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## VERIFICATION OF THE DEPLETION CALCULATION SCHEME OF AN HIGHLY HETEROGENEOUS PWR CORE DESIGN

S. Mengelle, S. Douce, F. Damian  
<sup>1</sup>CEA, DEN, Saclay, DM2S/SERMA  
F-91191 Gif-sur-Yvette, France

Tel: +0033169088327, Fax: +0033169089935, Email: [stephane.mengelle@cea.fr](mailto:stephane.mengelle@cea.fr)

*Abstract –In order to enhance the fuel utilization in Light Water Reactors and save resources, it is necessary to increase the conversion of fertile material ( $^{238}\text{U}$ ) and ( $^{239}\text{Pu}$ ). This can be obtained by designing low moderation PWR fuel assemblies which enhance the conversion of  $^{238}\text{U}$  into  $^{239}\text{Pu}$ . To ensure a high level of performance, the introduction of fertile elements is mandatory. This kind of design would therefore be complex to model. The flux gradient at the boundary between fissile fuel and fertile blankets is difficult to estimate by using a standard neutronic model based on transport-diffusion calculation schemes. The presence of fissile and fertile zones in the core leads to modify the standard calculation scheme based on a transport-diffusion calculation to take into account this heterogeneity. As a consequence, such transport calculations (first step of the calculation) which are performed in fundamental mode on a 3x3 cluster of fuel assemblies representative of the core loading pattern needs to be verified. Up to now, such verification was performed on static configurations by comparisons with the Monte-Carlo code TRIPOLI-4<sup>®</sup>. New capability for depletion calculation has been recently introduced in the reference Monte-Carlo code TRIPOLI-4<sup>®</sup> by coupling it with the depletion module of the MENDEL code. This allows now to model the burnup depletion of a complex 3D geometry with TRIPOLI-4<sup>®</sup>. This type of calculation is used as a reference to verify deterministic multi-groups calculations. This paper presents the comparisons between these two types of calculations in order to verify the performances and evaluate the safety criteria of highly heterogeneous core designs.*

### I. INTRODUCTION

To ensure a sustainable energy supply and face global warming, nuclear energy appears as a mandatory solution. Pressurized Water Reactors (PWRs), that represent the largest part of the French power plants, will produce the major part of the nuclear electricity during the current century. Thus the continued deployment of PWRs with their low uranium utilization leads to design alternative concepts.

The future of nuclear energy requires a new strategy for fuel management, particularly for the plutonium stockpile. In order to reach a better use of plutonium and save resources, a modified neutron spectrum, characterized by an increase of the average neutron energy is required to increase the conversion of  $^{238}\text{U}$  (fertile element) into  $^{239}\text{Pu}$  (fissile element). This can be obtained by designing low moderation PWR fuel assemblies (FA). Physical aspects of High Conversion Pressurized Water Reactors (HCPWR) are described in [1, 2, 3] and innovative high conversion PWR fueled with (U, Pu) mixed oxide is presented in [4]. The  $^{235}\text{U}$  enrichment in PWRs is about 3-5% and the typical conversion ratio\* is about 0.5. A lower moderation ratio allows enhancing the conversion ratio thanks to the reduction of the resonance escape probability and the

increase of the fertile capture rate in  $^{238}\text{U}$  and, therefore better uranium utilization.

However, core design going towards low moderation ratio presents several potential difficulties: positive moderator temperature coefficient, positive void coefficient, reduced control rod worth efficiency and thermal-hydraulic limitations.

Basic design studies of low moderation ratio PWR fuel assemblies have been performed with the purpose of achieving a high conversion ratio. A reasonable conversion ratio of 0.82 could be achieved with a MOX fuel and a moderation ratio of 1.27 (compared with a value close to 0.5 in a standard PWR). Furthermore, the quality of the discharged fuel is not too degraded with a low moderation ratio. This is a key point concerning the possibility of deploying such a concept in a nuclear plant.

The design of this type of reactor – heterogeneous core composed of fissile materials and fertile blankets – leads to complex phenomena. The flux gradient at the boundary between fissile fuel and fertile blankets is difficult to estimate using standard neutronic models based on transport-diffusion calculation schemes. The presence of fissile and fertile zones in the core (both radial and axial heterogeneities) leads to enlarging the calculation geometry used in the first step of the calculation scheme

\* In this paper, the conversion ratio is defined as the ratio between discharged fissile mass to loaded fissile mass

(transport calculation in fundamental mode). As a consequence, such transport calculations, which are performed on a 3x3 cluster of fuel assemblies representative of the core loading and heterogeneities, need to be verified.

Until a recent period, such verification was performed on static configurations by comparisons with the Monte-Carlo code TRIPOLI-4<sup>®</sup> [2]. Capabilities for depletion calculations have been recently introduced in TRIPOLI-4<sup>®</sup> [5]. TRIPOLI-4<sup>®</sup> is now coupled with the depletion module of the MENDEL [6] code and is able to model the burnup depletion of a complex 3D geometry. TRIPOLI-4<sup>®</sup> uses pointwise cross sections and doesn't make any geometrical approximations. These calculations are used as a reference to verify deterministic multi-groups calculations. This paper presents the comparisons between these two types of calculations in order to verify the performances and evaluate the safety criteria of highly heterogeneous core designs.

