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VALIDATION OF AN ADVANCED APOLLO3[®] DETERMINISTIC SCHEME FOR CHARACTERIZING OF THE JULES HOROWITZ IRRADIATION REACTOR CORE

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ABSTRACT

JHR is a new material testing reactor under construction at CEA Cadarache. Currently, the neutronic characteristics of the core are calculated thanks to the HORUS3D/N deterministic scheme. The industrial route of this scheme follows a two steps approach with first the APOLLO2 MOC lattice calculation and then the CRONOS2 core calculation based on diffusion theory. APOLLO3[®] is the new deterministic calculation platform at CEA, which incorporates advanced computation methods. In this paper, a new reference calculation scheme for JHR is being set up using the new methods brought by APOLLO3[®]. The calculation scheme is validated against reference stochastic simulations performed by TRIPOLI4[®]. Improvements at the lattice step allow a significant reduction of biases on absorption rates for fuel elements and Hf control rods when compared to results of a scheme that mimics, within APOLLO3[®], the HORUS3D/N scheme. The main changes in the new scheme are coming from the use of the subgroup self-shielding method instead of the Fine-structure equivalence method. These changes are associated to refined geometry meshes and to the 383 energy group structure. Condensed cross-sections from the lattice step are used to compute the neutron balance of a 2D JHR core configuration with five Hf control rods inserted. Core-reflector super cell has been added in the new calculation scheme to produce refined reflector cross sections. The MOC 2D core calculation performed with a coarser 41-group structure preserves the lattice calculation improvements and gives better predictions on reactivity and reactions rates. Next steps will use a 3D Sn MINARET full-core calculation with depletion including in-core experimental devices.

KEYWORDS: APOLLO3[®], JHR, Deterministic calculation scheme, Resonance self-shielding methods.

1. INTRODUCTION

The Jules Horowitz Reactor (JHR) [1] is a new material testing reactor under construction at CEA Cadarache in the south of France. The main goal of this research reactor is to test advanced materials and to demonstrate their ability to withstand proper characteristics under operation conditions and irradiation. This concerns the safety whether it is for new generations (GEN-III and GEN-IV) nuclear reactors or for current generation (GEN-II). Another goal is to produce ⁹⁹Mo for medical diagnostics. Neutronics calculations on JHR are routinely performed with the HORUS3D/N [2] calculation scheme. This design tool is based on a 2 steps APOLLO2[3]/CRONOS2[4] deterministic scheme and is validated at beginning of life against reference stochastic results provided by TRIPOLI4[®][5].

Currently, the industrial route of the HORUS3D/N scheme predicts JHR neutronics characteristics in 3D with depletion. It computes the lattice step with depletion for fuel elements with TDT solver [6] using the Method of Characteristics (MOC) on a refined 2D geometry and with 281 energy groups after a self-shielding treatment. For Be radial reflector, an APOLLO2, a whole core MOC calculation is lead on a 22-group energy mesh. For axial reflector, a Sn R-Z calculation is performed on a fuel assembly. The second step uses the CRONOS2-PRIAM solver based on diffusion theory using condensed/homogenized cross-section generated at first step. This second step is applied on a homogenized geometry with a 6-group condensed energy mesh. It allows full core depletion calculations.

The new APOLLO3[®] code [7] in development at CEA brings advanced options for deterministic calculations. New solvers are available, such as the unstructured conform MINARET Sn solver [8], a 2D/3D transport solver based on the discrete ordinates method (Sn) whose spatial discretization is relying on a Discontinuous Galerkin Finite Element Method (DGFEM). A subgroup method for resonance self-shielding coupled with flux calculation as it was done within ECCO code is implemented. It is also possible to create complex core geometry thanks to the SALOME platform [9].

The goal of this work is to define a new reference deterministic scheme based on APOLLO3[®] to improve the predictions of JHR neutronics characteristics. This new scheme will be compared to the APOLLO3[®] implementation of HORUS3D/N. It will be validated thanks to TRIPOLI4[®] [5] Monte Carlo simulations at beginning of life. Our objectives are to reduce as much as possible the biases of the reference route in respect with TRIPOLI4[®] and to ensure a computation time compatible with industrial uses. Today, the 2D beginning of life modelization has already been performed and is presented in this paper.

2. THE JULES HOROWITZ REACTOR

JHR is a 100MW pool research reactor. The core is made of 37 fuel assemblies loaded along concentric rings into alveolus of an aluminum matrix. Fuel assemblies are made of U_3SiO_2 fuel enriched up to 27 %. Three of these assemblies can be removed and replaced by an in-core experimental device. Twenty-seven hafnium rods are introduced at the center of fuel assemblies to control the reactivity. It is also possible to put experimental devices at the center of the remaining assemblies. Experiment devices can also be placed into the beryllium radial reflector. JHR reaches high flux, up to 5.10^{14} n.cm⁻².s⁻¹.

