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VALIDATION OF HORUS3D/N AGAINST TRIPOLI-4[®]D FOR CORE DEPLETION CALCULATION OF THE JULES HOROWITZ REACTOR

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ABSTRACT

The international Jules Horowitz material testing Reactor (JHR) is under construction at CEA Cadarache research center, in southern France. Its first criticality is foreseen by the end of the decade. In order to perform JHR design and safety studies, a specific neutronics calculation tool, HORUS3D/N, based on the deterministic codes APOLLO2 and CRONOS2 and on the European nuclear data library JEFF3.1.1, was developed to calculate JHR neutronics parameters taking into account fuel depletion: reactivity, power distribution, control rod reactivity worth, etc. Up to now, the biases and uncertainties on the different neutronics parameters computed with HORUS3D/N were assessed, in particular, by comparing HORUS3D/N deterministic calculations with reference route calculations based on APOLLO2-MOC and TRIPOLI-4[®]. The use for JHR of the recent Monte-Carlo TRIPOLI-4[®] in its new Depletion mode (TRIPOLI-4[®]D) will also allow providing biases for the main neutronics parameters under fuel depletion conditions. These biases will give a quantitative estimation of the impact of the approximations of the flux calculation in the deterministic route. This paper presents a contribution to the validation of HORUS3D/N based on the first comparisons between the calculations performed with APOLLO2-MOC and CRONOS2, and the ones from TRIPOLI-4[®]D. The study is performed on 2-D calculations for two different clusters in an infinite lattice configuration. It focuses on the main parameters of interest: isotopic concentrations, plate power distributions, reactivity, as functions of burnup. The results obtained show reasonable discrepancies with APOLLO2 calculation and allow to be confident on the APOLLO2.8/REL2005/CEA2005 package recommendations developed by CEA for light water reactor studies used in HORUS-3D/N. In particular, the main fuel isotopes are well predicted with TRIPOLI-4[®]D with discrepancies values lower than -1.5%.

Key Words: **Depletion calculation, Monte-Carlo, HORUS-3D/N, JHR, TRIPOLI-4[®]D.**

1. INTRODUCTION

The Jules Horowitz Reactor (JHR) is a new Material Testing Reactor (MTR) under construction at the CEA Cadarache research centre (south of France) [1]. Replacing the French MTR OSIRIS (shut down in December 2015), the JHR will contribute to the improved safety of the existing fleet of

reactors and to their optimization. This will be achieved through the development and qualification of nuclear fuel and materials exposed to high irradiation rates, thus leading to an accelerated ageing of the samples compared to the nominal exposure in a power plant. In the context of life-time extensions and the progressive deployment of Generation III reactors, the JHR will be a major tool for research and industry-driven investigations. The JHR will also be devoted to medical isotopes production for imaging and therapeutic purposes.

The design and safety studies have been carried out using the neutronics calculation tool HORUS3D/N, developed since the 2000s to meet the specific needs of JHR [2].

After a description of the JHR, this paper will focus on the dedicated HORUS3D/N neutronics package and on the recent Monte-Carlo Burnup transport code TRIPOLI-4[®]D. Then, the paper will provide the first results of the contribution to the validation of HORUS3D/N in depletion based on TRIPOLI-4[®]D and performed on two different clusters in an infinite lattice configuration.

2. DESCRIPTION OF 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. It 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 thermal power of 70 MW with possibility to reach 100 MW if needed. The core can be loaded with 34 to 37 fuel elements, inserted in an aluminum alloy rack (see Figure 1).

