JHR neutron deterministic calculation scheme improvement thanks to monte carlo analysis in depletion

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JHR NEUTRON DETERMINISTIC CALCULATION SCHEME IMPROVEMENT THANKS TO MONTE CARLO ANALYSIS IN DEPLETION

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ABSTRACT

The international Jules Horowitz Material Testing Reactor (JHR) is under construction at CEA Cadarache research center, in southern France. In order to perform JHR design and safety studies, a specific neutron calculation tool, HORUS3D/N, was developed. It is based on APOLLO2 and CRONOS2 deterministic codes and the European nuclear data library JEFF3.1.1. The validation step aims at quantifying the computation tool performances, i.e. the biases and uncertainties associated with HORUS3D/N computations. These biases and uncertainties were in particular assessed by comparing HORUS3D/N deterministic calculations with a reference computation route using a heterogeneous geometry in 2D and 3D.

The recent development of the new CEA's Monte Carlo burn-up code, TRIPOLI-4® version 10, offers the opportunity to study JHR configurations during depletion with a probabilistic computation code.

This paper presents, as a complement to the validation step, comparisons performed between HORUS3D/N and TRIPOLI-4® code with its new depletion capability. The study is performed on 2D and 3D computations for different JHR core configurations. It focuses on the reactivity discrepancies as functions of burnup and neutron leakage.

Finally, these comparisons will contribute to improve the computation options of the HORUS3D/N calculation scheme. It has been used in order to upgrade the depletion of the boron insert in the reflector and the axial neutron leakage. Improvements consist in an increased number of energy groups (in the homogenized cross section calculations), the removal of transport/diffusion equivalence factors, and a refined geometric modeling.

KEYWORDS: JHR, HORUS3D/N, TRIPOLI-4®, MONTE-CARLO DEPLETION

1 INTRODUCTION

The Jules Horowitz Reactor (JHR) [1] is the future Material Testing Reactor under construction in southern France. Its first criticality is foreseen by the beginning of next decade. It will be a major research infrastructure in Europe, designed to support existing power plant operations and lifetime extension, as well as future material studies. Its objectives are:

- to test the new structural materials and fuel behavior under irradiation for the development of the GEN-III and GEN-IV reactors,
- to demonstrate the satisfactory stainless steel behavior for current French Pressurized Water Reactor (PWR) lifetime extension,
- to supply 25% to 50% of the European demand for radio-isotopes, mainly ^{99}Mo, for medical applications [2].

The design and safety studies have been carried out using the neutron calculation tool, HORUS3D/N, developed since the 2000s to meet the specific needs of JHR [3]. It is a two-leveled deterministic calculation scheme using the JEFF-3.1.1 nuclear data library.
In this paper, after a brief description of JHR, the HORUS3D/N calculation scheme will be presented. Then, the paper will provide the first results of the comparison between HORUS3D/N and TRIPOLI-4® depletion computations. Currently, the validation process of HORUS3D/N uses, as references, Monte Carlo (3D) simulations at step 0, and APOLLO2-MOC (2D) simulations in depletion. The goal of the benchmark is to improve the validation process of HORUS3D/N by performing 3D calculations in depletion with a Monte-Carlo code and comparing it to the deterministic ones.
The study will be performed on 2D and 3D cases, for different JHR core configurations. It will focus on the main parameters of interest: reactivity, neutron leakage and boron concentration as functions of burnup. Finally, the paper will give prospects for HORUS3D/N scheme improvements brought by this first analysis.