## II. HCPWR: PRESENTATION OF DESIGN

### II.A. Problematics of plutonium recycling in PWRs

The recycling of plutonium in standard PWRs leads to a harder neutron spectrum. Core reactivity coefficients and reactivity control elements are therefore degraded. The limitations on the use of plutonium consist of keeping a negative coolant void coefficient, having acceptable soluble boron efficiency and keeping enough negative reactivity for shut-down.

Different options were considered in HCPWR in order to maintain negative neutronic coefficients to ensure core stability with a high plutonium content:

- The total plutonium content and consequently the burnup were limited to avoid any possibility for the voided core to be critical (around 20%).
- The reduction of the active core height compared to standard PWRs increases the surface over volume ratio and raises core leakage proportion which has a beneficial impact on the void coefficient.
- Modifications of the core content by adding fertile elements (depleted uranium ~0.2% of <sup>235</sup>U).

The soluble boron impact on the reactivity at hot and cold moderator conditions is reduced in HCPWR. It has implications on the beginning-of-cycle (BOC) critical boron concentration at refueling, cool-down and emergency shutdown. The use of enriched boron is considered in this design (50% of <sup>10</sup>B).

### II.B. Thermal-hydraulic considerations

The modification of the moderation ratio obtained by decreasing the ratio pitch / diameter leads to an increase of the Critical Heat Flux (CHF) and pressure drop in the core. Thermal-hydraulic analyses were performed to

demonstrate that HCPWR with moderation ratios ranging from 0.9 to 1.3 are technically feasible (both nominal operation and transient conditions). No major difficulties were observed with the tested core configurations.

## III. MAIN CHARACTERISTICS OF THE HCPWR

Several designs of HCPWRs using heterogeneous arrangement in the core are being evaluated at the CEA. Among these design, one of them is presented in this paper. It tries to combine the double advantage of a low moderation ratio and the presence of blanket elements in the core (arranged axially and radially). It is noteworthy that the external size of the core is consistent with the standard EPR vessel.

This HCPWR, with a moderation ratio of 1.27, is close to the standard PWR, but with a tight square pitch fuel rod 19x19 lattice to minimize moderation and to achieve a high conversion ratio of around 0.82 (HCPWR-19x19, see Figure 1 and table I). Two types of assemblies are inserted in the core:

- Heterogeneous fissile assemblies (208) composed of fissile material alternately with fertile material (see Figure 2).
- Homogeneous fertile assemblies (33) composed of fertile material only (see also Figure 2).

The double heterogeneity (radially and axially) leads to high performance relative to the void coefficient.

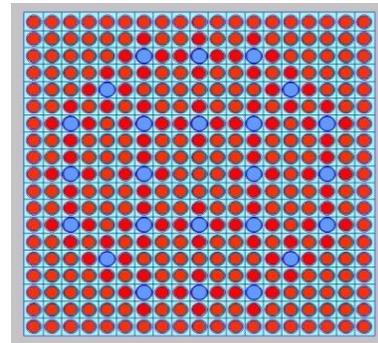


Fig. 1. Geometric description of the HCPWR 19x19 FA

TABLE I  
 Main characteristics of the HCPWR 19x19 FA

<b>Number of rods in x and y</b>	19
<b>Height (cm)</b>	360
<b>Assembly Pitch (cm)*</b>	21.61
<b>Number guide-tubes (GT)</b>	24
<b>Number rods (fissile or fertile)</b>	337
<b>Fuel rod pitch (cm)*</b>	1.13
<b>Pellet radius (cm)*</b>	0.41
<b>Clad radius (cm)*</b>	0.48
<b>Inner radius of GT (cm)*</b>	0.48
<b>Outer radius of GT (cm)*</b>	0.52
<b>Elementary moderation ratio**</b>	1.08
<b>Global moderation ratio**</b>	1.27
<b>Global moderation ratio***</b>	1.27

- (\*) Values are given in hot condition  
 (\*\*)  $Rmod_{elementary} = V_{mod} / V_{fuel}$  in a cell  
 $Rmod_{global} = V_{mod} / V_{fuel}$  in the assembly  
 (\*\*\*)  $Rmod_{global} = Nbre_{H2O} / Nbre_{heavy\ metal}$  in the assembly

Figure 2 presents on the left side the top view of the reactor core with the location of the two types of assemblies and on the right side the axial representation of the two different types of assemblies.

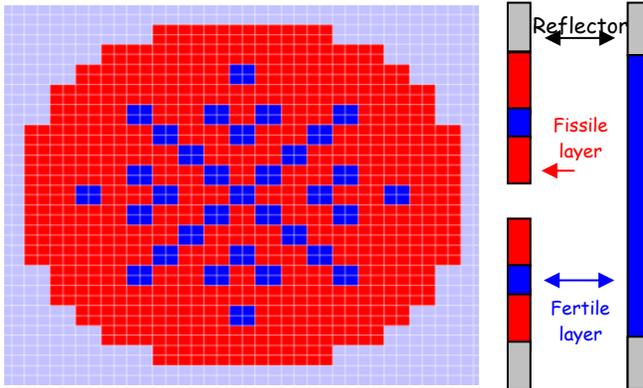


Fig. 2. Geometric description of the HCPWR 19x19 core

The plutonium vector used in the fissile layer contains 56% of fissile elements. The plutonium enrichment in the fuel is 19.7%. The isotopic composition of the plutonium vector is presented in table II.

