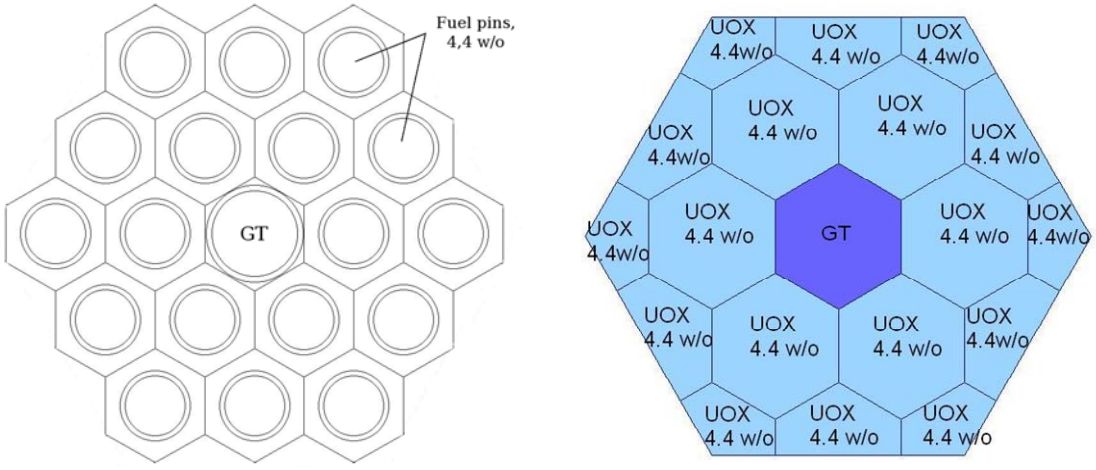


Figure 1: UOX-GT 19-pin cluster

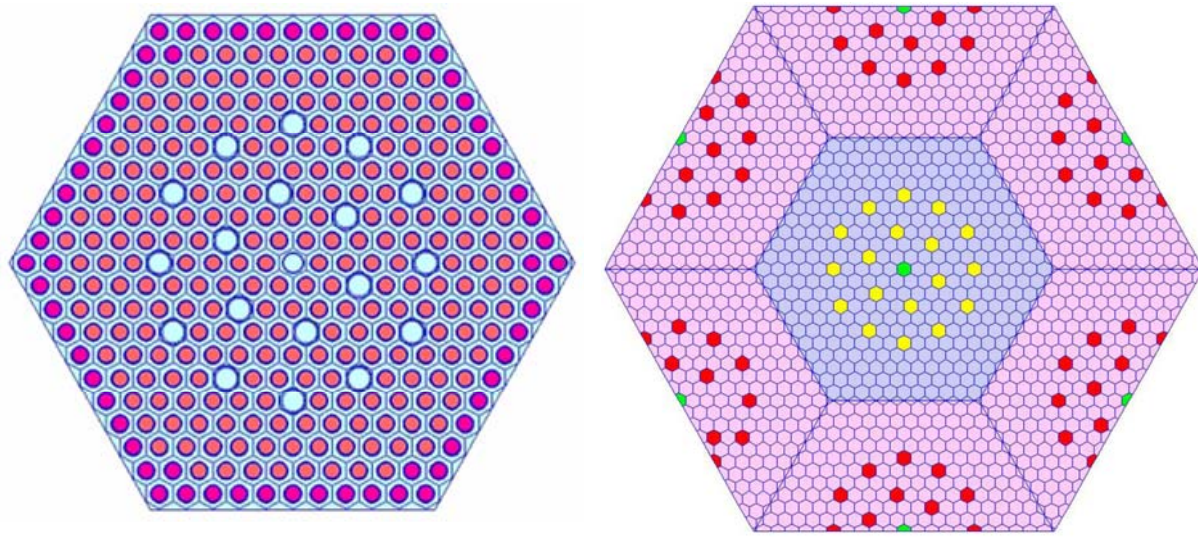


Figure 2:

a) UOX assembly of 4.23 w/o av. enrichment (246 pins of 4.4w/o and 66 pins of 3.6w/o)
b) 7-assembly UOX-CR /UOX-GT cluster of 4.23w/o with UOX-CR in the center

The NURISP VVER lattice benchmark [16] includes test problems for core simulators in structured and unstructured meshes. The structured mesh cases are 19-pin clusters as used for branch calculations with APOLLO2 to generate multi-parameter pin-by-pin libraries of neighborhood-dependent XS and IDF. The unstructured mesh problems consist of fuel assemblies and assembly clusters with inter-assembly water gaps.