2 THE JULES HOROWITZ REACTOR

The JHR is a tank-in-pool type reactor using light water as its coolant and moderator, with a maximum thermal power of 100 MW.
The reactor will start with a standard density low enriched U_3Si_2 fuel (e% ^{235}U = 19.75%, density 4.8 g.cm^{-3}), and a 70 MW thermal power. It will operate with a cold fuel (fuel temperature~100°C) and a slightly pressurized light water (mean pressure: 8 bars; inlet temperature: 30°C; flow rate: 7400 m^3/h). The core can be loaded with 34 to 37 fuel elements, inserted in an aluminum alloy rack (see Figure 1). The fuel elements (see Figure 1) are made of 3 sets of curved plates assembled with aluminum stiffeners and cladded with Al-Fe-Ni. A boron insert is positioned 1 cm above the active height in each plate to prevent nucleate boiling departure at the top of the core water channels. A hafnium control rod, connected to an aluminum follower (the follower is an aluminum tube replacing the absorber part of the control rod when it is withdrawn) can be loaded in the central hole of the fuel assembly. The core area is surrounded by a reflector made of beryllium blocks which optimizes the core cycle length and provides intense thermal fluxes in this area (~5×10^{14} n/cm^2/s).
Up to 20 experimental devices can be loaded and irradiated at the same time (see Figure 1), either in the core (in the cells of the rack or in the central hole of the fuel elements) or in the reflector (in static locations or on displacement systems) in order to investigate transient regimes occurring in accidental situations.
This flexible experimental capability can create up to 16 dpa/year for in-core material experiments (to be compared to the 2-3 dpa/year produced in industrial Light Water Reactors), and 600 W.cm^{-1} for simple 1% ^{235}U enriched fuel experiments in reflector, with 275 full power operation days per year.

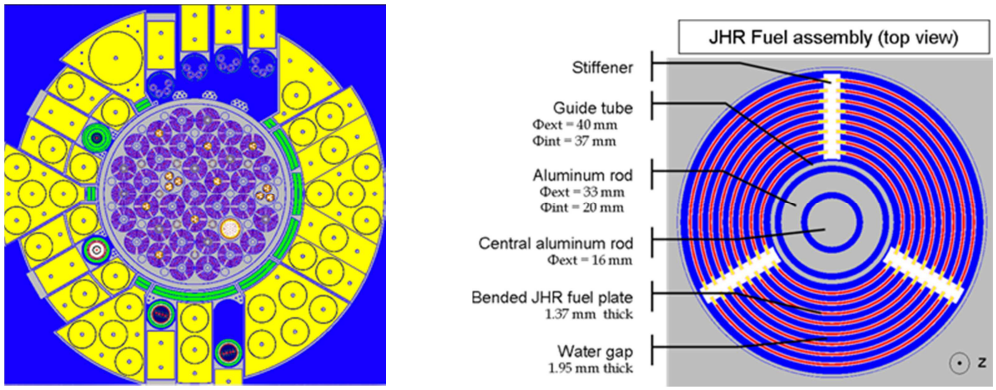

Figure 1. JHR core and assembly description

3 THE HORUS3D/N NEUTRONICS CALCULATION SCHEME

The JHR innovative characteristics led to the development of a specific neutron calculation scheme called HORUS3D/N (Horowitz Reactor simulation Unified System) [3] [4]. The HORUS3D/N deterministic scheme relies on the JEFF3.1.1 European nuclear data library [5]. It is based on a classical two-step APOLLO2 (Transport) [6]/ CRONOS2 (Diffusion) [7] deterministic calculation scheme.
The goal of HORUS3D/N is to predict, within a limited time (2 hours for 3D full core computations depleted up to 82 GWd/t_{HM} – mean end-of-cycle burn-up of the JHR core), neutron parameters with quantifiable confidence and across the JHR application domain. Thus, each new development of HORUS3D/N follows the Verification & Validation - Uncertainty Quantification process (or V&V-UQ process) [4]. This process aims at determining to what degree a calculation tool is an accurate representation of the "real world", i.e. it aims at quantifying the biases and uncertainties associated with the HORUS3D/N computations. These biases and uncertainties have two origins:

- the nuclear data which are physical parameters input and describe all the interactions between neutrons and matter,
- the models, and more generally, all the approximations used in the APOLLO2/CRONOS2 calculation scheme (approximation of the real geometry, energy meshing, resonance self-shielding, depletion, flux solver, etc.).