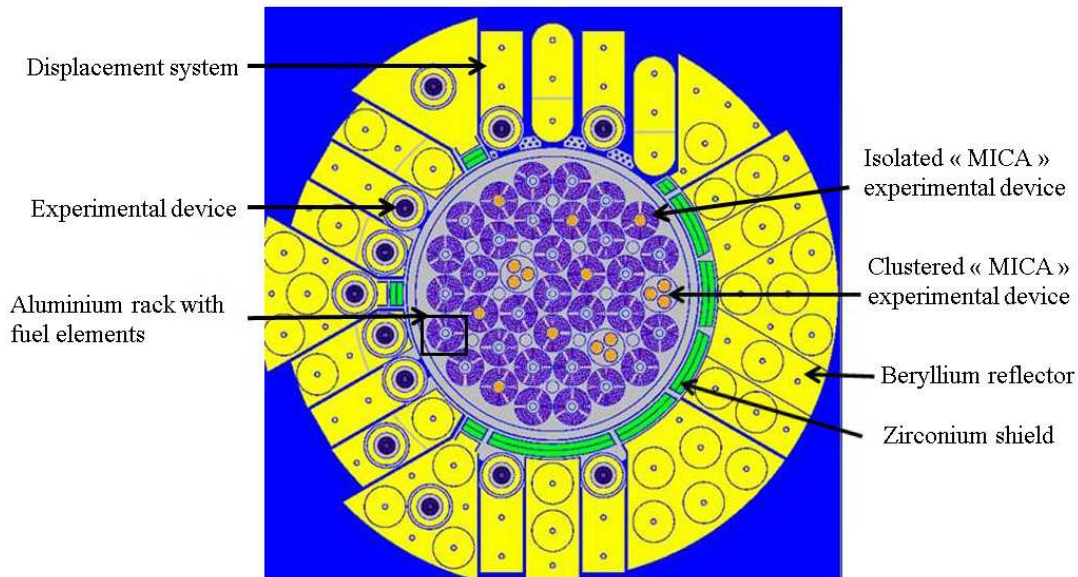


Figure 1. Layout of JHR core

Up to 20 experimental devices can be loaded in the core or in the reflector, and irradiated at the same time. In order to reach a high fast neutron flux level ($\sim 5 \times 10^{14} \text{ n/cm}^2/\text{s}$, $E \geq 0.907 \text{ MeV}$), the fuel elements (see Figure 2) are made of 3 sets of curved plates assembled with aluminum stiffeners and clad with Al-Fe-Ni. The core is surrounded by a reflector made of beryllium blocks which optimizes the core cycle length and provides intense thermal fluxes in this area ($\sim 5 \times 10^{14} \text{ n/cm}^2/\text{s}$,

$E \leq 0.625$ eV).

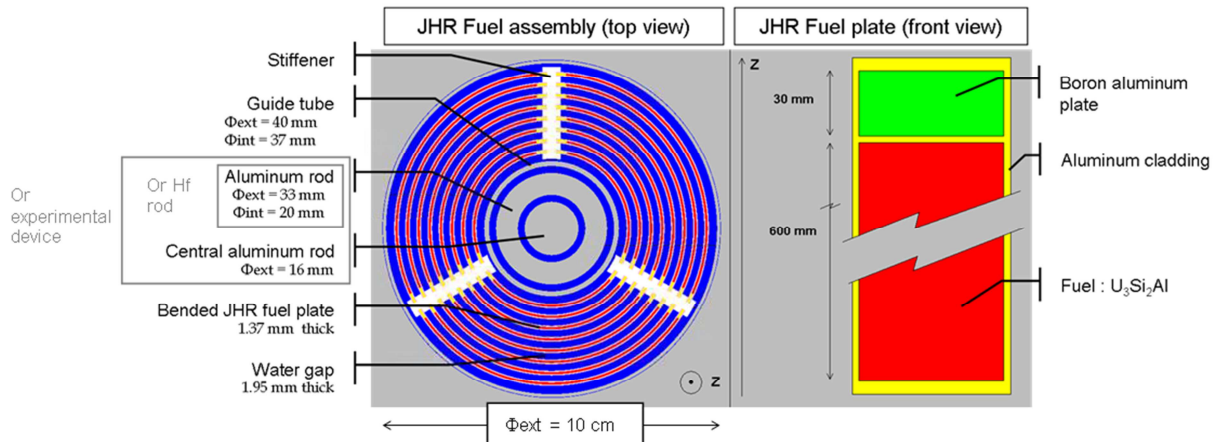


Figure 2. Schematics of JHR fuel element and fuel plate

3. DESCRIPTION OF THE HORUS3D/N NEUTRONICS CALCULATION SCHEME

The innovative character of the JHR led to the development of a specific neutronics calculation scheme called HORUS-3D/N (HOrowitz Reactor simulation Unified System). This scheme takes into account the specificities of the reactor when performing design and safety studies. The design scheme of HORUS-3D/N is based on an APOLLO2 [3] / CRONOS2 [4] deterministic calculation scheme and the JEFF3.1.1 European nuclear data library [5].

The HORUS-3D/N package is composed of 3 different routes:

- A “deterministic design” route for fresh fuel and for depletion, based on a two-step deterministic calculation with APOLLO2-CRONOS2. In the first step, the 2D APOLLO2 lattice code provides libraries of cross sections collapsed into 6 energy groups, tabulated versus burnup or fluence, for each kind of components present in the JHR. In the second step, these collapsed cross sections are introduced into a full 3D core calculation performed with the CRONOS2 diffusion code on a hexagonal spatial meshing.

- A reference route for fresh fuel, based on 2D and 3D continuous-energy Monte Carlo TRIPOLI-4[®] [6] calculation.

- A deterministic reference route taking into account depletion, based on 2D APOLLO2-MOC calculation.

To quantify all biases and associated uncertainties of HORUS3D/N calculations, its development follows the Verification & Validation – Uncertainty Quantification (V&V-UQ) process [2].