In this study, results for the following test cases are considered:

- 19-pin clusters
  - UOX-GT: guide tube surrounded by two rings of UOX pins (Figure 1)
  - UOX-CT: central tube surrounded by UOX pins
  - UOX-CR: control rod surrounded by UOX pins
- Fuel assemblies
  - UOX-GT: uncontrolled assembly
  - UOX-CR: controlled assembly
- 7-assembly cluster of a central UOX-CR assembly and 6 peripheral UOX-GT assemblies (forming a color set as shown in Figure 2).

The 19-pin clusters are to be calculated for fixed state parameters:
39.8MWd/kgHM, HZP at 574.15K, D_m=740kg/m^3, C_b =53ppm.

The UOX-CR assembly is to be calculated for five states listed in Table 1, as usually done for calculation of the reactivity effects.

Table 1: Assembly thermal-hydraulic states to be calculated

Conditions	Moderator		Fuel		Cladding		C_B ppm
	Temp,K	Density g/cm3	Temp, K	Density g/cm3	Temp, K	Density g/cm3	
S1: HZP state (ref)	552	0.76665	552	Ref	552	ref	600
S2: Fuel Doppler react	552	0.76665	924	Ref	552	ref	600
S3: Coolant reactivity	574	0.72527	552	Ref	552	ref	600
S4: 100% void	624	0.09610	552	Ref	552	ref	600
S5: Boron reactivity	552	0.76665	552	Ref	552	ref	0

The 7-assembly cluster is of fresh fuel and is to be calculated for fixed state parameters:
HZP at 574.15K, D_m=740 kg/m^3 and C_b =53ppm.

The task is to calculate the multiplication factor and the pin-by-pin fission reaction rates in comparison with transport reference solutions:

- APOLLO2 MOC 281g /JEFF3.1.1 solutions [16] validated against TRIPOLI4 results
- Well converged TRIPOLI4 /JEFF3.1.1 solutions [16] with σ (k) = ± 10-14 pcm

TRIPOLI4 [19] is a 3D Monte Carlo code, trademark of CEA.

The results presented here have been obtained with reflection boundary conditions on the external boundaries and zero buckling. Benchmarking of COBAYA3 pin-by-pin with XS and IDF from multi-parameter libraries obtained through pin-cluster branch calculations with critical buckling is subject of a separate analysis.

3. CROSS-SECTIONS AND INTERFACE DF

Accurate MOC based calculation schemes [16] with APOLLO2, validated against Monte Carlo solutions have been used to generate the pin-by-pin XS and IDF in 2, 4 and 8 energy groups for COBAYA3. Table 2 shows the adopted energy group structure.

Table 2: Broad energy group structure

2 group structure	4 group structure	8 group structure	Lower energy cut off (eV)
1	1	1	2.2313E+06
		2	8.2085E+05
		3	9.1188E+03
	2	4	1.3007E+02
		5	3.9279E+00
	3	6	6.2506E-01
2	4	7	1.4572E-01
		8	0.0000E+00

The pin-by-pin XS and IDF for the considered states are cell-position dependent and have been obtained with the CEA2005V4.1.2 library based on JEFF3.1.1, making use of the following modeling assumptions in APOLLO2:

19-pin clusters

- Reference two-step 281g Pij-MOC calculation scheme in APOLLO2 with SHEM [20] energy mesh
- Step MOC (UOX-GT, UOX-CT) or higher-order Linear Surface (LS) MOC [21] (UOX-CR)
- Fine MOC spatial mesh with 4 rings in the fuel, smeared gap-cladding, 3 radial meshes in the moderator, 12 azimuth sectors [16]
- Simplified LS MOC spatial mesh with 4 rings in the fuel, smeared gap-cladding, one ‘ring’ in the moderator and no azimuth sectors
- MOC parameters: tracking step dr=0.008cm, number of azimuth angles Nφ=48, number of polar angles Nψ=3, Bickley quadrature, P3 scattering anisotropy;
  LS MOC surface subdivision factor Ndiv=6, threshold size 0.74 cm

Fuel assembly

- Reference two-step 281g Pij-MOC calculation scheme in APOLLO2 with SHEM energy mesh
- Step MOC solver
- MOC spatial mesh with 2 rings in the fuel, smeared gap-cladding, 6 azimuth sectors only in CR and peripheral cells, 2566 regions in a whole assembly
- MOC parameters: dr=0.001 cm, Nφ =36, Nψ =3, Bickley, P0*