The biases and uncertainties of HORUS3D/N are assessed, in particular, by comparing the deterministic scheme with 2 reference routes:

- a reference route for the JHR beginning of life core calculations, based on 2D and 3D continuous-energy Monte Carlo TRIPOLI-4® [8] computations, on a heterogeneous geometry,
- a deterministic reference route for the JHR core calculations during depletion, based on 2D APOLLO2-MOC computations [9] [10], on a heterogeneous geometry.

Despite the good performances of HORUS3D/N in terms of bias and uncertainties [3], one has noticed in the validation process that the reference route in depletion is a weak point. Indeed, HORUS3D/N validation elements in depletion can be brought only for 2D calculations. The biases and uncertainties in depletion are the result of a convolution between 3D-time step 0 simulations and 2D depleting computations, thanks to advanced physical considerations.
However, currently, the axial reflector calculation scheme and the level of the cross sections library in CRONOS2 in depletion still cannot be validated. These aspects have only been studied at time step 0 by comparing HORUS3D/N calculation with 3D TRIPOLI-4® reference calculations. According to the discrepancies noticeable in Figure 2, an optimization of the the axial reflector calculation scheme is

needed. One has also to consider that discrepancies can be enlarged in depletion, unless there will be strong error compensation.

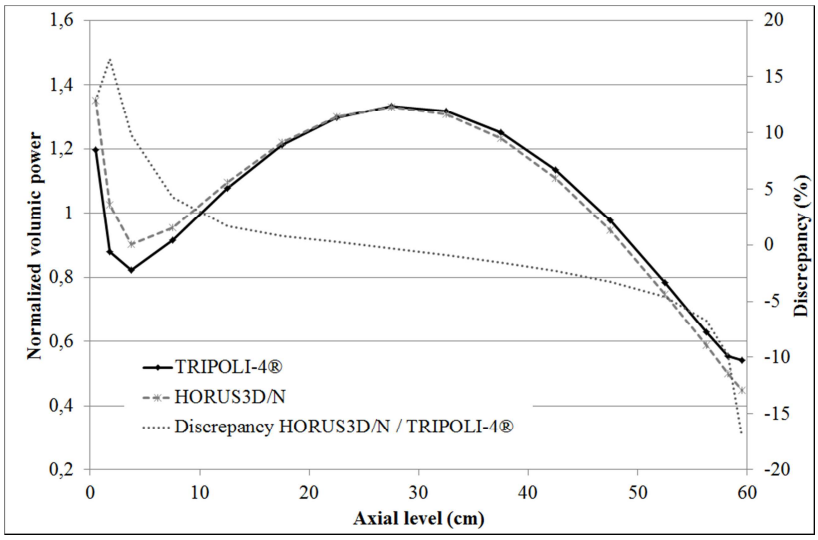

Figure 2. Axial power distribution of the JHR core – Comparison HORUS3D/N / TRIPOLI-4® at time step 0

4 COMPARISONS HORUS3D/N VS TRIPOLI-4® IN DEPLETION

The recent development of the new CEA's Monte-Carlo burnup code, TRIPOLI-4® version 10 [8] [11], offers the first opportunity to study 3D JHR core configurations in depletion with a Monte Carlo method. It relies on the use of TRIPOLI-4® for the Monte Carlo neutron transport part, and on MENDEL [11] nuclide depletion solver for the burnup calculation.

The study presented in this paper is based on the results of the first HORUS3D/N benchmark versus TRIPOLI-4® [12] [13]. The analyses are carried out on several JHR core configurations, using the same JEFF-3.1.1 nuclear data library. It quantifies the capability of HORUS3D/N to calculate neutron parameters in 3D during depletion at nominal power. Two core configurations are considered for the benchmark:

- the "test core", with 37 fuel elements, without any Hafnium rods, without any experimental device
- the "experimental core", with 34 fuel elements, 8 Hafnium rods, and the maximal core experimental loading: 7 fuel elements with experiments, and 3 cells loaded with experiments replacing fuel assemblies

The "test core" is only made of fresh fuel assemblies without any perturbation (experimental device or absorber): this is the simplest configuration. This core is studied to evaluate the HORUS3D/N performances on a simple case. The "experimental core" is much more complex because hafnium control rods and several experimentations are introduced. This core has been chosen because it is representative of the equilibrium state.

