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# HTGR Actinide Burner Feasibility Studies: Calculation Scheme Related Considerations

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## Abstract

At the CEA, the actinides burner version of the prismatic block-type reactor is currently investigated, including studies about the design proposed by General Atomics. The purpose of this paper is essentially to evaluate the capability of the deterministic methods to calculate a wide range of core configurations. In the first part of the paper, the analysis is carried out on the «Deep Burner» fuel element geometry. The fuel element calculations are performed with both Transport code APOLLO2 and Monte-Carlo code TRIPOLI4. This preliminary analysis shows the reliability of the deterministic code APOLLO2 to calculate heterogeneous fuel element configurations (fuel element loaded with plutonium and minor actinides). In the second part, the analysis deals with the core geometry in order to estimate the impact of some physical assumptions on the fine fuel isotopic depletion. Due to the strong spectrum transient in the core, it turns out that the transuranic mass balances in a GT-MHR cannot be estimated easily from fuel element calculations but rather need the use of a core modeling approach taking into account the presence of the graphite reflectors. Two different methods based on a fine core Diffusion calculation in CRONOS2 and a simplified Transport calculation in APOLLO2 are investigated in this paper.

**Keywords** ***High Temperature Gas-Cooled Reactor, Deep-Burner Concept, Fuel Depletion Calculation***

## 1. Introduction

For a few years, the High Temperature Gas cooled Reactor (HTGR) technology has gained worldwide new interest due to its specific characteristics. It is a promising reactor concept for the next generation of nuclear power applications. In addition to the studies performed on the industrial concept (uranium core type), there is a strong interest in the development of a «Deep Burner» version of HTGRs, dedicated to minor actinides destruction. At the CEA the actinides burner version of the prismatic block-type reactor is currently investigated, including studies about the design proposed by General Atomics [1]. Advanced HTGRs allow a simplification of safety through reliance on innovative features and passive systems. One of the innovative features in HTGRs is the ceramic-coated fuel particle, which can retain the fission products even under severe accident conditions. The other original feature is the annular configuration of the core, surrounded by internal and external graphite reflectors able to evacuate decay heat in accidental conditions. The growing interest in HTGRs activities has shown the need to validate the tools and techniques developed for reactor physics calculations. The physics of the deep-burn transmutation concept is still complicated due to the fact that two fuel types, driver and transmuter, are loaded in the core. Same ceramic-coated particle technology is used to fabricate both fuel types but particles are sized differently so as to favour immediate fissions in the driver fuel, or absorption followed by fissions in the transmutation fuel. Furthermore, self-shielding effects are of great importance to calculate HTGR fuel cycle or temperature coefficient correctly.

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The purpose of this paper is essentially to evaluate the capability of the deterministic methods to calculate a wide range of core configurations. In the first part of the paper, the analysis is carried out on the «Deep Burner» [2] fuel element geometry. In the second part, the analysis deals with the core geometry in order to estimate the impact of some physical assumptions on the fine fuel isotopic depletion.

## 2. Computational methods and nuclear data

For the calculations, the CEA reactor physics code system SAPHYR is used. SAPHYR gathers several CEA codes such as APOLLO2 [3] (transport) based on a database produced with THEMIS/NJOY, CRONOS2 [4] (diffusion-transport) which are interconnected. The Monte-Carlo Transport code TRIPOLI4 [5] is also used for the analysis. All the data used for the calculations are issued from JEF2.2.

## 3. Analysis of the fuel element loaded with plutonium and minor actinides based fuel

The purpose of the analysis is to compare the results obtained using the transport code APOLLO2 with the reference calculations performed with the Monte-Carlo code TRIPOLI4.

### 3.1. Brief description of a fuel element

In the actinides burner concept, the standard fuel element is loaded with two different compact types (see Figure 1). The driver fuel compact is composed of kernels that are loaded with first generation plutonium and neptunium. The transmuter compact consists of degraded plutonium and minor actinides. The compositions of the fuel kernels in both cases are given in Table 1. The standard fuel element is loaded with 144 driver fuel rods and 72 transmuter fuel rods (axially, one rod contains 15 fuel compacts).