Assembly cluster

- Reference two-step 281g Pij-MOC calculation scheme in APOLLO2 with SHEM energy mesh
- LS MOC solver
- LS MOC spatial mesh with 2 rings in the fuel, smeared gap-cladding, one 'ring' and no azimuth sectors in the moderator except for CR cells where 6 azimuth sectors are used; 1070 regions in 1/6 color set
- LS MOC parameters: dr = 0.008, Nφ = 36, Nψ = 2, P1; Ndiv= 6, threshold 0.74 cm

The same nuclear data and calculation parameters have been used to obtain the APOLLO2 deterministic reference solutions [16] for the considered cases.

4. RESULTS

4.1 19-pin clusters

This configuration allows the use of structured spatial mesh in COBAYA3. Table 3 summarizes the comparison of COBAYA3 vs. APOLLO2 computed multiplication factors and normalized pin-by-pin fission reaction rates (FRR). The results show that the impact of the number of broad energy groups is small compared to that of the transport correction of homogenization errors. Table 4 shows a comparison with TRIPOLI4 reference solutions.

Table 3: Biases of COBAYA3 vs. APOLLO2 reference results

Code	UOX-GT			UOX-CR		
	k-inf	Δk(C3-A2) pcm	maxΔFRR (C3-A2)*100	k-inf	Δk(C3-A2) pcm	maxΔFRR (C3-A2)*100
APOLLO2 ref	0.96217			0.61971		
C3 2g, no IDF	0.96302	+85	0.22	0.61367	-604	0.11
C3 4g, no IDF	0.96230	+14	0.19	0.60688	-1283	0.06
C3 8g, no IDF	0.96199	-17	0.22	0.60745	-1227	0.11
C3 2g, GET	0.96214	-2	0.02	0.61972	+0.3	0.02
C3 4g, GET	0.96214	-2	0.02	0.61971	-0.2	0.02
C3 8g, GET	0.96214	-2	0.02	0.61971	-0.2	0.02

Table 4: Multiplication factors and biases to TRIPOLI4 reference solution

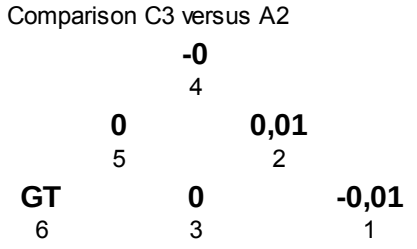
Code	UOX-GT		UOX-CR	
	k-inf	Δk, pcm	k-inf	Δk, pcm
TRIPOLI4 ref	0.96253 ± 11E-5	-	0.61981± 11E-5	-
APOLLO2 LS MOC 281g	0.96216	-37	0.61971	-10
COBAYA3 8g, GET IDF	0.96214	-39	0.61971	-10

Table 5 presents the computed pin fission rates for 1/6 19-pin clusters at 39.8 MWd/kgH. The COBAYA3 results show a perfect reproduction of the APOLLO2 reference solutions when using side- and cell position dependent GET IDF. The solutions with IDF are nearly the same in 2, 4 and 8 energy groups.

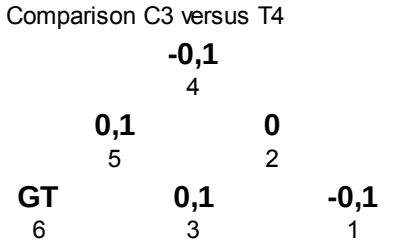
Table 5: COBAYA3 2g vs. APOLLO2 ref solutions for 1/6 pin clusters at 39.8MWd/kgH

Cell N	UOX-CT		UOX-GT		UOX-CR	
	C3 FRR	ΔFRR, %	C3 FRR	ΔFRR, %	C3 FRR	ΔFRR, %
1	0.991	0.00	0.993	-0.01	1.018	0.02
2	0.992	-0.01	0.994	0.01	1.014	-0.01
3	1.013	0.00	1.010	0.00	0.976	-0.01
4	0.991	0.00	0.993	-0.01	1.018	0.00
5	1.013	0.00	1.010	0.00	0.975	0.00

Figures 3 - 5 illustrate the biases of COBAYA3 to APOLLO2 and TRIPOLI4 computed pin-by-pin fission rate distributions.