The propagation of the statistical uncertainty of TRIPOLI-4® on the isotopic concentration is evaluated in this study with independent replicas [13] [14]. It is about 0.5% at 1σ[1]. The standard deviation on the effective multiplication factor during depletion is around 25 pcm (1σ).

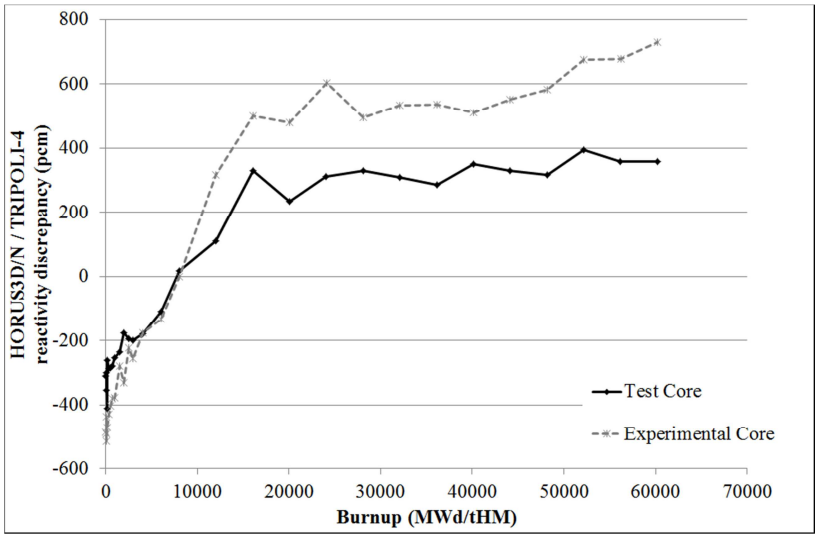

Figure 3. Multiplication factor calculations for 3D core configurations – comparison between HORUS3D/N and TRIPOLI-4® computations

Figure 3 presents the reactivity discrepancies between HORUS3D/N and TRIPOLI-4® as a function of the burnup for each of the 3D core configurations. For the studied cases, HORUS3D/N computations, when compared to TRIPOLI-4® tends to underestimate the reactivity for low burnup, and to overestimate it for burnup over ~10 GWd/t_{HM}. An increase of the reactivity discrepancies can be observed when control rods and experiments are loaded, reaching 370 pcm at the end of the irradiation phase.

Table I summarizes the main results of the benchmarks between HORUS3D/N and TRIPOLI-4®. The two cores configurations have also been studied in 2D in order to evaluate the impact of the axial modeling in CRONOS2.
One can notice that we have important discrepancies on the reactivity between the 2D and 3D calculations. This is the consequence of the inaccurate axial leakage modeling (including the boron absorption rate) in deterministic calculations. The current axial reflector library limits the performance of the calculation scheme. This point is the topic of the next part of the paper through the study of the boron consumption in the upper axial reflector part. This is of a safety issue for the JHR because boron is there to prevent nucleate boiling departure at the top of the core water channels.

[1] We performed 8 independent replicas for each case simulating $1{,}5 \times 10^6$ neutron histories per replica.

Table I. Comparison of multiplication factors: HORUS3D/N vs TRIPOLI-4® at 60 GWd/t_{HM}

		Δk HORUS3D/N vs. TRIPOLI-4®	Statistical uncertainty
Test core	**2D**	+117 pcm	13 pcm (1σ)
	3D	+358 pcm	31 pcm (1σ)
Experimental core	**2D**	+98 pcm	12 pcm (1σ)
	3D	+728 pcm	30 pcm (1σ)

5 IMPROVEMENT OF THE AXIAL REFLECTOR MODELING

The main objective of this part is to study the impact of homogenized cross sections calculation schemes with APOLLO2 on the axial reflector modeling in CRONOS2, and to determine in what extent TRIPOLI-4® depletion calculations can help to choose the best options.