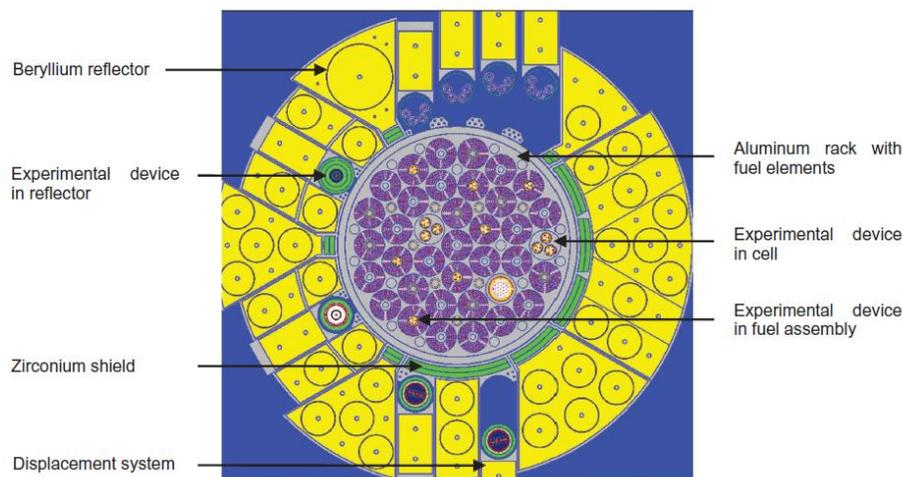


Figure 1. JHR Core Description

The JHR fuel assemblies consist of 24 curved concentric plates maintained together thanks to an aluminum stiffener. Light water circulates into these fuel assemblies to refresh and moderate the fuel.

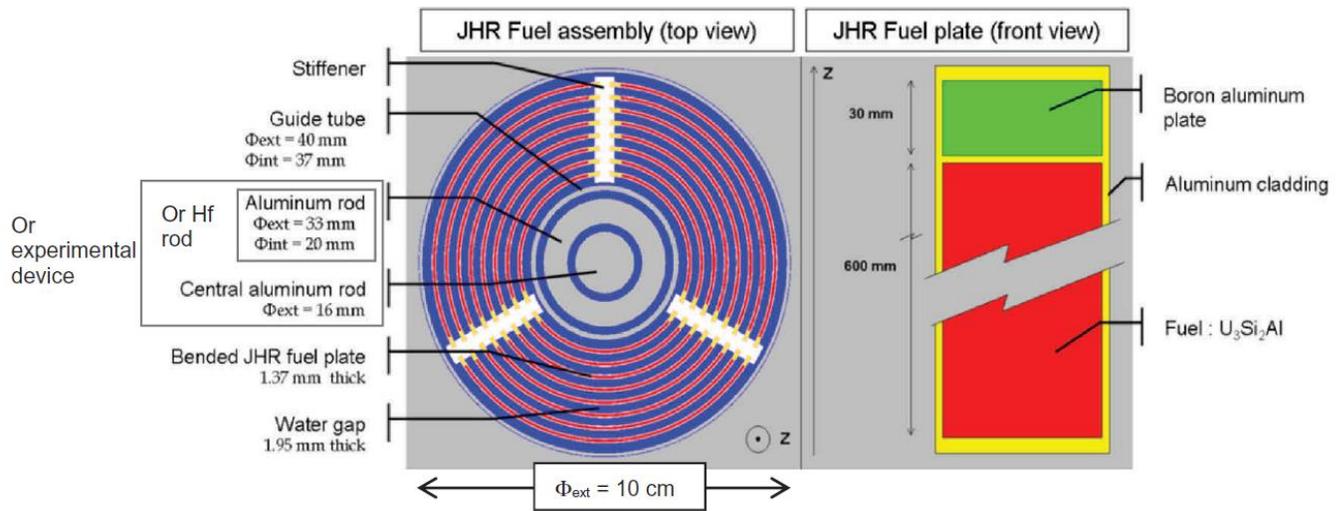


Figure 2. JHR fuel element and JHR Fuel Plate Description.