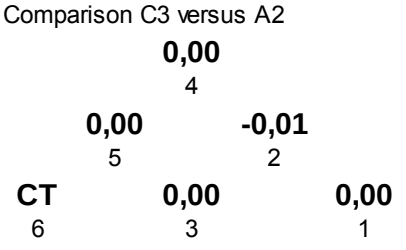


Dev Kinf (A2), pcm	1
Max dev FRR, %	0,0108
Average dev FRR, %	0,01
Kinf A2	0,96267
Kinf C3	0,96268

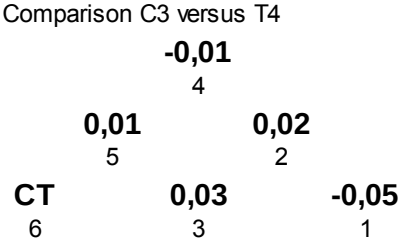


Dev Kinf (T4), pcm	15
Max dev FRR, %	0,08
Average dev FRR, %	0,05
Kinf T4	0,96253
Kinf C3	0,96268

Figure 3: Biases of COBAYA 8g GET to APOLLO2 MOC and TRIPOLI4 ref results for 19-pin UOX-GT cluster



Dev Kinf (A2), pcm	1
Max dev FRR, %	0,0075
Average dev FRR, %	0,00
Kinf A2	0,98668
Kinf C3	0,98668



Dev Kinf (T4), pcm	20
Max dev FRR, %	0,0461
Average dev FRR, %	0,0234
Kinf T4	0,98648
Kinf C3	0,98668

Figure 4: Biases of COBAYA 8g GET to APOLLO2 MOC and TRIPOLI4 ref results for 19-pin UOX-CT cluster

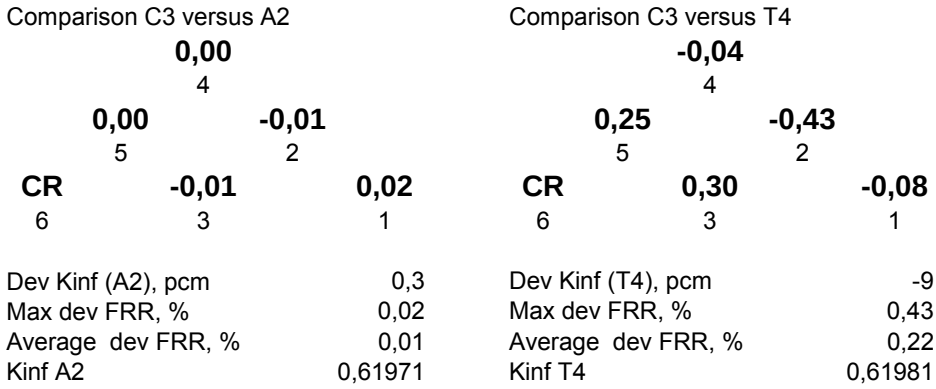


Figure 5: Biases of COBAYA 8g GET to APOLLO2 LS MOC and TRIPOLI4 ref results for 19-pin UOX-CR cluster

4.2 Fuel assembly

A profiled VVER-1000 assembly of 4.23 $^{w}/_{o}$ average initial enrichment is considered:

a) UOX-CR assembly at 39.8 MWd/kgHM
b) UOX-GT assembly at zero burn-up

In order to model the peripheral water gap, unstructured spatial mesh must be used. Table 6 summarizes the comparison of COBAYA3 vs. APOLLO2 solutions for UOX-CR assembly when using GET discontinuity factors for the interior cells and the irregular peripheral cells.

Table 6: COBAYA3 vs. APOLLO2 results for UOX-CR assembly at 39.8MWd/kgHM

State	Code	k-inf	Δk (C3-A2), pcm	max ΔFRR*100
S1	A2 MOC 281g P0*	0,73812	-	-
	COBAYA3 2g GET	0,73827	15	0,27
	COBAYA3 4g GET	0,73820	7	0,37
	COBAYA3 8g GET	0,73820	8	0,34
S2	A2 MOC 281g P0*	0,73010	-	-
	COBAYA3 2g GET	0,73024	14	0,27
	COBAYA3 4g GET	0,73017	7	0,32
	COBAYA3 8g GET	0,73017	7	0,35
S3	A2 MOC 281g P0*	0,73062	-	-
	COBAYA3 2g GET	0,73075	13	0,26
	COBAYA3 4g GET	0,73067	5	0,33
	COBAYA3 8g GET	0,73067	5	0,33
S4	A2 MOC 281g P0*	0,42612	-	-
	COBAYA3 2g GET	0,42612	0	0,03
	COBAYA3 4g GET	0,42611	-1	0,03
	COBAYA3 8g GET	0,42611	-1	0,04
S5	A2 MOC 281g P0*	0,77432	-	-
	COBAYA3 2g GET	0,77441	9	0,31
	COBAYA3 4g GET	0,77433	1	0,36
	COBAYA3 8g GET	0,77433	1	0,38