Currently, the calculation scheme dedicated to the production of collapsed cross section libraries for the axial reflector with APOLLO2 is the following:

- Computation of self-shielded cross sections for the fuel assembly with a Livolant-Jeanpierre + resonant mixture method, on the 281 group SHEM [15] energy mesh,
- Collapsing on a 6 group energy mesh,
- Flux calculation in depletion with a SN solver using 6 energy groups,
- Computation of Transport/Diffusion coefficients.

The geometry used in APOLLO2 to produce collapsed cross sections libraries for the axial reflector is presented in Figure 4. It is a classical 1D-RZ geometry which represents a simplified JHR assembly made of cylinders disposed concentrically.

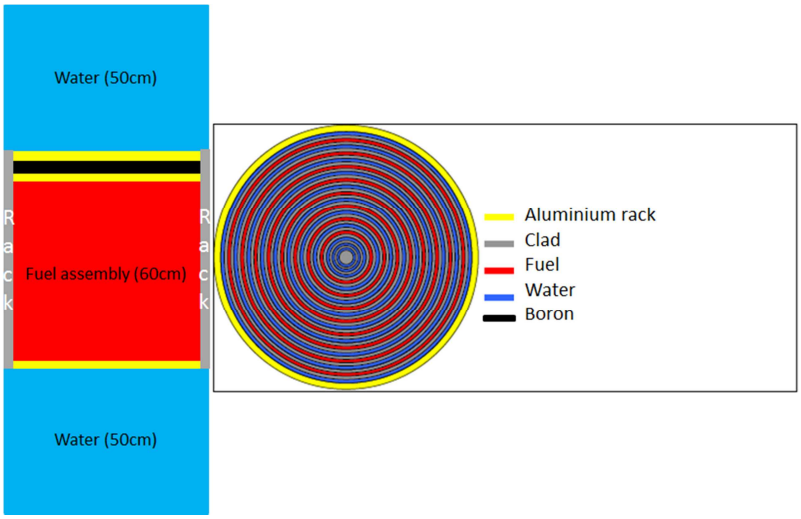

Figure 4. 1D-RZ geometry used in APOLLO2

The library contains cross sections, concentrations and equivalence factors of homogenous media that will be used in CRONOS2 to describe the axial reflector. This scheme is named “6G” in this paper.
Transport/diffusion equivalence on a 6-group mesh is sometimes quite hazardous because equivalence factors can diverge, meaning that the physical problem is not well described by the calculation.
Thus one can prefer the following calculation scheme applied on the same geometry:

- Computation of self-shielded cross sections for the fuel assembly with a Livolant-Jeanpierre + resonant mixture method, on the 281 group SHEM [15] energy mesh,
- Collapsing on an optimized 22 group energy mesh,
- Flux calculation in depletion with a SN solver using 22 energy groups,
- Cross sections collapsing on the 6 group energy mesh.

The optimized 22 group energy mesh is designed to minimize errors on main isotopes reaction rate compared to a MOC calculation (on 281 groups). This mesh is also used for the radial reflector calculation. This new scheme is named “22G”.

Moreover, CRONOS2 and TRIPOLI-4® JHR modeling differs by a geometrical characteristic: the hafnium control rod in the upper part of the reflector is not represented in CRONOS2, whereas, as shown in Figure 5, TRIPOLI-4® modeling takes it into account. Indeed, even in its upper position, the hafnium control rod is still present in the upper reflector. This will have a strong impact on the neutron leakage, the boron consumption and axial power due to the increased absorption rate in the medium representing the reflector. This is corrected in the new deterministic calculation scheme “22G-HF”.

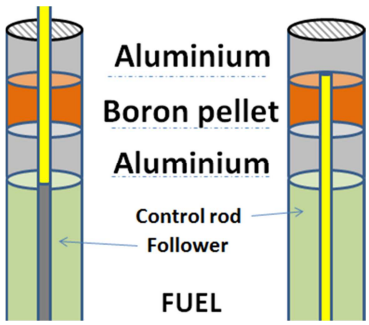

Figure 5. Schematic view of the control rod insertion in an assembly in TRIPOLI-4®

As an example, Table II presents the ^{10}B collapsed cross sections determined with the two sets of calculation scheme options in APOLLO2: “6G” and “22G-HF”. One can see significant differences in the thermal energy range. In the 5th group the discrepancy is 12.4%, and reaches 21.0% in the 6th group.