3. APOLLO3[®] REFERENCE DETERMINISTIC NEUTRONIC SCHEME

3.1. General Description of the Studied Configuration and Scheme

The studied configuration is made of 37 fuel assemblies and 5 Hf control rods inserted. It is a 2D study at time 0 led with the solver TDT-MOC that used the Method of Characteristics in APOLLO3[®]. The geometry is generated with the SALOME [9] platform. The radial reflector is modelled by a homogenized Be-H₂O-Al composition. The neutronics calculation scheme developed with APOLLO3[®] is a reference 2 stepped MOC-MOC scheme. The first step is lead on a refined lattice geometry and on a refined energy mesh. During this step, the self-shielding treatment is performed by using collision probabilities (CPs) calculated on the same TDT geometry than the MOC fluxes. The scalar fluxes are used to homogenize and condense cross sections. In the second step, these cross sections are used to compute neutronics characteristics of the entire core with MOC. The lattice and core results are compared in 2D to Monte-Carlo TRIPOLI4[®] simulations to validate them. In what follows, dataset options are presented for the two steps for a scheme that re-used current options of APOLLO2 dataset transposed in APOLLO3[®] (called “iso-HORUS3D/N”) and for the new deterministic scheme developed with APOLLO3[®]. All the cross sections used for the simulations come from the JEFF3.1.1 library [10].

3.2. First Step: Lattice Calculation and Selfshielding

The goal of this step is to compute homogenized, condensed and self-shielded cross sections. The main options of the datasets are presented in table I for two types of assembly, with or without Hf control rod inserted.

The main modifications made to the HORUS3D/N scheme concern the self-shielding options, the energy mesh and the geometry. The new REL-383 energy mesh [11] is based on SHEM-361 [12], itself based on SHEM-281 [13] energy one. Several groups have been added in the epithermal domain to allow accurate treatment of LWR fuel and usual absorbers using the subgroup method [7]. For self-shielding, the HORUS3D/N scheme uses the Livolant-Jeanpierre method on a cylindrical geometry that does not depict stiffeners. Main resonances of ²³⁵U, ²³⁸U, ²³⁶U and structures elements (²⁷Al, ⁵⁶Fe, ⁵²Cr and Zr) are self-

shielded above 22.5 eV [14]. If needed, Hf isotopes are mixed and self-shielded between 1.06 keV and 22.5 eV. For the new scheme, the subgroup method is used on 1/6th assembly that depicts stiffeners. U and Hf are mixed and self-shielded from 5 MeV to 2.55 eV. Self-shielding is extended down to 2.55 eV rather than the 22.5 eV energy boundary to account for Hf thermal resonances that are not finely described by the energy mesh. However, in the absence of equivalence, it is not sufficient to deal with large Γ_n resonances (such as ¹⁷⁸Hf 7.8 eV), since the non-correlation assumption between reactions and sources of the subgroup method is not valid; a more refined energy mesh is unavoidable in this case.

For the description of the geometry of core assemblies, the new calculation scheme uses a more refined mesh description in water and in fuel as it is depicted on figures 3 to 6. For core assemblies with Hf control rod inserted, the infinite lattice approximation is not really justified, and hence a cluster geometry is adopted to compute this type of configuration. On HORUS3D/N scheme, the surrounding composition is coming from the homogenization of a fuel element without Hf control rods (figure 5), while for the new scheme, the exact environment is adopted (figure 6). These cluster geometries are used to compute cross sections for core calculation. But to validate the lattice calculation with Hf control rod inserted, a single fuel element with Hf has been used with reflective boundary conditions.

Table I. Self-shielding and flux solver options for lattice calculation.

		Iso-HORUS3D/N	New APOLLO3® scheme
Self-shielding calculation	Method	Livolant-Jeanpierre - CPs	Subgroups - CPs [11]
	Energy Mesh	SHEM – 281	REL – 383
	Geometry (without Hf)	1D Cylindrical	Real 6 th assembly 433 meshes
	Geometry (with Hf)	1D Cylindrical	Real 6 th assembly 565 meshes
Lattice calculation	Method	TDT-MOC2D	TDT-MOC2D
	Energy Mesh	SHEM – 281 [13]	REL – 383
	Geometry (without Hf)	Real 6 th assembly 195 meshes	Real 6 th assembly 433 meshes
	Geometry (with Hf)	Real 6 th assembly 291 meshes	Real 6 th assembly 565 meshes
	Anisotropy	P3	
	Tracking options	$\Delta r = 0.01$ cm $N\Phi = 40$ $N\Psi = 3$	

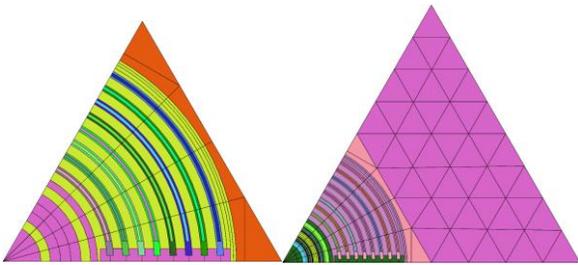


Figure 3. Iso-HORUS3D/N Without/With Hf Lattice Geometry.