4. MONTE-CARLO VALIDATION IN DEPLETION WITH TRIPOLI-4[®]D

Up to now, the validation process of the scheme only relied on TRIPOLI-4[®] Monte-Carlo calculations for fresh fuel and on APOLLO2-MOC deterministic calculations in depletion. The adaptation for the JHR of the recent TRIPOLI-4[®]D Monte-Carlo Burnup transport code developed by the CEA will also allow providing biases for the main neutronics parameters (reactivity, power factors, etc.) under fuel depletion conditions. Therefore such biases will give a quantitative estimation of the im-

part of the approximations used in the deterministic depletion route.

4.1. TRIPOLI-4[®]D Code

TRIPOLI-4[®]D was developed by coupling the probabilistic code TRIPOLI-4[®] and the new CEA depletion code system MENDEL [7] based on a deterministic solver. Both interfaces are linked to the C++ interpreter CINT allowing to build advanced coupling schemes between transport and burnup solvers, which are either run interactively, or compiled and executed with coupling scripts. This interpreter belongs to the ROOT libraries developed at CERN under a LGPL public license [8]. In order to solve the transport/depletion coupling, two different methods are available for the time discretization: an explicit Euler method and a Predictor-Corrector method. For a given time t , the Euler approach consists in calculating the flux ϕ_t and reaction rates corresponding to the isotopic vector at this time; then, a depletion calculation using this flux ϕ_t provides the isotopic vector at the end of the time step. Concerning the 2nd order Predictor-Corrector method, two schemes are available: one called “midpoint” based on the assumption that the flux calculated at the middle of the time step gives the best description of the flux behaviour during the whole time step; and one called “mean” which consists in calculating the new isotopic vector by averaging the vectors obtained at the beginning and at the end of the time step respectively.

Figure 3 describes the TRIPOLI-4[®]D architecture.

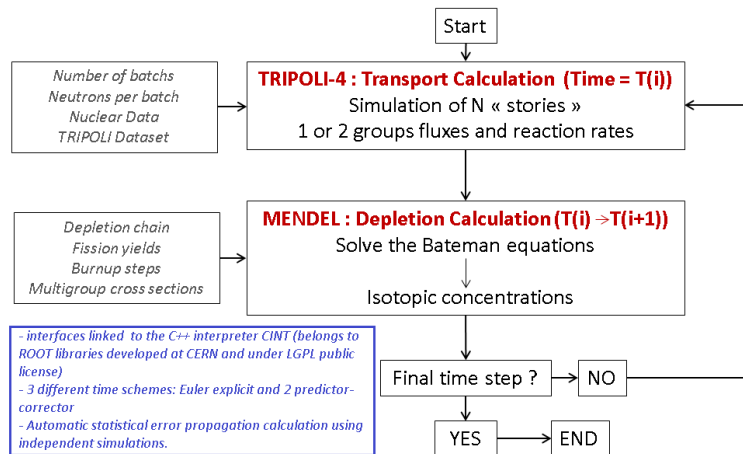


Figure 3. TRIPOLI-4[®]D architecture

Two different depletion methods are implemented in the MENDEL code: an analytical one which consists in an exact mathematical solution of the Bateman equations in a matrix format; and a numerical one based on the Runge-Kutta method (4th order). In the context of the coupling, the Runge-Kutta method is used. This method which does not depend on the isotopes relationships is well suited to treat pure depletion problems. The depletion chain used by MENDEL is translated from the APOLLO2 standard depletion chain. 160 isotopes are tracked in the burnup calculation including 26 actinides and 126 fission products. Although the MENDEL depletion solver does not allow statistical errors propagation, errors on isotopic concentrations can be taken into account thanks to perturbative methods or independent simulations.

4.2. Preliminary Results of the Benchmark APOLLO2 / CRONOS2 / TRIPOLI-4[®]D

Two different assemblies in an infinite lattice configuration were chosen for the first step of this validation study:

- an heterogeneous standard assembly (referred to as STD) hosting a control rod aluminum follower;

- an heterogeneous assembly with a control rod inserted (referred to as CNT) and surrounded with homogeneous standard assemblies (fresh fuel) in order to represent an infinite lattice. A 27% enriched fuel is considered. This corresponds to the enrichment value needed to operate at 100 MW, with cycle duration equal to 25 days at least.

Calculations were performed using a pattern of 7 assemblies that is representative of the central area of the reactor core. The central assembly of this pattern is either a STD or CNT one, and it is surrounded by 6 heterogeneous standard assemblies (see Figure 4.).

The APOLLO-2 MOC assembly calculations use the SHEM-281 groups energy cutting [2].

The TRIPOLI-4[®]D 2D assembly calculations were performed using 1500 batches of 1500 neutrons per simulation. These simulation parameters allow obtaining a standard deviation on the infinite multiplication factor of 85 pcm for each replica of the calculation which could not be reduced due to calculation time constraints. For the purpose of the comparison, the TRIPOLI-4[®]D burnup steps were chosen as the APOLLO-2 ones. 32 independent replicas were run in order to treat the issue of statistical error propagation. In the context of the validation study, all the results are given for a temperature of 20°C.