Table II. Comparisons of ^{10}B condensed total cross sections calculated with APOLLO2

(Group number) – Energy range		6G SN-RZ + equivalence			22G-HF SN-RZ
		σ (barns)	Equivalence factors	σ (barns) w. Eq. Factor	σ (barns)
(1)	**[0.951 MeV ; 19.640 MeV]**	1.78	0.875	2.03	2.06
(2)	**[7.470 keV ; 0.951 MeV]**	4.77	1.000	4.77	4.81
(3)	**[4.000 eV ; 7.470 keV]**	81.78	1.079	75.79	77.51
(4)	**[0.625 eV ; 4.000 eV]**	495.51	1.033	479.68	529.09
(5)	**[0.138 eV ; 0.625 eV]**	1112.16	1.082	1027.87	1152.73
(6)	**[10^{-10} eV ; 0.138 eV]**	4844.27	2.598	1864.62	2256.23

In this latest part of the paper, we are considering the JHR "experimental core" configuration. Two kinds of calculation are considered:

- The Monte Carlo ones: TRIPOLI-4® in depletion (the statistical uncertainty associated to the axial power is below 0.1%),
- The deterministic ones: CRONOS2. The libraries used in CRONOS2 have been determined with the three calculation schemes: "6G", "22G" and "22G-HF". Thus we have three types of CRONOS2 computations named after these schemes.

We achieved the study on a parameter that could not be validated during depletion in 3D at core scale: the boron consumption in the upper reflector part. Here, TRIPOLI-4® is going to be the starting point for a future Monte-Carlo validation in depletion.
The paragraph §5.1 is focused on the cross section library verification in 2D. In the paragraph §5.2, boron consumption on 3D core configuration is studied. Finally, consequences on reactivity are presented in the paragraph §5.3

5.1 Boron 10 consumption in upper boron plates at assembly scale

At standard assembly scale, in the CRONOS2 calculations, a large difference between the calculation schemes: "6G", "22G" and "22G-HF" is observed. It is the consequence of a combination of 3 main effects: the number of energy groups, the transport/diffusion equivalence factors and the refined hafnium rod modelling. In this chapter, we performed a separated analysis of these effects.

In Table III, the impact of the number of groups in the APOLLO2 lattice calculation can be deduced from the observation of the "APOLLO2" column. Here, we notice that the number of groups has a small influence on the total amount of boron consumed at 60 GWd/t_{HM}. The difference is only 1%.
The influence of the combination of the number of groups and equivalence factors in the CRONOS2 core calculation is seen in the "CRONOS2" column. The number of groups has a similar influence in APOLLO2 and CRONOS2 and we can say here that the equivalence factors reduce the boron consumption by around 2%. The application of equivalence factor increases the boron capture rate which leads to an overconsumption.
The analysis of the fourth column of Table III indicates that the discrepancy between CRONOS2 and APOLLO2 is reduced from 5.1% to 2.7% when the "22G" is used. This validates the CRONOS2 calculation in depletion (APOLLO2 being the reference scheme for depletion) and show that the new scheme improves our results for a standard assembly.

Table III. Impact of the transport/diffusion equivalence factors and the number of energy groups on the boron consumption at 60 GWd/t_{HM} (in % of initial mass)

	APOLLO2	CRONOS2	APOLLO2/CRONOS2 discrepancy
"6G" scheme with T/D in CRONOS2	37.3%	42.4%	+5.1%
"22G" scheme	38.3%	41.0%	+2.7%
Impact of the scheme evolution	+1.0%	-1.4%	-

Furthermore, we have studied the influence of the hafnium rods presence in the axial reflector as illustrated in Figure 5. Table IV gives the impact of the hafnium rod modelling on the boron consumption at 60 GWd/t_{HM} in the deterministic codes APOLLO2 and CRONOS2. As expected, the control rod induces an important reduction of the boron consumption by around -8%. The neutron flux in the reflector is strongly reduced and then the boron capture rate is proportionally decreased.
Concerning the validation, the bias between CRONOS2 and APOLLO2 is still around 2%.