TABLE II  
 Plutonium vector used in the MOX HCPWR 19x19 FA

<sup>238</sup> Pu	<sup>239</sup> Pu	<sup>240</sup> Pu	<sup>241</sup> Pu	<sup>242</sup> Pu	<sup>241</sup> Am
3,03%	48,73%	30,63%	7,34%	9,80%	0,74%

The core loading pattern presents an IN/OUT arrangement and refueling is done by quarter (see Figure 3). It leads to a reduction of the fluence received by the vessel by positioning fresh fuel in the inner part of the core.

The main characteristics of the HCPWR 19x19 core are summarized in table III. Thermal power and core diameter correspond to the standard EPR reactor. The total quantity of fertile elements in the core is about 27%.

It is important to note that the number of control rod cluster assemblies is greater than in the EPR core (89). The design of the RCCAs pattern was done by considering only the respect of safety criteria during a shut-down margin evaluation.

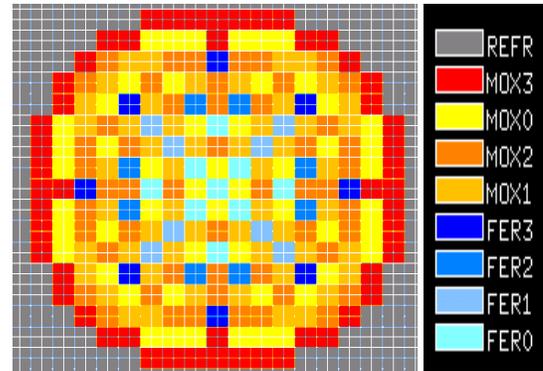


Fig. 3. Loading pattern of the HCPWR 19x19 core

TABLE III  
 Main characteristics of the HCPWR 19x19 core

Thermal Power (MWth)	4250
Electric power (MWe)	1450
Number of loop	4
No. of Assemblies (fissile/fertile)	241 (208/33)
Active height (m)	3.60
Fissile height (m) in MOX FA	3.05
Fertile height (m) in MOX FA	0.55
Fertile % in core	26.9
No. of RCCA (AIC + B4C)	100

### III. CALCULATION MODELS

#### III.A. Lattice calculation using the deterministic code APOLLO2

The calculation code used for deterministic lattice calculations is APOLLO2, developed at the CEA [7, 8, 9]. One of the major objectives of this code is to produce multi-parameterized cross section libraries, collapsed in space and energy, devoted to core calculations. The core calculations are performed using CRONOS2 [10]. APOLLO2 and CRONOS2 are part of the SAPHYR code package [11] developed by French Atomic Energy Commission. It is used and qualified for diverse neutronics applications (PWR, VVER, BWR,...). Nuclear cross-section libraries are derived from the JEFF3.1.1 evaluation [12].

APOLLO2 is a modular code for multi-group transport calculations in 2-D geometries and for depletion calculations. The code calculates the heterogeneous flux inside the fuel assembly, the critical buckling and the depleted compositions. The code solves the multi-group transport equation either by the collision probability method, the SN method or the method of characteristics (MOC).

The depletion calculation used in this study is based on a single level calculation scheme using the characteristics method and 281 energy group mesh. At the end of the

calculation all the depleted media are stored in order to perform restarted calculations.

To reduce calculation time, the calculation scheme used for restarted steps is a double level calculation. The first level uses the collision probability method with a 281 energy group mesh [8] to generate microscopic cross-sections collapsed on a 26 energy group mesh. These cross sections are used in a second level by the characteristics method.

The calculation is performed on a 2-D geometry representing 1/8<sup>th</sup> of a 3x3 cluster of assemblies (see Figure 4) with reflective boundary conditions.

The number of calculation meshes in the fuel is optimized to accurately take into account the rim effect (four rings to represent self-shielding and depletion effects)

A fertile assembly is positioned at the center of this cluster to simulate realistic core conditions. Fertile pins are represented in green in Figure 4, guide-tube cells in gray and fissile pins in red.

A self-shielding calculation is performed on the cluster described in Figure 4 (multicell  $P_{ij}$  method) for eleven isotopes in the fuel ( $^{235}\text{U}$ ,  $^{238}\text{U}$ ,  $^{238}\text{Pu}$ ,  $^{239}\text{Pu}$ ,  $^{240}\text{Pu}$ ,  $^{241}\text{Pu}$ ,  $^{242}\text{Pu}$ ,  $^{241}\text{Am}$ ,  $^{243}\text{Am}$ ,  $^{243}\text{Cm}$ , and  $^{237}\text{Np}$ ) and the self-shielding mixture model is applied to take into account shadow effects between the main resonant isotopes ( $^{238}\text{U}$ ,  $^{239}\text{Pu}$ ,  $^{240}\text{Pu}$ ,  $^{241}\text{Pu}$ ) [12]. The Doppler Effect is systematically calculated for the fission products. A self-shielding calculation is performed during the depletion calculation when the concentrations are higher than  $10^{-10}$  ( $10^{23}\text{At./cm}^3$ ).