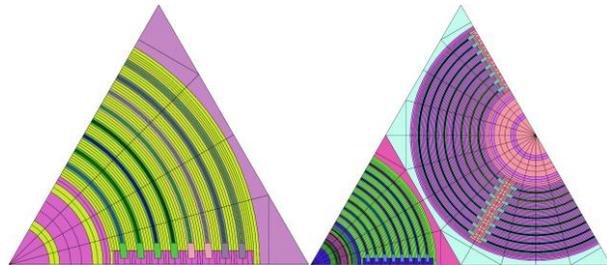


Figure 4. New Scheme Without/With Hf Lattice Geometry.

3.3. Second Step: Core Calculation

The core step re-uses the cross sections obtained at the lattice step but condensed in a few tens of groups in order to perform the 2D full-core calculation (no spatial homogenization). The main options are presented in table II

Table II. MOC solver option for core calculation.

		Iso-HORUS3D/N	New APOLLO3 [®] scheme
Core calculation	Flux solver	TDT-MOC2D	TDT-MOC2D
	Energy Mesh	22 groups	41 groups
	Reflector self-shielding	No	Yes (Zr and ²⁷ Al)
	Geometry	32388 meshes	35345 meshes
	Anisotropy	P3	
	Tracking options	$\Delta r = 0.01 \text{ cm } N\Phi = 40 \text{ } N\Psi = 3$	

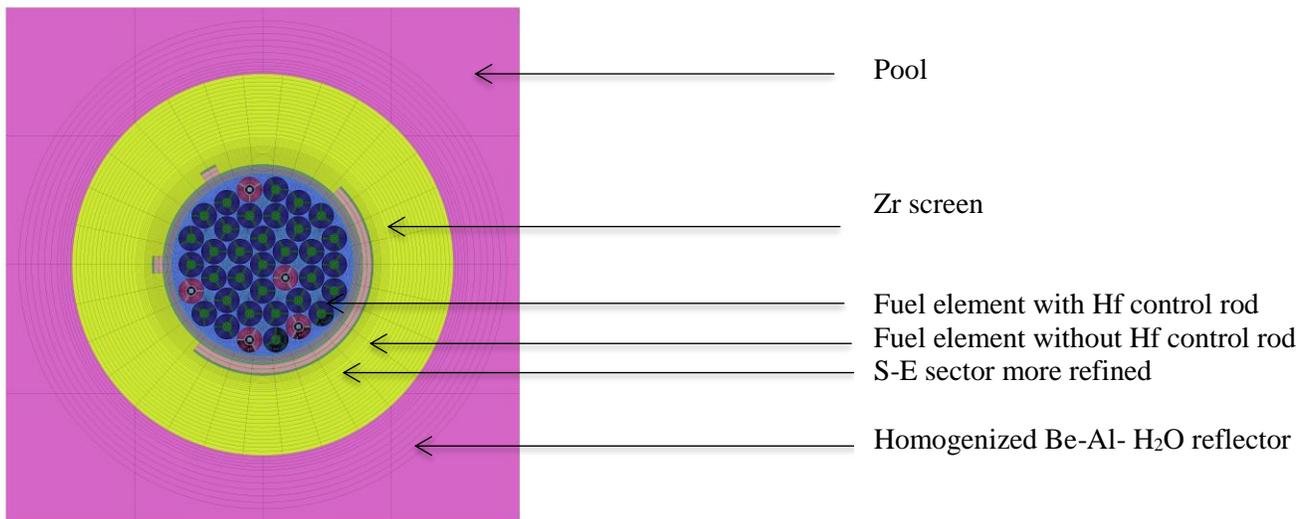


Figure 5. Meshed Core Geometry for New APOLLO3[®] Scheme.

A 41-group energy mesh has been used for the new calculation scheme instead of the previous 22-group one. It allows a more refined computation in the epithermal domain to improve ²³⁸U absorption calculation in the first two resonances. Geometry studies contains 32 fuel elements without Hf control rod inserted and 5 fuel elements with Hf control rod inserted. To condense reflector cross-section down to 22 or 41 groups, a 1/6th reflector geometry is adopted, with a homogenized core. For the new APOLLO3[®] scheme, a self-shielding treatment is also applied to the Zr and ²⁷Al resonances.