***Table 1: Isotopic compositions (% w.o) of driver and transmuter fuel kernel***

| Isotope | Driver kernel (10,36 g.cm$^{-3}$) | Transmuter kernel (10,0 g.cm$^{-3}$) |
|---|---|---|
| $Np^{237}$ | *0* | *5,8* |
| $Pu^{238}$ | *1,5* | *4,5* |
| $Pu^{239}$ | *57* | *2,4* |
| $Pu^{240}$ | *23* | *20,9* |
| $Pu^{241}$ | *8,3* | *15,8* |
| $Pu^{242}$ | *5* | *19,9* |
| $Am^{241}$ | - | *21* |
| $Am^{242M}$ | - | *0,2* |
| $Am^{243}$ | - | *7,7* |
| $Cm^{244}$ | - | *1,7* |
| $Cm^{245}$ | - | *0,1* |

***Red compact:*** Driver fuel
***Green compact:*** Transmuter fuel

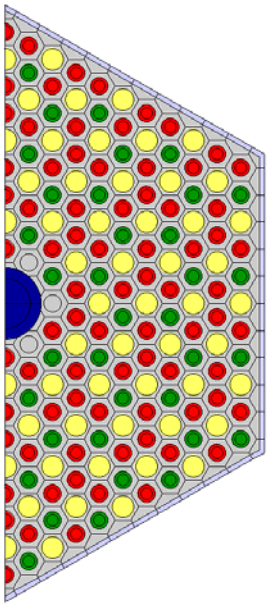


***Figure 1: Fuel element geometry in the transport code APOLLO2***

In APOLLO2, the calculations are performed in transport theory (172gr) using the collision probability method in general geometry. The double heterogeneity of the driver and transmuter fuel compacts is explicitly taken into account. In TRIPOLI4, it is necessary to describe the fuel particles in

each fuel compact. The assumptions that are made on the coated fuel particles modeling must be evaluated in this strong heterogeneous configuration such as in usual HTGR configurations [6]. The calculations are performed using pointwise cross-sections.

## 3.2. Impact of the stochastic medium modeling in Monte-Carlo code

### *3.2.1. Description of the problem*

The use of the Monte-Carlo method as a reference for the HTR calculations underscores the problem of the stochastic medium modeling in such a code. In this first part, different methods were investigated. In the first case, the coated fuel particles were uniformly placed on a regular lattice. The choice of the lattice parameters (type of lattice, distance between coated fuel particles…) was discussed. In the second case, the coated fuel particles were randomly distributed in the fuel compact. For this kind of description, it is not possible to describe each particle in the fuel element but only a small amount of a few hundreds particles. Therefore, the number of particles explicitly described, characterized in the study by the ratio [*Height of the compact modelled versus Outer radius of the particle*], is another parameter which was investigated.

### *3.2.2. Results and discussion on the fuel cell geometry*

A preliminary analysis was performed on a fuel cell geometry for both Driver and Transmuter fuel compact. The results are shown in Figure 2. Only the random distribution calculations are characterized by the ratio between the modeling height and the diameter of the fuel (this parameter is represented on the x-axis).

No significant variation of the $k_{infinity}$ values could be observed for various H/D ratios, however, the results obtained with a regular lattice distribution were strongly dependant on the lattice parameter. On the one hand, the results of the driver fuel cell obtained with an improved hexagonal lattice (distance between coated fuel particles equal to 1,13 mm) do not agree with the random distributions ones. On the other hand, for the transmuter fuel cell, the difference in $k_{infinity}$ between the improved hexagonal model and the random model is within the statistical uncertainty. More details of the Monte Carlo models and their interpretation, e.g. uranium based fuel are presented at [6] (this conference).