The following two sub-sections will present the first results of the validation work. All the discrepancies will be given taking into account the results of the APOLLO2-MOC calculations as reference ones.

4.2.1. 2D Standard Assembly (STD) Calculations

The calculations were performed up to 150 GWd/t_{HM}, which corresponds to the maximum average burnup of the assembly during operating conditions. Concerning the TRIPOLI-4[®]D modelling, 1/6th of an assembly was considered (see Figure 4). Each of the eight fuel plates is described as a different medium for the depletion calculation.

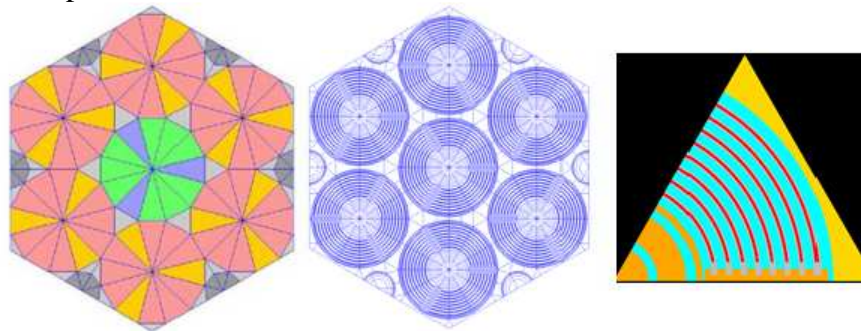


Figure 4. STD assembly with environment geometric pattern for CRONOS2 (left) and APOLLO2 (in the center) and TRIPOLI-4[®]D (right)

It is important to emphasize that, for this type of calculations, up to a burnup of 150 GWd/t_{HM}, using the Predictor-Corrector option, the required TRIPOLI-4[®]D calculation time was about 6 weeks, corresponding to 2.5 weeks of CPU time.

As mentioned above, two different methods are available for time discretization in TRIPOLI-4[®]D. A previous comparison between the results given by the Euler and the Predictor-Corrector method performed on the same kind of assembly, showed a progressive shift of the TRIPOLI-4[®]D results as function of burnup [9]. This effect starts from a burnup of 100 GWd/t_{HM}. For a burnup of 150 GWd/t_{HM}, a discrepancy of 300 pcm ± 25 pcm (2σ) is observed.

Figure 5 presents the evolution of the infinite multiplication factor during depletion and the evolution of the bias due to the time discretization method, as estimated from both the earlier and the current work. The TRIPOLI-4[®]D calculations from the earlier work [9] are also included in the plot. Errors bars indicate the value of 2 standard deviation taking into account the 32 replicas which is multiplied by 100 to make it readable. The results obtained show that the bias increases quasi-exponentially with the burnup.

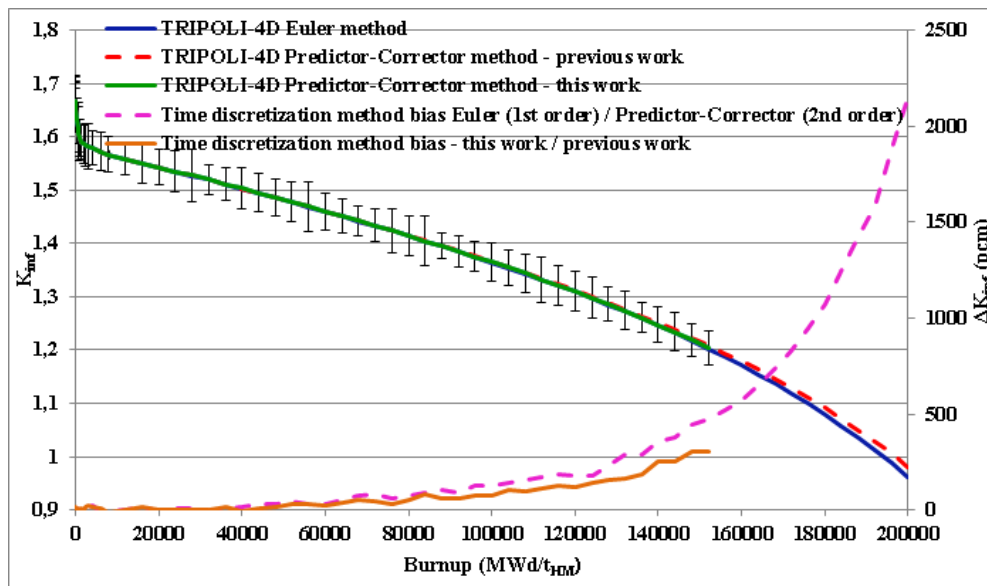


Figure 5. Evolution of the infinite multiplication factor in depletion and evaluation of the bias due to the time discretization methods: Euler (1st order) and Predictor-Corrector (2nd order) – STD assembly case