For the HORUS3D/N scheme, each fuel element is meshed into 12 angular sectors. The fuel plates and the water gaps are radially meshed, as shown in figure 3 and 5. The first results have shown that the most important bias in the assemblies was located in the 3rd ring of the S-E sector. This sector have been refined to improve the prediction. A mesh as refined as the lattice mesh has been adopted to model these fuel elements (figure 4 and 6).

4. NUMERICAL RESULTS

In this part, the results obtained with the two APOLLO3[®] schemes are compared to a TRIPOLI4[®] stochastic simulations. The biases for different physical quantities are presented below, firstly for the lattice simulation, and secondly for the core one.

4.1. Lattice Results

For the lattice simulations, we have studied the two configurations with or without Hf control rod inserted. It is possible because even the configuration with Hf is supercritical, as depicted below.

4.1.1. Fuel assemblies without Hf control rod

The results have been synthesized for the lattice step according to the 6 factors formula (table III and IV). It is an extension of the 4 factors Fermi formula that takes into account (n, 2n) reactions, and keeps separate fast fissions on odd/even isotopes: $k_{\infty} = \chi_{n/2n} \cdot \epsilon_{\text{odd}} \cdot \epsilon_{\text{even}} \cdot p \cdot f \cdot \eta$. The thermal cut-off is set to 0.625 eV.

Table III. Six factors results on the fuel element without Hf.

Factors	TRIPOLI-4 [®] values	Iso-HORUS3D/N scheme bias (pcm)	New AP3 scheme bias (pcm)
$X_{n/2n}$	1.00021	+ 3	+ 3
ϵ_{odd}	1.00296	- 1	- 1
ϵ_{even}	1.06631	+ 2	- 2
p	0.83797	- 31	- 31
f	0.91144	+70	+ 43
η	2.04199	- 5	- 4
k_{∞}	1.66829	+ 38	+ 7

The impact of the new scheme seems to be small on the fuel element without Hf. Only a significant improvement is observed on the factor that represents thermal neutrons absorption outside fuel (f). Improvement on f factor comes from the more refined geometry in moderator for the new scheme.

To studies more precisely the influence of the scheme on reactions rates, we have also compared fuel absorption and fission rates on a 6-group energy mesh. Only the most important biases in a plate are shown, for groups with an upper than 5 % contribution to the total absorption/fission rate.

Table IV. AP3-T4 rates comparison on fuel plates for the non-rodded assembly.

	Energy groups	$\pm \Delta_{\text{max}} $ /plates iso-HORUS3D/N scheme	$\pm \Delta_{\text{max}} $ /plates new AP3 scheme	Contribution to total absorption rate in fuel
Non fissile absorption rate	4.10 keV – 22.4 eV	- 1.0 %	+ 0.8 %	21.4 %
	22.4 eV – 2.55 eV	+ 1.1 %	+ 0.1 %	25.1 %
	0.625 eV – 0.0001 eV	- 0.5 %	- 0.3 %	47.2 %
Fission rate	20 MeV – 0.0001 eV	- 0.4 %	- 0.3 %	100 %

We observe again that the impact of the new scheme is limited in the fuel element without Hf. In fact, a great bias compensation occurs between [22.4 eV – 2.55 eV] group where the absorption is over-predicted and [4.10 keV – 22.4 eV] where it is under-predicted in iso-HORUS3D/N. With the new scheme, the extended self-shielding cancels bias in [22.4 eV – 2.55 eV] group, and overestimates the absorption rate in [4.10 keV – 22.4 eV] group. Overall, the prediction of absorption and fission rates is not significantly improved, but some of bias compensations are cancelled.

4.1.2. Fuel assemblies with Hf control rod

Table V. Six factors results on the fuel element with Hf.

Factors	TRIPOLI-4 [®] values	Iso-HORUS3D/N scheme bias (pcm)	New AP3 scheme bias (pcm)
$X_{n/2n}$	1.00033	+ 5	+ 5
ϵ_{odd}	1.00585	+ 1	- 2
ϵ_{even}	1.14438	+ 113	+ 44
p	0.64960	- 484	- 216
f	0.76691	-103	- 30
η	2.04093	- 6	- 6
k_{∞}	1.17077	-473	- 204

An important improvement of the prediction can be observed in this case on the factor which represents the effect of resonant absorptions during the slowing down (p) and on the factor which represents thermal neutrons absorption outside fuel (f). Once again, the improvement on f factor comes from the more refined geometry for the new scheme. On p factor, it mainly comes from self-shielding treatment and energy mesh. The modification of the self-shielding treatment particularly affects the prediction in Hf.