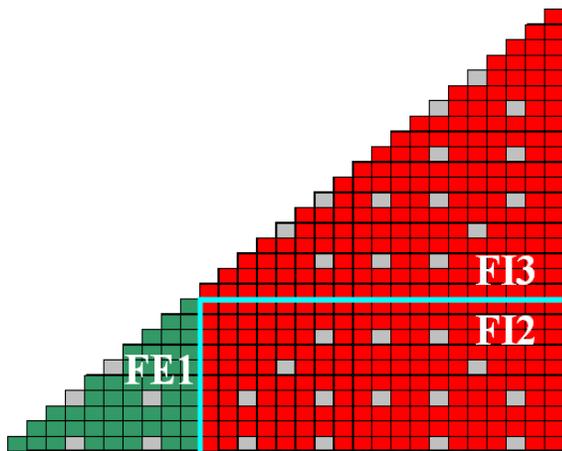


Fig. 4. Cluster of assemblies used to generate collapsed cross sections for CRONOS2

Concerning the flux calculation, the characteristics method is used with the following options:

- Linear flux on the geometric mesh [14]
- Tracking with a distance between two tracks  $\Delta R=0.1$  cm and number of azimuthal angles  $\Delta\phi=24$

- Cross sections are developed as 5<sup>th</sup> order Legendre polynomials.

The flux calculated is different for each physical medium but in order to optimize the CPU time, depletion regions with a similar trend with regards to the flux distribution are grouped. Five types of cells are thus defined per assembly: corner (blue), cell with water gap (light blue), direct contact with guide-tube (red), in diagonal with guide tube (orange) and central cell without direct contact with guide tube (yellow) – see Figure 5). During the depletion a flat flux is assumed between two burnup steps to insure the consistency with the time scheme selected for the TRIPOLI-4<sup>®</sup> calculation.

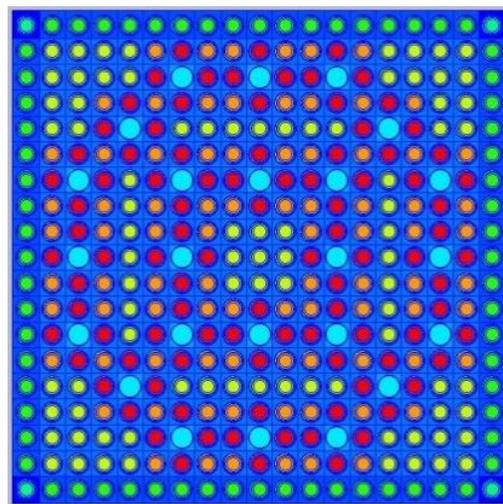


Fig. 5. Assembly Geometry used for depletion calculation

The APOLLO2 code generates N-group macroscopic cross-sections to be used in the CRONOS2 core code. These cross-sections are tabulated as a function of burn-up, boron concentration, water density, fuel temperature and rod cluster insertion.

For these calculations, the cross-section libraries generated by APOLLO2 contain microscopic cross-sections for 28 isotopes (heavy nuclides and fission products of the Xenon and Samarium chains) in order to evaluate very accurately the mass balance in the core (microscopic depletion model).

When libraries are created, cross-sections are collapsed on few energy groups and spatially homogenized. Three sets of macroscopic cross-sections are produced on this cluster (FE1, FI2, and FI3 – see Fig 4) for core diffusion calculations. A step of transport/diffusion equivalence is performed allowing for the preservation of the reference reaction rates.

### III.B. Core calculations using the deterministic CRONOS2 code

The CRONOS2 code has been designed for providing all the computational tools needed for reactor calculations. The code can perform 3D core calculations including steady state, kinetic and transient multi-group calculations. Thermal-hydraulic feedback is modeled using specific modules.

The following options are used in this study:

- Diffusion method
- 2 or 8 energy group cross section libraries presented in appendix
- Gauss integration along the X, Y and Z axes for the flux and the current
- Parabolic interpolation in the X, Y and Z directions for the current
- Four spatial meshes per assembly
- A depletion chain containing 28 isotopes (20 heavy nuclides and 8 fission products)

### III.C. Reference calculation using the Monte Carlo based code TRIPOLI-4<sup>®</sup> code

The Monte-Carlo depletion calculation is based on the coupling between TRIPOLI-4<sup>®</sup> and the MENDEL depletion solver. The first step consists of calculating the microscopic reaction rates with TRIPOLI-4<sup>®</sup>. These microscopic reaction rates are then normalized to the core power level. In the second step the MENDEL depletion solver uses these data to compute the new concentrations for each medium. These concentrations are transmitted to TRIPOLI-4<sup>®</sup> for a new transport calculation. This process is reproduced all along the depletion calculation. The Bateman equations are solved assuming a flat flux between two Burnup steps. In order to propagate the uncertainties on the flux at each calculation step, a set of independent depletion calculations are performed in parallel; the values of concentrations obtained with these depletion calculations are then averaged.

For each burnup step of every simulation, 200 batches of 2000 neutrons are processed and the first twenty batches are discarded to improve the statistics. The standard deviations on the K infinity are obtained with 30 depletion calculations.

### III.D Methodologies used for the verification process

To verify the calculation scheme three kinds of models of the cluster of assembly are compared (fig. 4):

1. **TRIPOLI-4<sup>®</sup> depletion calculation:** This model is considered as the reference one. Reflective boundary conditions are considered. TRIPOLI-

4<sup>®</sup> calculations are performed with no leakage (and no critical buckling search).