Good performance of the COBAYA3 pin-by-pin solver across the mesh irregularities is displayed. The results show that:

- the biases of the inside assembly pins are very low, similar to those for structured mesh
- the average absolute bias is below 0.05 %
- a single corner pin #1 shows bias of app. 0.3%

Figure 6 illustrates the COBAYA3 2g computed pin-by-pin fission rate distribution for irradiated UOX-CR assembly in State 1 and the biases to APOLLO2 ref solution, if no discontinuity factors are used. The bias in k-infinity is - 973 pcm. The maximum bias in pin fission rates is -1.70 (expressed as ΔFRR*100) for pin #40 near a CR, or -1.82 % for pin #15 (with relative FRR of 0.928) next to a CR.

Figure 7 shows the COBAYA3 2g GET computed pin-by-pin fission rate distribution for the same UOX-CR assembly in State 1 and the biases to APOLLO2 ref solution.

Figure 8 shows the COBAYA3 8g BBH computed pin-by-pin fission rate distribution for a fresh UOX-GT assembly in State 1 and the biases to APOLLO2 ref solution.

2 energy groups, no DF

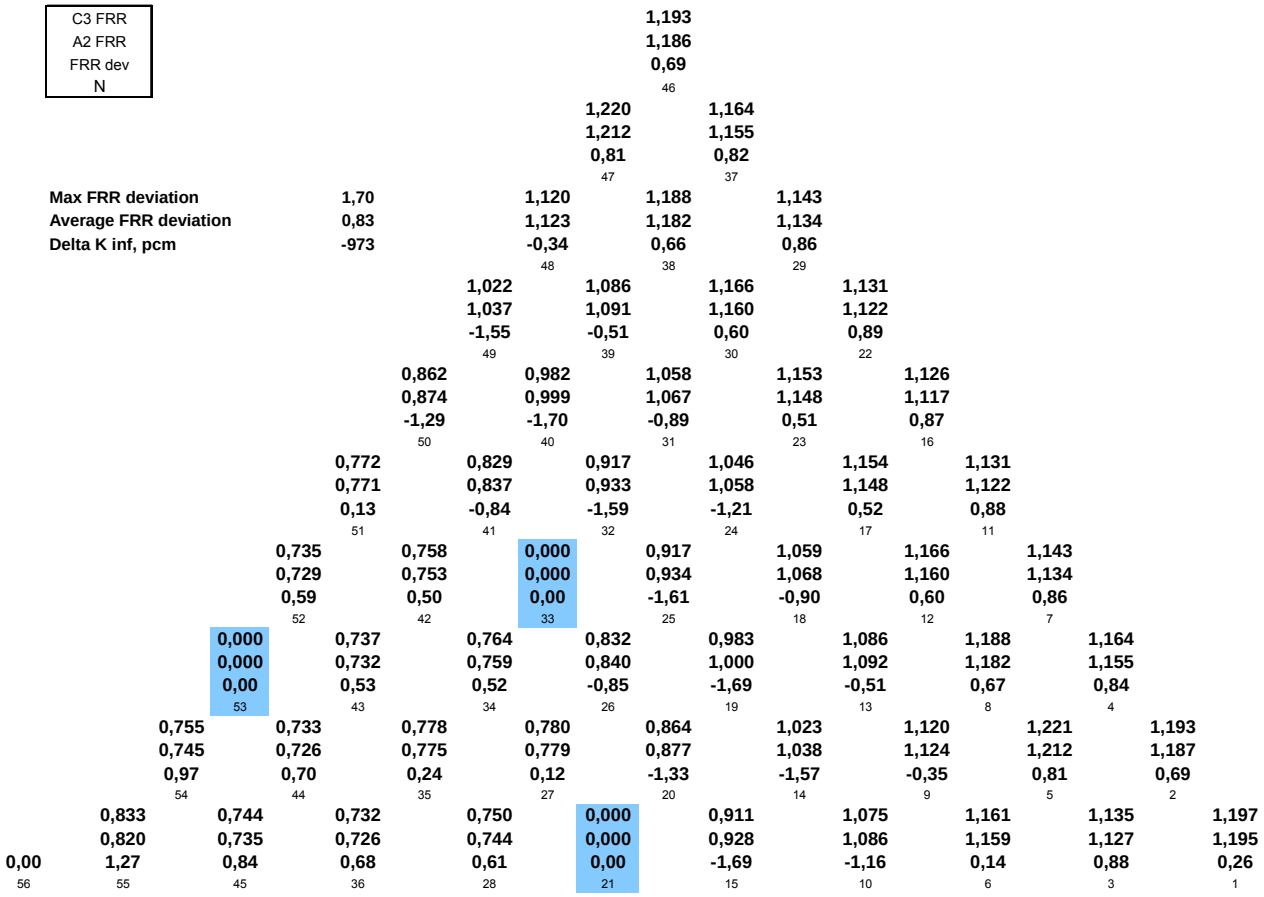


Figure 6: Pin-by-pin fission rates and biases (C3 2g no DF - A2ref)*100 for UOX-CR assembly at 39.8 MWd/kgHM, in State 1: HZP at 552K

2 energy groups, GET DF

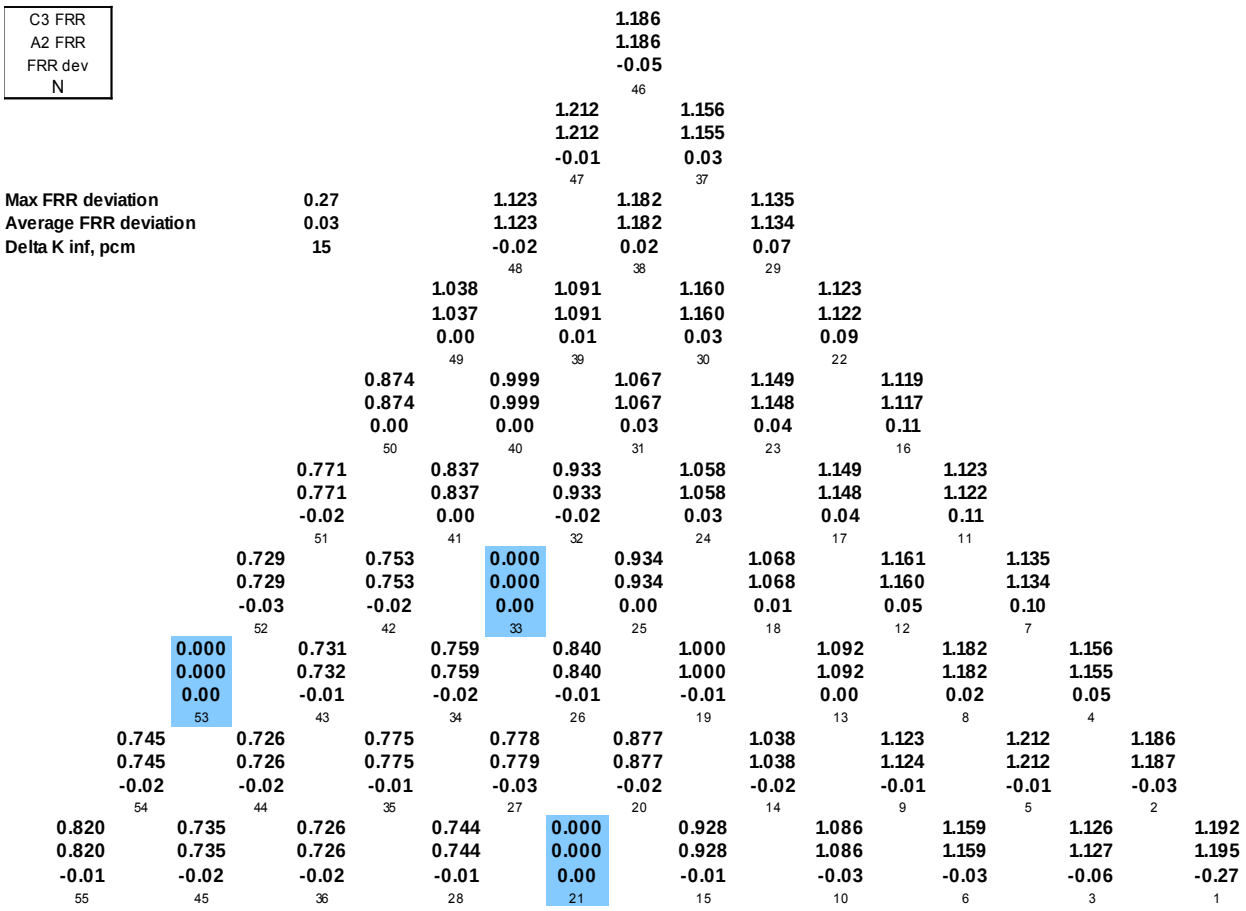


Figure 7: Pin-by-pin fission rates and biases (C3 2g GET - A2ref)*100 for UOX-CR assembly at 39.8 MWd/kgHM, in State 1: HZP at 552K