The difference between the discrepancies estimated in this work and in the previous one (respectively orange full line and pink dashed line in Figure 5) is due to the cluster time constraint which has an impact on the concentration data loading, however the same trend is found. Indeed, using the Predictor-Corrector method, two flux calculations are needed in order to calculate the new concentrations for the next transport calculation. Nevertheless, if one of these two calculations is not performed within the allocated 24h hours, only the first flux calculation is used. As a result of using this flux for the concentration calculation, the new inventory seems to have been obtained thanks to the Euler method. This study highlighted that the implementation of such a TRIPOLI-4[®]D calculation using the available cluster is a compromise between the loading of the concentration for each

new calculation step and the targeted standard deviation.

The Predictor-Corrector method using the “mean” scheme was selected for this study because it is second-order accurate. In addition, this choice has the advantage to avoid numerical issues that are typical of the explicit Euler method and that may require severe limitations in terms of the maximum allowable time-step. It should be mentioned that this method is consistent with the APOLLO2 one.

The comparison of the discrepancies respectively between the APOLLO2-CRONOS2 (7 assemblies considered) and APOLLO2-TRIPOLI-4[®]D calculations (1/6th assembly considered) with the Predictor-Corrector method, is given in Figure 6. The results from previous investigations [9] are also included. The discrepancy between APOLLO2 and CRONOS2 is due to the diffusion and homogenization approximations, as well as the behavior ¹⁴⁹Sm and ¹³⁵Xe in the depletion process (i.e., concentrations build up to their equilibrium values) for a burnup value lower than 10 GWd/t_{HM}. Using TRIPOLI-4[®]D, a good consistency is obtained in comparison with APOLLO2, with a positive shift lower than 90 pcm ± 37 pcm for a burnup of 120 GWd/t_{HM} in the previous and than 40 pcm ± 37 pcm in the current work.

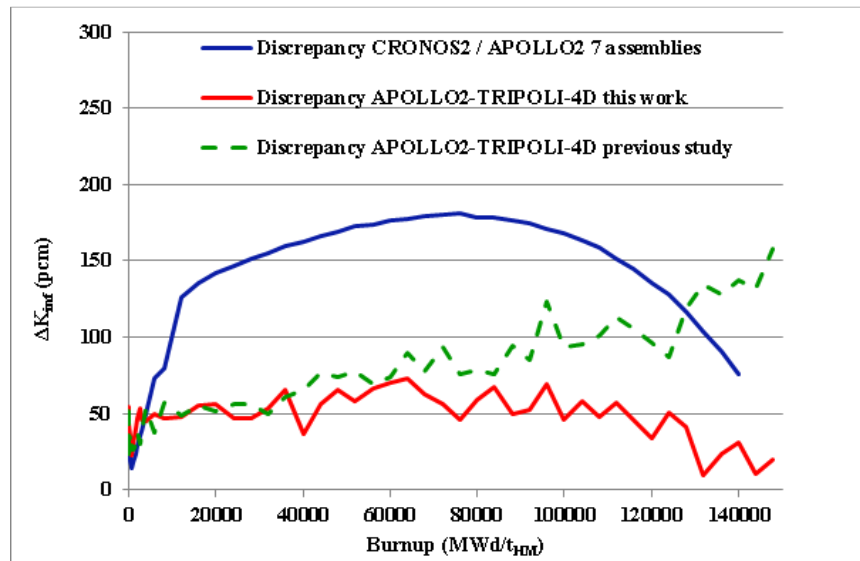


Figure 6. k_{inf} calculations for the STD assembly– comparison between APOLLO2, CRONOS2 and TRIPOLI-4[®]D

The second parameter of interest is the evolution of the masses of the main isotopes in depletion: ²³⁵U, ²³⁸U, ^{239,240,241}Pu, ¹³⁵Xe and ¹⁴⁹Sm. All the comparisons are performed on an assembly sector. The masses given by CRONOS2 for the heavy nuclides are estimated by an interpolation of the APOLLO2 data for the corresponding burnup value of the considered mesh. In JHR, the burnup corresponds, on a first order approximation, to the number of ²³⁵U nuclei consumed so the ²³⁵U inventory in depletion has to be well predicted. Even for high burnups, the observed discrepancy does not exceed -0.5 % between the APOLLO2 and the TRIPOLI-4[®]D calculations and -3.0% between the APOLLO2 and the CRONOS2 calculations (see Figure 7).