Table IV. Impact of the hafnium rod modelling in the upper reflector on the boron consumption at 60GWd/t_{HM}

	APOLLO2	CRONOS2	APOLLO2/CRONOS2 discrepancy
"22G" scheme	38.3%	41.0%	+2.7%
"22G-HF" scheme	30.8%	32.8%	+2.0%
Impact of the Hf rod	-7.5%	-8.2%	-

Finally, Figure 6 presents a summary of the previous results showing the graphical comparison of the "6G", "22G" and "22G-HF" calculation schemes at the assembly scale to the TRIPOLI-4® computation. We can notice that the evolutions of the boron calculated with TRIPOLI-4® and the "22G-HF" deterministic calculation scheme are equivalent. The boron consumption is reduced by 9.6% in CRONOS2 and now fit the Monte Carlo depletion.

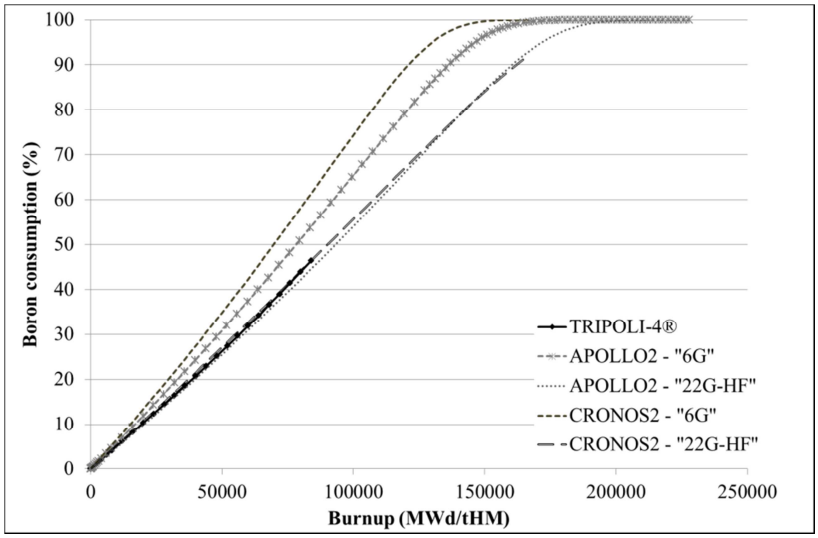

Figure 6. Comparison the boron consumption evolution in a standard assembly

5.2 Boron 10 consumption in upper boron plates at 3D full core level

Although we performed several improvements of the calculation scheme, at 3D core level, we are still noticing a difference between the deterministic route and TRIPOLI-4®. As shown in Figure 7, at 60GWd/t_{HM}, the discrepancy between TRIPOLI-4® and CRONOS2-"22G-HF" is still around 10%. Despite the large value, it is worth to mention that the discrepancy compared to the "6G" scheme is halved: this is coherent with the observation on the 2D assembly in an infinite lattice. Current studies are focused on explaining that remaining difference in the whole core calculation and to set better modeling hypothesis in the deterministic computations using TRIPOLI-4® as a comparison point.