2. **APOLLO2 depletion calculation:** A single level calculation using the characteristics method and 281 energy groups is performed. No leakage is considered in order to compare Monte Carlo and deterministic methods on the cluster of assemblies.
3. **CRONOS2 depletion calculation:** Few groups diffusion calculations using four meshes per assembly are performed. Multi-parameterized cross sections are produced using the calculation scheme presented in Chapter §III.A (including the critical leakage calculation to reproduce the standard calculation chain). A microscopic depletion model (using 28 particularized isotopes) is used. The diffusion coefficient is calculated using the critical leakage term and the buckling with the following formula:

$$D = \text{leakage} / B_{\text{crit}}^2.$$

The temperature of the medium and the boron concentration are fixed identically in the three models.

For this kind of comparison it is important to use similar cross-section libraries. For all these calculations, a library produced by the GALILEE project [15] based on the JEFF3.1.1 release is used.

These triple comparisons allow validating the calculation process and evaluating the discrepancies introduced by the following points:

- the self-shielding model,
- the efficiency of the characteristics method,
- the double level calculation during the libraries process,
- the diffusion method and the choice of the reduced number of energy groups.

## IV. COMPUTATIONAL TIME

The calculations with APOLLO2 and CRONOS were performed with a Linux PC Intel Xeon CPU E6-2680 V2 2.8 GHz and those with TRIPOLI-4<sup>®</sup> on a cluster using the same processors.

TABLE IV: Computational time

CRONOS2 2 groups	43 s
CRONOS2 8 groups	60 s
APOLLO2	48 h
TRIPOLI-4 <sup>®</sup>	30 x 43 h

Concerning the APOLLO2 calculation, two thirds of the calculation time is used by the flux solver and one third by the self-shielding process.

For TRIPOLI-4<sup>®</sup>, the 43 hours represents the time for one elementary depletion calculation, but in order to have a significant statistic, the process needs to be repeated several times to insure convergence. To determine the duration of the calculation it is necessary to multiply the elementary time by the number of independent simulations. These calculations are made in parallel to reduce the real time.

### V. RESULTS OF THE COMPARISON – FIRST RECOMMANDATIONS

Figure 6 presents the values of K infinity obtained with the three models presented in Chapter §III.D during the depletion.

Concerning the CRONOS2 models, the results are given for 2 and 8 energy groups. It is to be noted that static verification [4] confirms the interest of using a refined 8 group energy mesh for diffusion calculations to model voided configurations when the neutron spectrum is harder than in a nominal condition.

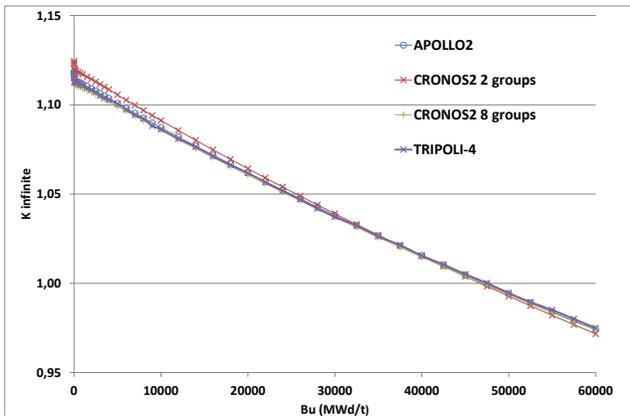


Fig. 6. Evolution of K infinity during depletion

Figure 7 presents the discrepancies on K infinity in pcm. The reference is TRIPOLI-4<sup>®</sup> and the associated error bars at three sigma are indicated on the graph.

*The two curves obtained with CRONOS2 verify the use of an energy mesh containing eight groups. The discrepancies between APOLLO2 and TRIPOLI-4<sup>®</sup> are always lower than the three sigma standard deviation. This result confirms that APOLLO2 with the MOC can be considered as a deterministic reference for this type of very heterogeneous calculation.*

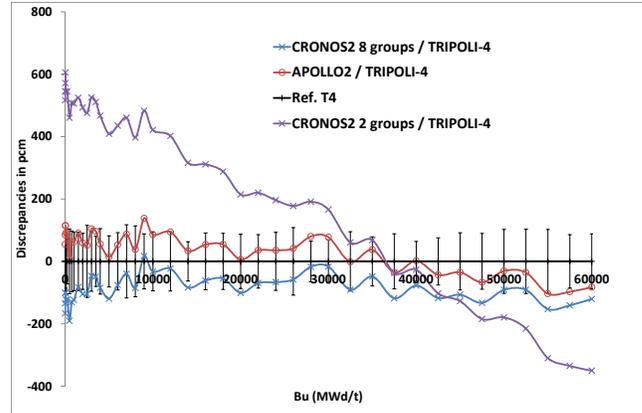


Fig. 7. Evolution of the discrepancies on K infinity and standards deviation

The following tables present the power maps and the relative discrepancies to TRIPOLI-4<sup>®</sup> results collapsed on each assembly of the cluster (the tables correspond to the geometry presented in Figure 4: one eighth of the 3x3 cluster of assembly, fertile in green and fissile in red) at 0 and 60 GWd/t.