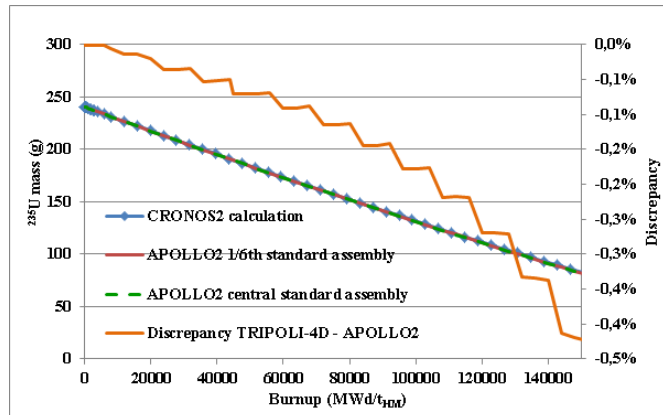


Figure 7. Evolution of the ^{235}U mass in depletion – comparison of the APOLLO2, CRONOS2 and TRIPOLI-4[®]D results in the STD assembly case

Concerning the ^{238}U chain isotopes, the same good consistency of the results can be noticed (see Figure 8). For a burnup 150 GWd/ t_{HM} , the maximum bias does not exceed -0.6 % in the case of APOLLO2 – TRIPOLI-4[®]D comparison. The higher values, observed at low burnups for $^{239,240,241}\text{Pu}$, are only due to the small amount of these isotopes in the fuel at the beginning of the irradiation period.

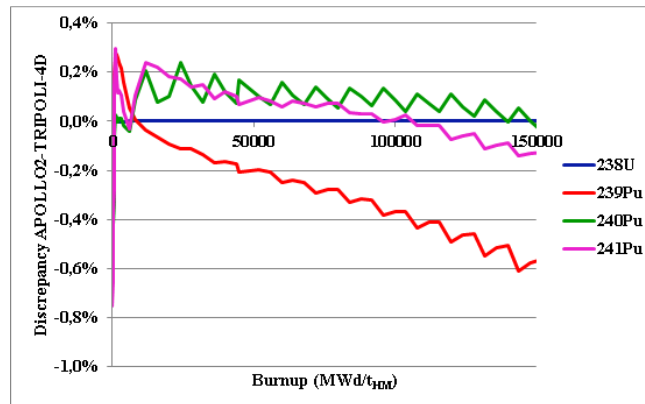


Figure 8. Evolution of the ^{238}U chain isotopes masses in depletion: discrepancies APOLLO2-TRIPOLI-4[®]D – STD assembly case

Despite the value of the standard deviation in TRIPOLI-D calculations, the comparison with APOLLO2 shows a good consistency of the two modellings. The relevance for JHR of the APOLLO2.8/REL2005/CEA2005 package recommendations developed by CEA for light water reactor studies used in HORUS-3D/N (refined SHEM energy mesh and resonant mixture self-shielding treatment for ^{235}U , ^{238}U , ^{239}Pu and ^{240}Pu in the intermediate energy range) [2] is not called into question.

Concerning the two main fission products studied, ^{135}Xe and ^{149}Sm , the discrepancies between the APOLLO2 and TRIPOLI-4[®]D results, within a burnup range up to 150 GWd/ t_{HM} , do not exceed -1% and -1.5%, respectively (see Figure 9). The consistency on material balance confirms the ap-

plicability of the SHEM mesh for a MTR light water reactor as well as for other light water reactor systems.

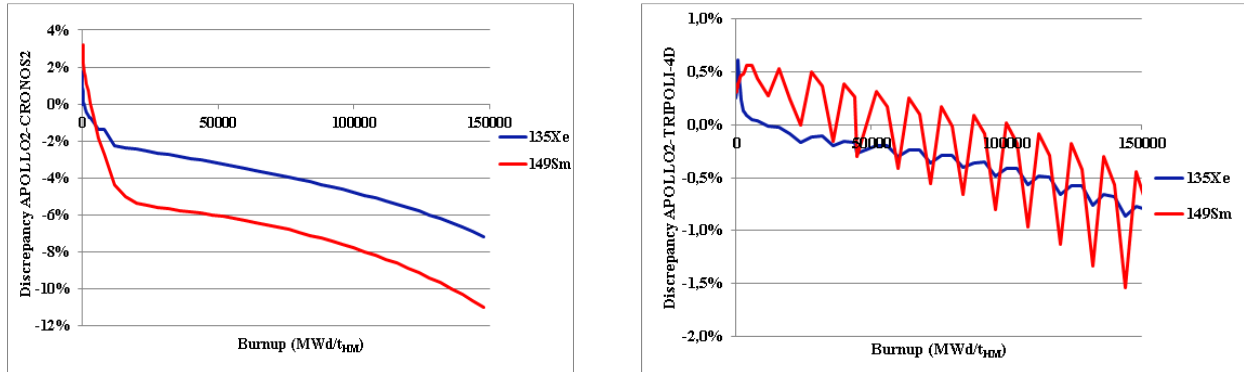


Figure 9. Evolution of the ^{135}Xe and ^{149}Sm masses in depletion: discrepancies APOLLO2-CRONOS2 and APOLLO2-TRIPOLI-4[®]D – STD assembly case