8 energy groups, BBH DF

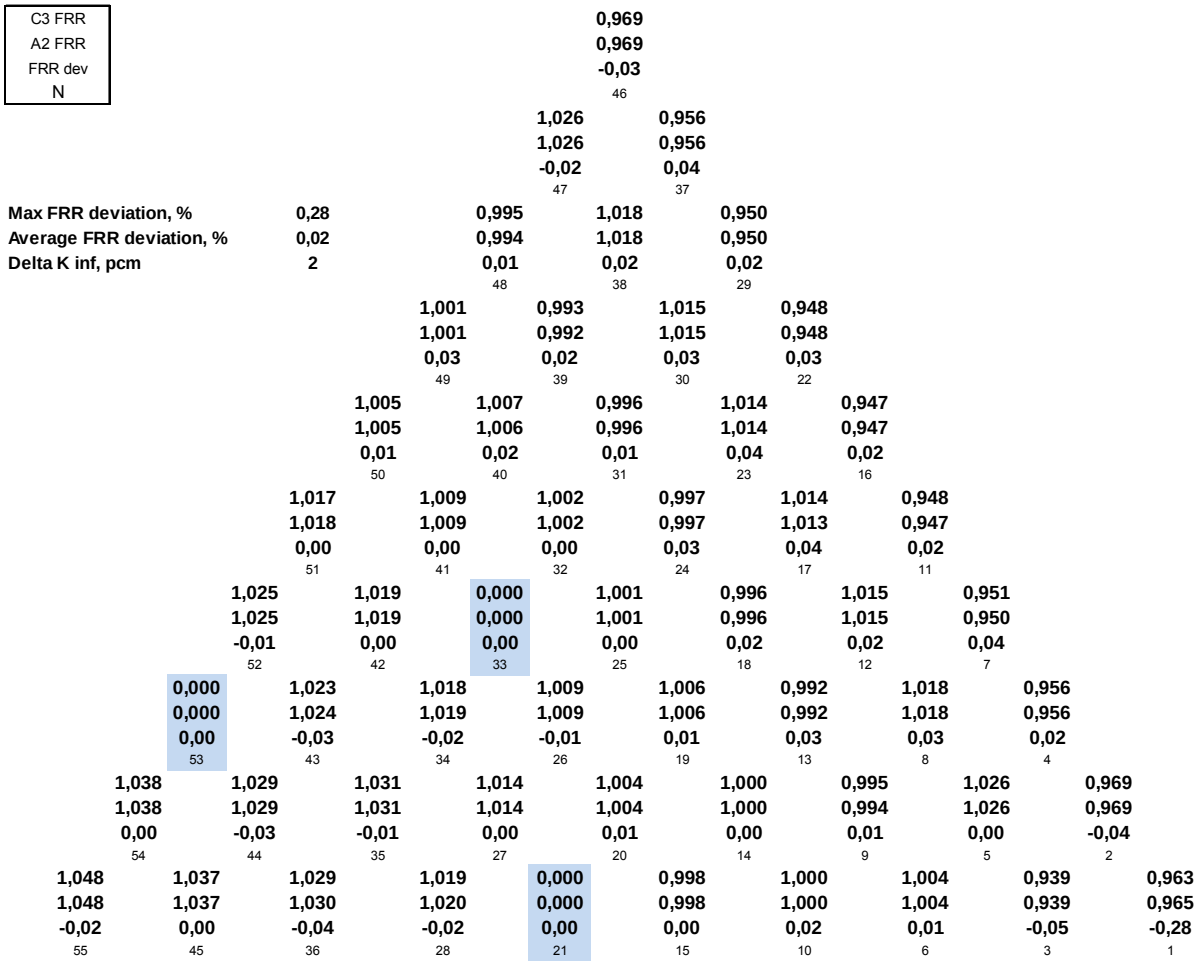


Figure 8: Pin-by-pin fission rates and biases (C3 8g BBH - A2ref)*100
for a fresh UOX-GT assembly in State 1: HZP at 552K

4.3 Color set results

The hexagonal color set consists of a central UOX-CR assembly and 6 halves of peripheral UOX-GT assemblies with 4.23 w/o average enrichment. This is a challenging test problem characterized by radial variation of the enrichment and steep thermal flux gradients near the CR as well as in the water holes (GT, CT) and the inter-assembly water gaps. The modeling of inter-assembly water gaps requires the use of unstructured spatial mesh.