TABLE V: TRIPOLI-4<sup>®</sup> power map at 0 and 60 GWd/t (With error bars at three sigma)

	1,099 ± 1,72 %	1,058 ± 1,58 %
0,141 ± 3,62 %	1,061 ± 1,63 %	0,603 ± 1,29 %
		1,039 ± 1,09 %

TABLE VI.A: APOLLO2 vs TRIPOLI-4<sup>®</sup> at 0 and 60 GWd/t (Power maps AP2 and relatives discrepancies)

	1,096 -0,28 %	1,058 -0,51 %
0,154 9,30 %	1,051 -0,94 %	0,603 1,80 %
		1,039 -0,53 %

TABLE VI.B: CRONOS2 2 group vs TRIPOLI-4<sup>®</sup> at 0 and 60 GWd/t (Power maps CR2 and relatives discrepancies)

	1,099 0,02 %	1,032 -2,41 %
0,152 7,78 %	1,049 -1,06 %	0,603 7,38 %
		1,020 -1,83 %

TABLE VI.C: CRONOS2 8 group vs TRIPOLI-4® at 0 and 60 GWd/t

(Power maps CR2 and relative discrepancies)

	1.100	1.017
	0.12 %	-3.86 %
0,159	1.041	1.005
13.02 %	-1.85 %	-3.29 %
	0.678	
	12.43 %	

A significant increase of power is observed in the fertile assembly during the depletion due to the production of  $^{239}\text{Pu}$  and  $^{241}\text{Pu}$ .

We can note that the discrepancies between APOLLO2 and TRIPOLI-4® are always lower than error bars in the fissile assembly. For CRONOS2 the discrepancies are a little higher; they reach -3.86% at the end of the cycle. For the fertile assembly the discrepancies are the most important at the beginning of the cycle but the powers are low.

To complete the comparison, an analysis of the deviation on the concentrations between APOLLO2 and TRIPOLI-4® on three elementary cells is performed (see Figure 8 for the positions and names of the studied cells → FISSILE1, FISSILE2 and FERTILE).

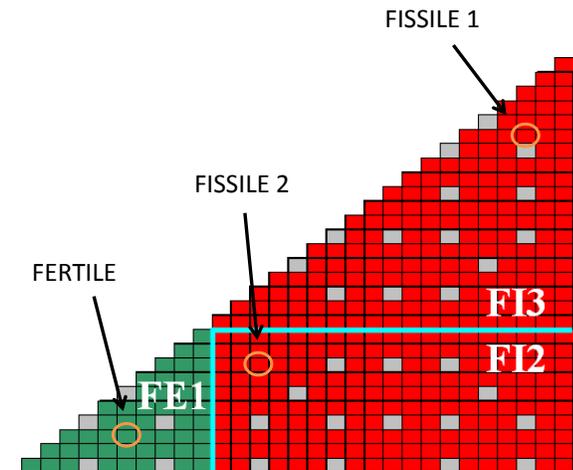


Fig. 8. Positions of the studied cells in the cluster of assembly

To take into account the rim effect all the cells are modeled with 4 rings. As shown in the following figures (Figures 9 and 10) the discrepancies between APOLLO2 and TRIPOLI-4® in the internal and the external rings are not significant for the cell named FISSILE 1 (Fig. 8). It produces a correct self-shielding and flux calculation in APOLLO2.

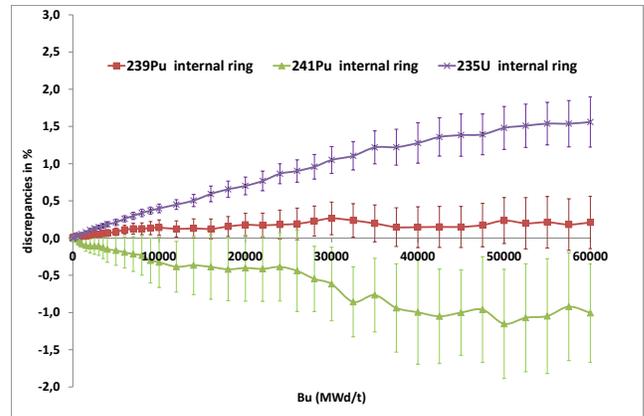


Fig. 9. Relative discrepancies on the concentrations between APOLLO2 and TRIPOLI-4® [cell named FISSILE 1 - internal ring]

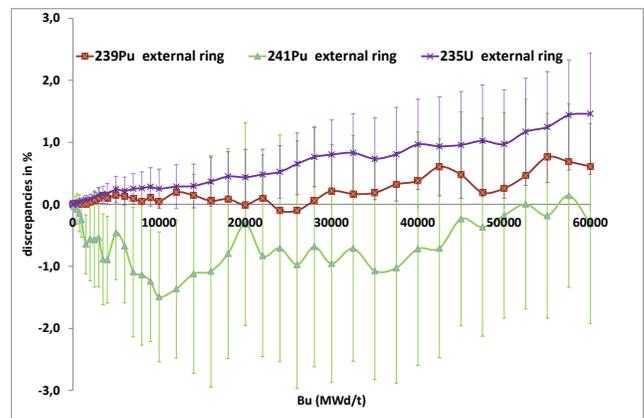


Fig. 10.