From the APOLLO2-CRONOS2 comparison of the predicted mass of ^{135}Xe , the discrepancies reach +2% at the beginning of the irradiation period, and -7% for a burnup of 150 GWd/t_{HM}. As regards ^{149}Sm , the bias between APOLLO2 and CRONOS2 is +3.2% at the beginning of the irradiation period and -11% for a burnup of 150 GWd/t_{HM}. These deviations are due to the concentrations build up of the two isotopes to the equilibrium value, and to the different modelling methods. The results concerning the discrepancies in absolute values of power per plate are directly linked to the observed trends of ^{235}U inventory as shown in Table 1. A systematic bias is observed.

Table 1. Power per plate discrepancies – comparison APOLLO2-TRIPOLI-4[®]D in the STD assembly case

Plate No	APOLLO2-TRIPOLI-4 [®] D discrepancy			
	BU = 37,5 MWd/t _{HM}	STD 2σ	BU = 150 GWd/t _{HM}	STD 2σ
1 (internal)	-2,53%	± 0,05 %	-1,56%	± 0,06 %
2	-2,07%	± 0,07 %	-1,57%	± 0,04 %
3	-1,59%	± 0,05 %	-1,43%	± 0,04 %
4	-1,76%	± 0,04 %	-1,78%	± 0,04 %
5	-1,45%	± 0,03 %	-1,69%	± 0,03 %
6	-1,61%	± 0,04 %	-1,97%	± 0,05 %
7	-1,53%	± 0,05 %	-2,19%	± 0,04 %
8 (external)	-1,77%	± 0,04 %	-2,31%	± 0,04 %

4.2.2. 2D Assembly with Inserted Control Rod (CNT)

In the CNT case, the TRIPOLI-4[®]D and APOLLO2 models consider the same 7 assemblies geometric pattern. In every fuel assembly, each of the eight fuel plates is described as a different medium for the depletion calculation.

As for the STD configuration, the first results, given for low burnup values, show a good agreement between the three k_{inf} trends in depletion (see Figure 10). For a burnup value of 56 GWd/t_{HM}, the difference of the APOLLO2 prediction against CRONOS2 and TRIPOLI-4[®]D is about 300 pcm. This discrepancy is due to: the homogeneous/heterogeneous transport equivalence; the homogenization; and the reduction of energy groups considered in the CRONOS2 calculation. The effect is such that APOLLO2 underestimates the neutronic worth of the control rod. The underestimation of the control rod worth involves a local overestimation of the flux.

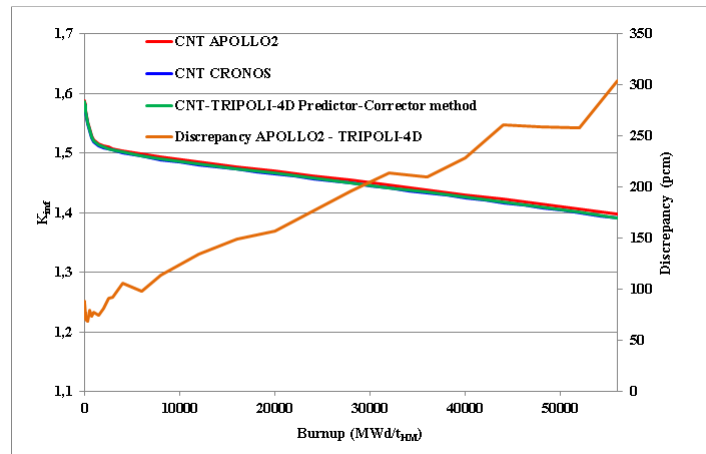


Figure 10. k_{inf} calculations for the CNT assembly – comparison between APOLLO2, CRONOS2 and TRIPOLI-4[®]D

This can also be illustrated by the similar evolution of the ²³⁵U mass in depletion. Figure 11 shows a discrepancy which increases with the burnup and reaches 4.3% in the case of the APOLLO2-TRIPOLI-4[®]D comparison.

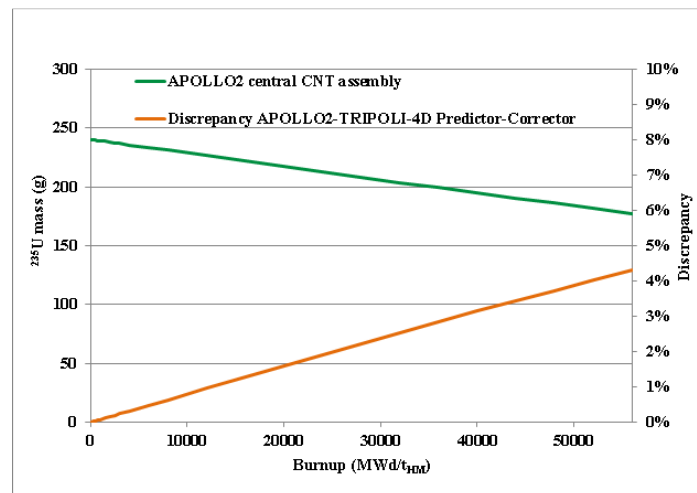


Figure 11. Evolution of the ²³⁵U mass in depletion – comparison of APOLLO2 and TRIPOLI-4[®]D results in the CNT assembly case