Table 7 shows the biases of COBAYA pin-by-pin to APOLLO2 LS MOC 281g results when using GET discontinuity factors for the interior cells and the irregular inter-assembly cells. Good agreement with the reference results is displayed.

Figure 9 illustrates the deviations of COBAYA3 2g to the reference pin fission rates in 1/6 of the central UOX-CR assembly normalized over the whole color set.

Table 7: Summary of COBAYA3 vs. APOLLO2 LS MOC results with 60^{o} rot. symmetry

APOLLO2	COBAYA3 2g GET	Δk(C3-A2), pcm	max ΔFRR*100	max ΔFRR*100
			Central UOX-CR	Peripheral UOX-GT
1.30908	1.30892	-16	1.02	1.24

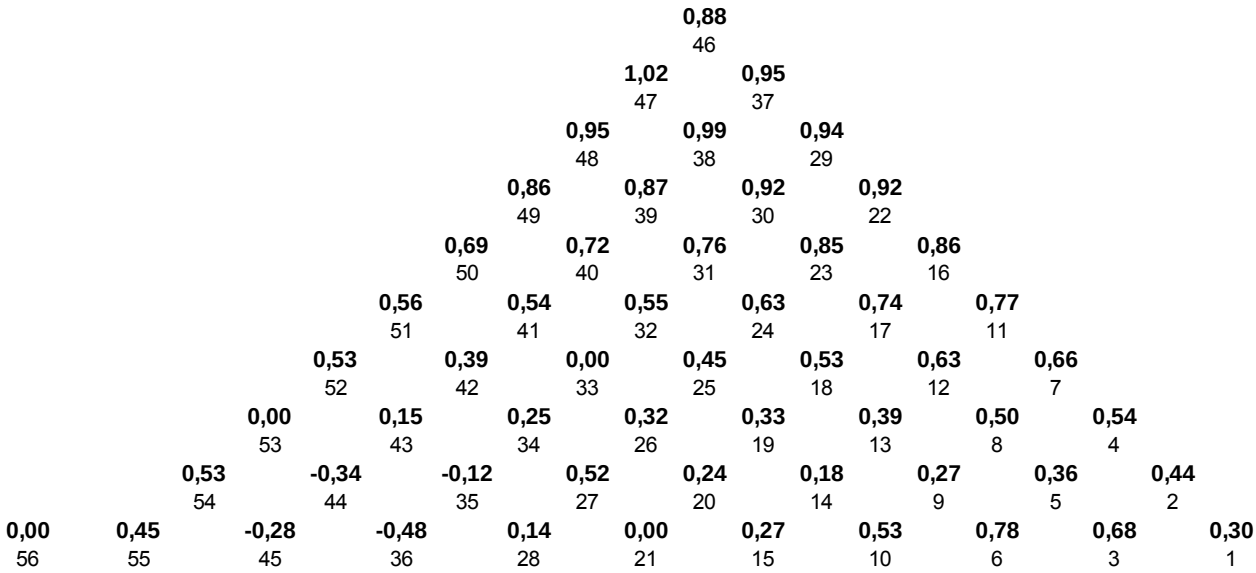


Figure 9: Central UOX-CR assembly of the color set:
Biases (COBAYA3-APOLLO2)*100 in normalized pin fission reaction rates

5. SUMMARY AND CONCLUSIONS

The results show that:

- COBAYA3 pin-by-pin successfully performs unstructured mesh calculations with Interface DF
- The transport-corrected diffusion theory solutions for 2D sub-sets of the core with neighborhood-dependent XS and DF are very close to the reference results
- The impact of the number of broad energy groups is small compared to that of the transport correction of homogenization errors
- COBAYA3 pin-by-pin is an accurate and computationally efficient core simulator for hexagonal geometry

The analyzed benchmark solutions prove that the use of side-dependent interface discontinuity factors allows achieving the target pin-by-pin fidelity for safety analysis.

ACKNOWLEDGEMENTS

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