Relative discrepancies on the concentrations between APOLLO2 and TRIPOLI-4® [cell named FISSILE 1 - external ring]

The second comparison between APOLLO2 and TRIPOLI-4® concerns the cell named FISSILE 2 which is closer to the fertile area. We only present the discrepancies for the external ring of the fuel. The discrepancies are always included in the three sigma standard deviation for  $^{239}\text{Pu}$ . Concerning the  $^{235}\text{U}$  and  $^{241}\text{Pu}$  isotopes the concentrations obtained with APOLLO2 are consistent with those evaluated by TRIPOLI-4® (see Fig 11 - discrepancies always lower than 3%).

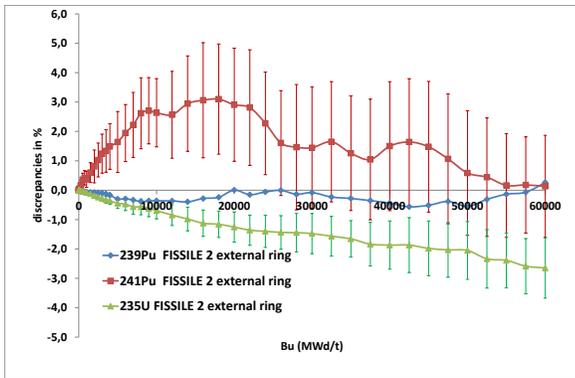


Fig. 11.

Relative discrepancies on the concentrations between APOLLO2 and TRIPOLI-4® [cell named FISSILE 2 - external ring]

The results obtained on the cell FERTILE 1 show less consistency than the previous comparisons. The concentrations of  $^{239}\text{Pu}$  during the depletion calculation with APOLLO2 are greater than the concentration of TRIPOLI-4®. This deviation can have several origins. The APOLLO2 model groups the cells and gives averaged concentrations (see Figure 5) whereas for TRIPOLI-4® all cells are independent. A different strategy of collapsing should be defined to improve the representation of the flux gradient. Moreover, the TRIPOLI-4® calculation may not be sufficiently well converged to give accurate results in the fertile area due to limited sources of neutrons.

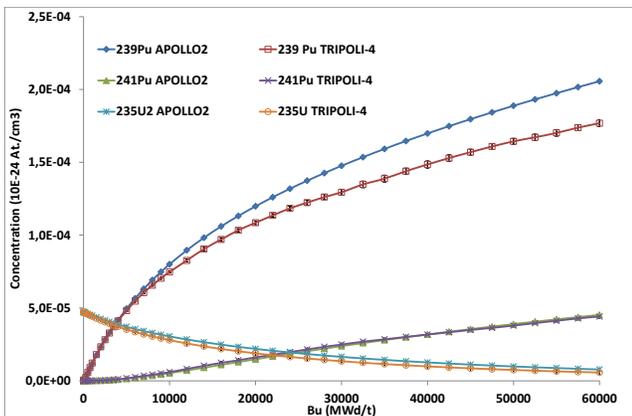


Fig. 12.

Relative discrepancies on the concentrations between APOLLO2 and TRIPOLI-4® [cell named FERTILE - internal ring]

Figures 13 and 14 present the relative discrepancies between the averaged concentrations at the scale of the assembly obtained with APOLLO2 and CRONOS2 (with 8 energy groups) for the  $^{239}\text{Pu}$ ,  $^{241}\text{Pu}$  and  $^{235}\text{U}$  isotopes. The results are presented only for the assembly named FI2 (cf. Figure 8 for the position of the assembly). The conclusions are similar for the assembly named FI3.

Good agreement is observed for the fissile assembly but the relative FE discrepancies are higher for the fertile assembly FE1 (cf. Figure 14). For  $^{239}\text{Pu}$  we can note a

relative discrepancy of 5% at the end of the depletion. The relative discrepancies observed at the beginning of the depletion for the  $^{241}\text{Pu}$  isotope is not relevant because absolute values of concentrations are particularly low. This comparison confirms the possibility to use a reduced depletion chain (containing 28 nuclides) within the diffusion calculation at the core scale (depletion chain in APOLLO2 uses 168 nuclides).

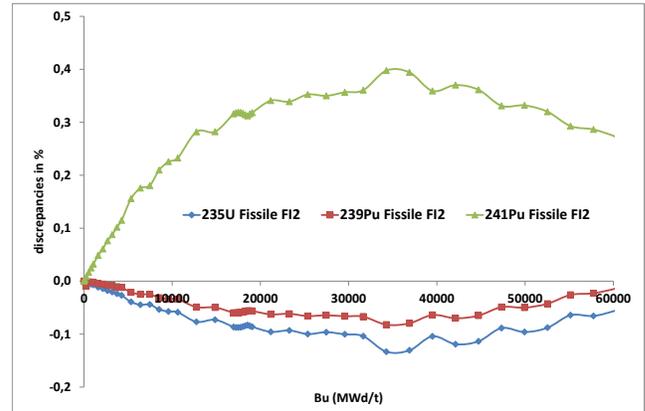


Fig. 13. Relative discrepancies on averaged concentrations in the FI2 assembly between APOLLO2 and CRONOS2 8 group