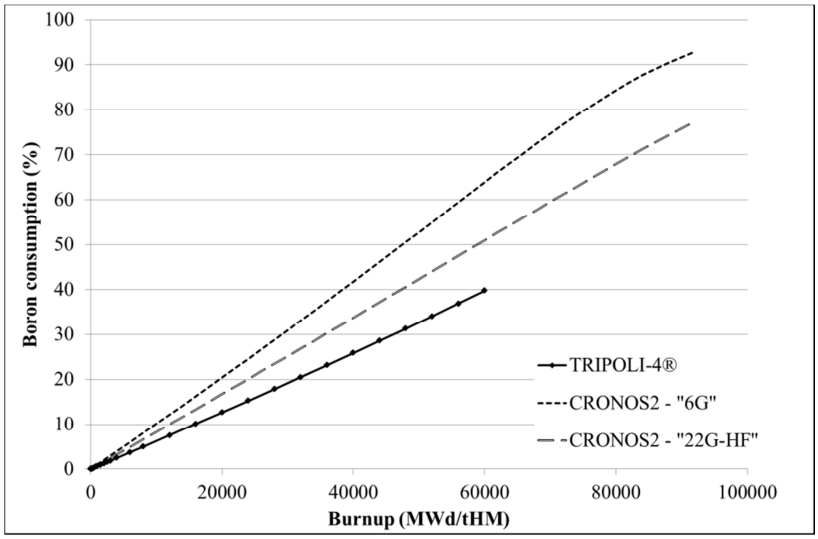

Figure 7. Comparison the boron consumption evolution in the experimental core

5.3 Impact on the multiplication factor for 3D configurations

Finally, as mentioned in the paragraph §4 and shown in Figure 8 , the new calculation scheme, “22G-HF”, allows to stabilize the discrepancy between HORUS3D/N and TRIPOLI-4® at a value around -750 pcm. The main cause is the presence of the absorber rod in the upper part of the core leading to an increased absorption rate. The boron is also consumed at a slower speed in the “22G-HF” calculation. This leads to a lower loss of reactivity.

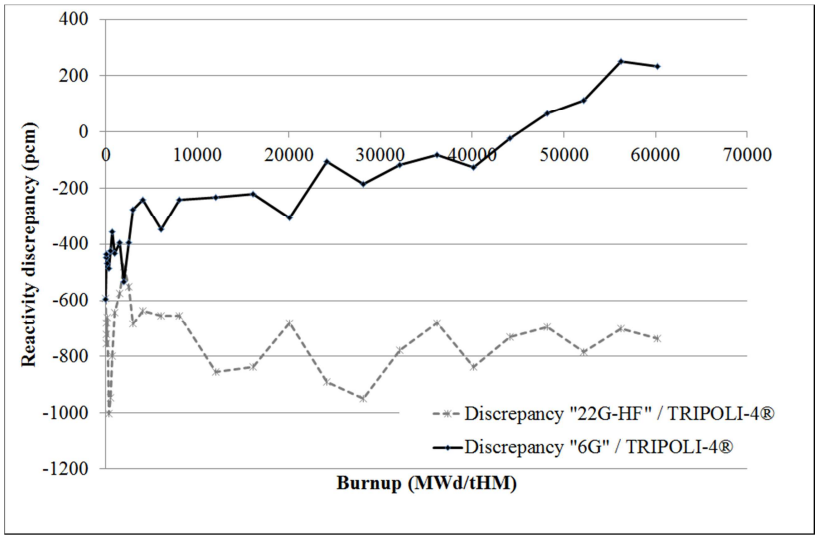

Figure 8. Deterministic to probabilistic reactivity comparison of the 3D experimental core in depletion

6 CONCLUSIONS

In this article, we presented an overview of HORUS3D/N calculation scheme dedicated to JHR neutron simulation. We also mentioned the validation process that was followed to determine the biases and uncertainties associated to the main results.

Then, a benchmark between HORUS3D/N and TRIPOLI-4® in its new depletion mode was performed. The main goal was to prove the feasibility of a 3D full core depletion computation with TRIPOLI-4® and compare it to the performances of our deterministic calculation scheme. We showed a good agreement between TRIPOLI-4® and HORUS3D/N on the reactivity evolution and boron content of axial insert.

Finally, this benchmark will contribute to improve the computation options of the scheme when future developments will be performed. In particular, we recommend the modification of the current axial reflector calculation scheme. Both at step 0 and during depletion, cross sections for the axial reflector have to be calculated with a direct transport calculation with APOLLO2 on a geometry including the control rod in the upper part of the reflector, and one should not use Transport/Diffusion equivalence factors. This leads to improve significantly the results concerning the depletion of the boron insert in the reflector.

The new neutron calculation tool dedicated to JHR operation and loading studies that will be developed on HORUS3D/N basis will benefit from these improvements.

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