Below, we compare the absorption and fission rates on a 6-group energy mesh in the fuel plates and Hf rod. Only the most important biases in a plate are shown, in groups with a contribution greater than 5 % to the total absorption/fission rate.

Table VI. AP3-T4 fuel plates rate comparisons for assembly with Hf control rod inserted.

	Energy groups	$\pm \Delta_{\text{max}} $ /plates iso-HORUS3D/N scheme	$\pm \Delta_{\text{max}} $ /plates new AP3 scheme	Contribution to total absorption rate in fuel
Non fissile absorption rate	4.10 keV – 22.4 eV	- 0.8 % / + 0.9 %	+ 0.4 %	25.3 %
	22.4 eV – 2.55 eV	+ 1.4 %	+ 0.3 %	27.6 %
	0.625 eV – 0.0001 eV	- 0.7 % / + 0.1%	- 0.2 % / + 0.1 %	40.1 %
Fission rate	20 MeV – 0.0001 eV	- 0.5% / + 0.2%	- 0.1 % / + 0.1%	100 %

For the fuel element with Hf, the prediction in [4.10 keV – 22.4 eV] group is clearly improved with the new scheme thanks to the new self-shielding treatment. The extended self-shielding improves again prediction in [22.4 eV – 2.55 eV] group. In addition, for this type of fuel element, the prediction of absorption and fission rates in the thermal group is better with the new APOLLO3[®] scheme. Globally, the reactions rates in the fuel plates of a fuel element with Hf are better predicted with the new scheme.

Table VII. AP3-T4 comparisons on absorption rate in Hf control rod for the rodded assembly.

	Energy groups	Δ iso-HORUS3D/N scheme	Δ new AP3 scheme	Contribution to total absorption rate in rod
Absorption rate	4.10 eV – 22.4 eV	+ 3.4 %	+ 0.4 %	23.6 %
	22.4 eV – 2.55 eV	+ 2.0 %	+ 1.1 %	20.4 %
	2.55 eV – 0.625 eV	+ 0.8 %	+ 0.9 %	18.6 %
	0.625 eV – 0.0001 eV	+ 0.8 %	+ 0.3 %	34.3 %

In the Hf control rod, the impact of the new APOLLO3[®] scheme is even better than with the iso-HORUS3D/N scheme. In the [4.10 keV – 22.4 eV] group, the bias on absorption rate goes from 3.4 % to 0.4 % with the new scheme. It is the most important improvement of the new scheme. The prediction in group [22.4 eV – 2.55 eV] is strongly improved thanks to the extended self-shielding. In fact, the absorption rates in Hf thermal resonances are better predicted with self-shielding as we can see on Figure 8, which represents the bias on absorption rates in REL383 groups in the range 22.5 eV and 2.55 eV.

However, the new methodology does not improve the absorption rate around 7.8 eV in ¹⁷⁸Hf and ¹⁷⁶Hf resonances. A more detailed study have shown that the absorption rate of ¹⁷⁶Hf is improved significantly, but remain the same for ¹⁷⁸Hf. In fact, the ¹⁷⁶Hf resonance is essentially a capture resonance, while the scattering and capture components of the ¹⁷⁸Hf resonance are almost equal. So the subgroup method hypothesis of non-correlation between neutron source and reactions is not valid because neutrons absorbed in the resonance can come from scattering in the resonance itself. The subgroup method is not applicable here and a solution could be a more refined energy mesh at this energy. [15].