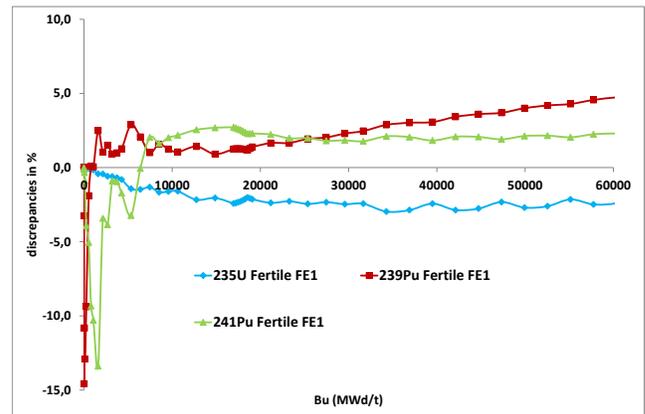


Fig. 14. Relative discrepancies on averaged concentrations in the FE1 assembly between APOLLO2 and CRONOS2 8 group

For the main fission product we obtain a relatively good prediction in the fissile fuel. A deviation is to be noted for samarium-149 (see Figure 15).

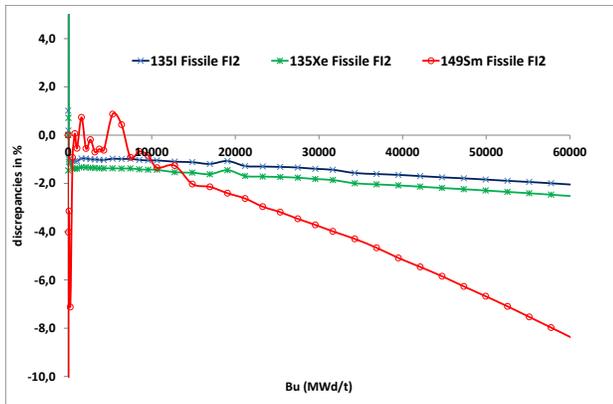


Fig. 15. Relative discrepancies on averaged concentrations for some fission products between APOLLO2 and CRONOS2 8 group [FI2 assembly]

In the fertile fuel the concentrations of xenon and samarium are correctly predicted (see Fig 16). The initial relative discrepancies observed for iodine-135 correspond to very low concentrations and can therefore be considered as non-significant.

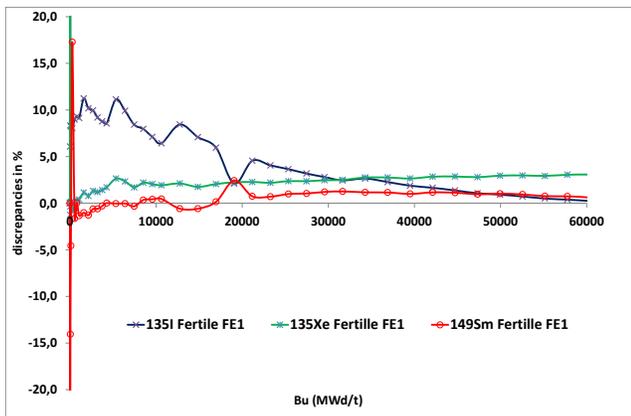


Fig. 16. Relative discrepancies on averaged concentrations for some fission products between APOLLO2 and CRONOS2 8 group [FE1 assembly]

## VII. CONCLUSIONS

This work allows recommendations to be made for the calculation options to be used to model highly heterogeneous core. Good agreement between the APOLLO2 and TRIPOLI-4<sup>®</sup> calculations is obtained in terms of reactivity and power maps at the scale of the assembly.

APOLLO2 with the characteristic method, a SHEM mesh and the self-shielding mixture method could be considered as a reference for this type of heterogeneous calculation.

This study also shows the limit of homogeneous diffusion to model this type of complex geometry. An 8 group energy mesh in CRONOS2 gives better results than a 2 group energy mesh.

This calculation performed at the scale of a cluster of assemblies could be considered as a benchmark to test various calculation schemes in CRONOS2. To go further, calculations based on a heterogeneous description of the geometry (pin by pin with homogeneous cells) could be performed using different solvers (transport  $S_N$ ,  $P_N$  or simplified transport  $SP_N$ ).

The depletion calculations with TRIPOLI-4<sup>®</sup> are still costly in calculation time but accessible with HPC computers.

For the analysis of the concentration, the uncertainty bars are sometimes quite high. This could be solved by the improvement of the number of processors and the number of neutrons simulated.

Additional analyses should be performed to evaluate the accuracy of the model to the core-wide. These analyses could show that the model accurately takes into account both radial and axial heterogeneities of the core. Indeed, collapsed macroscopic cross sections used to model axial layers of the core are produced using the same process and this calculation hypothesis needs to be verified.

The modelling of this 3x3 cluster of assemblies in 3D including fissile and fertile layers could be a first step before moving toward the core-wide calculation.

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## APPENDIX

Two and eight group energy meshes used in the CRONOS2 calculation.

Group	Energy higher
1	1.96403E+01
2	1.33694E+00
3	1.95008E-01
4	9.11882E-03
5	4.00000E-06
6	1.25094E-06
7	6.25000E-07
8	1.38000E-07

Eight group energy mesh

Group	Energy higher
1	1.96403E+01
2	6.25000E-07

Two group energy mesh