The second step of this validation work, is currently under study, and deals with core calculations in two different configurations, respectively for average burnups of the core up to 20 GWd/t_{HM} and up to 60 GWd/t_{HM}. The two configurations of interest are defined as follows:

- 34 fuel elements, 5 fixed absorbers in the rack between the assemblies, 13 control rods, and aluminum experimental devices loaded in the core (starting core configuration);
- 34 fuel elements, 8 control rods, with reference experimental loading that is arranged in 7 fuel elements and 3 cells.

The performed tests showed that 72 hours are required for a core calculation up to 20 GWd/t_{HM} using 500 batches of 5000 neutrons per simulation. These simulation parameters allow obtaining uncertainty standard deviation on the infinite multiplication factor of 80 pcm for each replica. In spite of the system size, the difference in computational time between assembly and core calculation is due to the difference in the simulation parameters used between the two cases.

5. CONCLUSIONS

The HORUS3D/N neutronics calculation tool is dedicated to JHR design and safety analysis. Up to now, the validation process of the scheme only relied on TRIPOLI-4[®] Monte-Carlo calculations for fresh fuel. The adaptation for the JHR of the recent TRIPOLI-4[®]D Monte-Carlo Burnup transport code developed by the CEA will also allow provide biases for the main neutronics parameters (reactivity, power factors, etc.) under fuel depletion conditions. The first step of the validation study consisted in a comparison between the calculations performed with APOLLO2 and TRIPOLI-4[®]D, and the ones from CRONOS2, in 2D, for two different assemblies in an infinite lattice configuration: a standard one (STD) and an assembly with a control rod inserted (CNT). The 2nd order Predictor-Corrector method using the “mean” scheme was chosen for time discretization in the TRIPOLI-4[®]D calculation because it is second-order accurate and to avoid numerical problems. Despite the significant standard deviation of the TRIPOLI-4[®]D calculations, the results show reasonable discrepancies with APOLLO2 calculation and allow to be confident on the APOLLO2.8/REL2005/CEA2005 package recommendations developed by CEA for light water reactor and used in HORUS-3D/N. In particular, the discrepancies between TRIPOLI-4[®]D and APOLLO2 in terms of the main fuel isotopes are lower than -1.5%. The investigation of the CNT configuration highlights an increase of the bias when a disturbance is introduced in the modelling, even for low burnup values, due to an underestimation of the control rod reactivity weight with APOLLO2. The main results of the work are summarized in Table 2.

Table 2. HORUS3D/N validation against TRIPOLI-4[®]D: summary of the first results

	STD (up to 150 GWd/t_{HM})	CNT (up to 56 GWd/t_{HM})
T4D Euler/Predictor bias	$\Delta k_{inf} = 300 \text{ pcm} \pm 25 \text{ pcm} (2\sigma)$	/
Δk_{inf} APOLLO2/CRONOS2	Max = 170 pcm at 80 GWd/t _{HM}	340 pcm
Δk_{inf} APOLLO2/ TRIPOLI-4[®]D	$< 50 \text{ pcm} \pm 37 \text{ pcm} (2\sigma)$	$300 \text{ pcm} \pm 30 \text{ pcm} (2\sigma)$
Isotopic content (mass) APOLLO2/TRIPOLI-4[®]D discrepancy	$-0.5\% < {}^{235}\text{U} < 0\%$	$0\% < {}^{235}\text{U} < 4.5\%$
	$-1\% < {}^{238}\text{U}, \text{Pu isotopes} < 1\%$	$0\% < {}^{238}\text{U} < 0.5\%$
	$-1.5\% < {}^{135}\text{Xe}, {}^{149}\text{Sm} < 1\%$	$-15\% < {}^{135}\text{Xe} \text{ and } {}^{149}\text{Sm} < -4\%$
Power per plate	$-3\% < \text{AP2/T4D discrepancy} < 0\%$	/

Core calculations for configurations of interest are currently under study as a second step of this validation work.

The outcome could provide recommendations for the development of the HORUS-3D/N scheme concerning the depletion model.

As a future complement of the work, a benchmark between TRIPOLI-4[®]D and MCNPX-ORIGEN (for the same selected configurations) is planned so that the capability of the TRIPOLI-4[®]D depletion solver can also be assessed against a different Monte-Carlo burnup tool using the same nuclear data library.

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