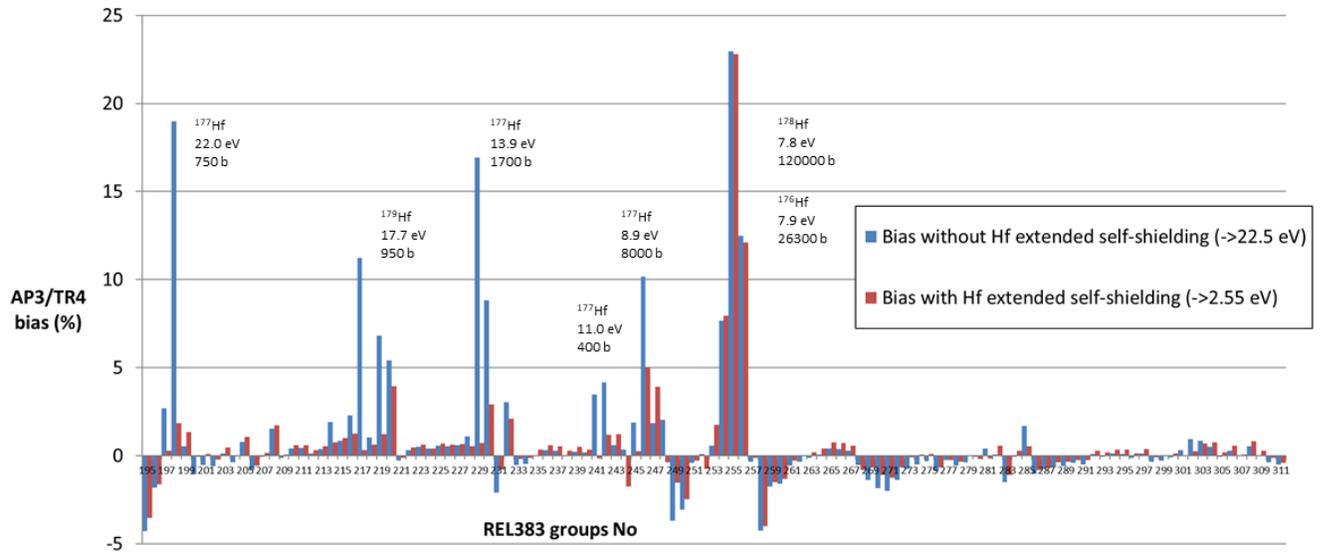


Figure 6. AP3/TR4 Absorption rate Bias in Hf

To conclude on infinite lattice predictions, iso-HORUS3D/N gives good results for the prediction of fuel elements without Hf despite biases compensations, which are avoided with the new APOLLO3[®] scheme. For the prediction of the fuel element with Hf, the new scheme significantly improves the agreement on reaction rates with respect to iso-HORUS3D/N prediction, especially for Hf control rod.

4.2. 2D Core Results

In this sub-section, we presents results on the core configurations described previously. The results for the six factors and absorptions/fissions rates are compared between iso-HORUS3D/N scheme and the new APOLLO3[®] scheme.

In the infinite lattice calculation, factor $X_{n/2n}$ corresponds to the ratio between the neutrons production rate during generation (n-1) and the neutron absorption rate during generation n. In an infinite lattice, all neutrons are absorbed into a medium. In a full-core situation, neutron can leak out of the geometry and not be absorbed; the leakage factor is lower than one. The product $X_{n/2n}$.leakage is larger than one, so we can suppose that the leakage factor out of the geometry is negligible.

Table VIII. Six factors results on core geometry

Factors	TRIPOLI-4 values	Iso-HORUS3D/N scheme bias (pcm)	New AP3 scheme bias (pcm)
$X_{n/2n}$.leakage	1.00811	+ 8	+ 25
ϵ_{odd}	1.00368	- 2	- 1
ϵ_{even}	1.08633	- 3	- 4
p	0.84585	- 183	- 146
f	0.73454	+ 235	+ 88
η	2.04256	- 8	- 7
k-eff	1.39490	+ 46	- 45

The results on reactivity show a positive bias for the iso-HORUS3D/N scheme while it is negative for the new APOLLO3[®] scheme. On the six factors, we can observe with the iso-HORUS3D/N scheme a bias compensation of about ± 200 pcm between the factor that represents the effect of resonant absorptions during the slowing down (p) and the factor that represents thermal neutrons absorption outside fuel (f). The new scheme significantly improves the prediction of the thermal absorption outside fuel with a bias reduced from +235 pcm to +88 pcm. Factor p is also better predicted compared to the iso-HORUS3D/N scheme. Therefore, the new APOLLO3[®] scheme improves the prediction of the six factors formula.

Fission rates predictions are close, but slightly better, for the iso-HORUS3D/N scheme as it can be seen on figures 7 and 8. For the two schemes, the most important bias is observed near the Zr screen where the fission rate is over-predicted. Spatial refinement near the Zr screen and its self-shielding do not improve the fission rate results. A more precise analysis of this bias is required in terms of energy, and isotopes. Zr isotopes cross sections have many resonances (particularly ⁹¹Zr) which are not especially taken into account in the current group structure. ⁹¹Zr cross section hold many scattering resonances between 200 eV and 5 keV. As it was observed for ¹⁷⁸Hf, subgroup method is not totally applicable for these resonances because neutrons scattered in these resonances can come from scattering in the same resonance. A more refined energy mesh in these resonances is considered again to improve the predictions.

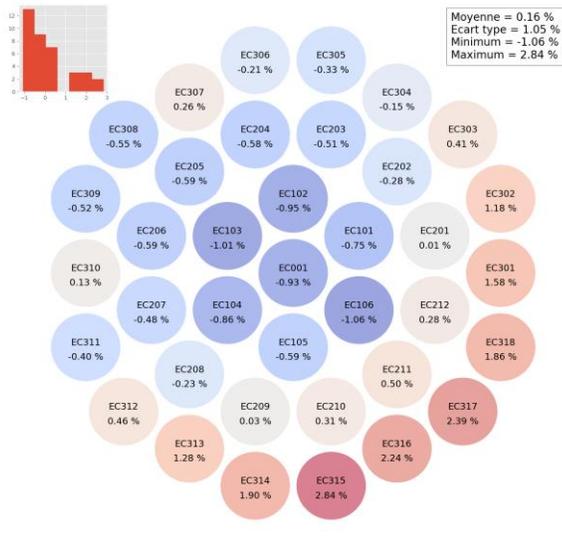


Figure 7. AP3-TR4 Bias on Fission Rates per Assembly iso-HORUS3D/N Scheme.

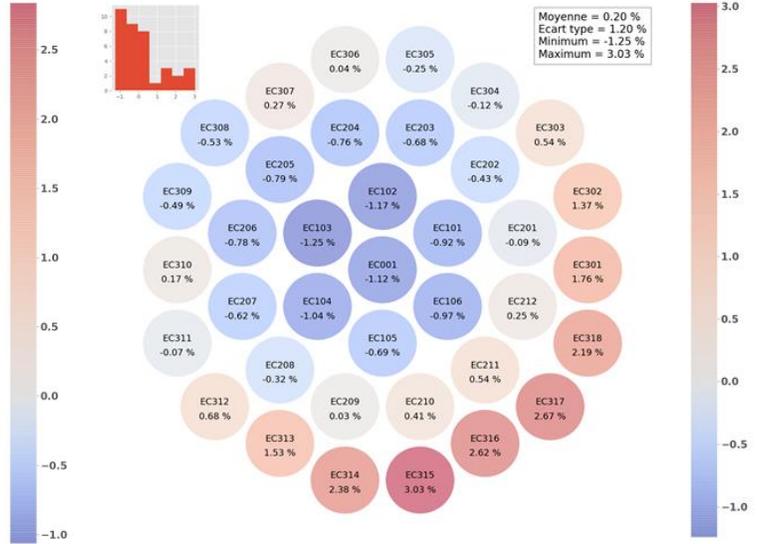


Figure 8. AP3-TR4 Bias on Fission Rates per Assembly new APOLLO3® Scheme.

In table IX, the first column represents the number of the assembly where the Hf control rod is inserted. We observe that the new scheme improves the predictions of the absorption rate in Hf as observed on the lattice results.

Table IX. AP3-TR4 comparisons on absorption rate in Hf control rods

Assembly element control rod	Bias on absorption rate in Hf control rods, iso-HORUS3D/N scheme	Bias on absorption rate in Hf control rods, new AP3-scheme
EC106	+ 2.1 %	+ 1.2 %
EC306	+ 2.5 %	+ 1.7 %
EC311	+ 2.6 %	+ 1.9 %
EC314	+ 4.4 %	+ 3.8 %
EC316	+ 4.7 %	+ 4.1 %

5. CONCLUSION

With this work, a first step in defining a reference APOLLO3® neutronics scheme to model the JHR reactor has been developed. The changes in the new APOLLO3® scheme compared to the former HORUS3D/N scheme come from the self-shielding, the energy groups and spatial mesh refinements. The first comparisons at the lattice step and core step show an overall good performance. The main improvements are observed for the Hf control rod efficiency with a better prediction of the resonant absorption rates. However, it appears that this neutronics scheme requires improvements in the treatment of the ¹⁷⁸Hf 7.8 eV resonance which is poorly represented by the group scheme itself and in the Zr screen reflection which requires both accurate slowing down and spatial treatment.

At that stage of its development, the new scheme is dealing with a 2D core slice at beginning of life. This step is used to check improvements in homogenized and condensed cross sections for the fuel assembly and the radial reflector. The objective is now the development of a 3D neutronics scheme with depletion

thanks to the Sn solver MINARET. This will lead to a reference deterministic scheme with APOLLO3[®] able to model JHR core characteristics and its experimental assemblies with high accuracy without the need to refer to Monte Carlo calculations hence in a friendlier and quicker way.

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APOLLO3[®] and TRIPOLI-4[®] are registered trademarks of CEA. We gratefully acknowledge Framatome and EDF for their long-term partnership and their support.

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