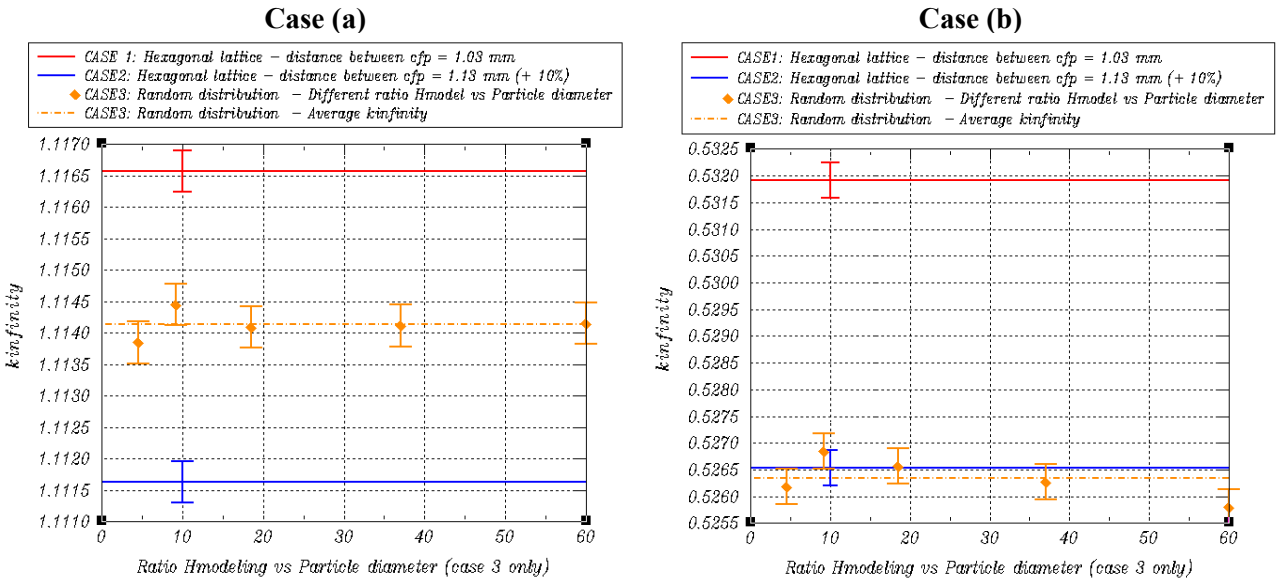



***Figure 2: Impact of the coated fuel particles description in Monte-Carlo code TRIPOLI4 case (a): DRIVER fuel cell – case (b): TRANSMUTER fuel cell***

### *3.2.3. Results and discussion on the fuel element geometry*

The analysis is done on the fuel element geometry by comparing the $k_{infinity}$. The results obtained from the above-mentioned TRIPOLI4 models (random distribution and regular lattice) and APOLLO2 calculations are gathered in Table 2. As previously said, a discrepancy remains between the two models but in the case of the fuel element, the discrepancy is in the range of the 3σ, which indicates compensating effects. The results obtained from APOLLO2 (172 energy groups) agree very well with the TRIPOLI4 results using the random distribution (maximum discrepancy of 250 pcm). The $k_{infinity}$ value (99 energy groups) underestimates the reference values by 700 pcm.

***Table 2: Fuel element $k_{infinity}$***

| | $k_{infinity}$ | Discrepancy [pcm] |
|---|---|---|
| **TRIPOLI4 - Random distribution** | 1,0095 ± 50 pcm (1σ) | *reference* |
| **TRIPOLI4 - Hexagonal lattice Distance between cfp = 1,13 mm** | 1,0115 ± 45 pcm (1σ) | *+ 200* |
| **APOLLO2 – 172 gr** | 1,00696 | *– 250* |
| **APOLLO2 – 99 gr** | 1,00243 | *– 700* |

## 4. Fuel depletion calculations

This part of the work presents the fuel depletion calculations of the entire reactor. The system reactivity ($k_{effective}$) and isotopic concentrations as a function of burn-up are calculated with 2 models using different methods. The results are compared with results from a fuel assembly calculations.

The first method is based on 3-dimensional calculations with diffusion theory, where top and bottom reflectors are described. The second method uses the transport theory with the collision probability method where the core geometry is represented as a slab/slice. It allows one step calculation but is limited in 2-dimensions.

Both methods used to calculate core characteristics take into account radial reflectors, which strongly disturb the neutron flux distribution.

### 4.1. Methodology and modeling details

CRONOS2 is a 3-dimensional, multigroup code for reactor physics. It is able to take into account thermal-hydraulics feedbacks and transient problems using diffusion theory. CRONOS2 needs burn-up-dependent microscopic or macroscopic cross sections, provided by assembly calculations in infinite medium, in order to calculate neutrons fluxes and reaction rates and perform depletion calculations. Although fine calculation schemes are currently developed for HTGR core calculations at the CEA [6], a simplified 2-dimensional RZ core geometry model was used to facilitate the physical analysis and to save computing time. Diffusion calculations were performed with 13 energy groups. Assumptions on geometry and energy mesh were validated at beginning of cycle with TRIPOLI4 multigroup calculations using the same 2D-RZ description of the core and 172 groups energy structure. The discrepancy between CRONOS2 and TRIPOLI4 on $k_{eff}$ was less than 0,001. Concerning core calculations with the APOLLO2 transport code, a slab/slice representation of the reactor was described with square cells containing fuel compacts, helium channels or graphite. The internal reflector, the core and the external reflector are described in a “quasi-1D” cartesian geometry. Neutron fluxes and self shielding effects are calculated with the collision probability method (multicell approximation). A library with 172 energy groups was used. Assembly calculations are also performed with APOLLO2 . All details – from the grain structure of the fuel over the different position of the fuel and transmuter compact to the outer boundary of the assembly are modelled in detail, in order to calculate accurately the neutron flux in and between the different compact types. The obtained cross section were condensed to 13 energy groups for the CRONOS2 core calculation and the 172 cross

section data set was kept for the above mentioned APOLLO2 slab model and as input data for TRIPOLI4. Figure 3 summarizes the different steps of each method:

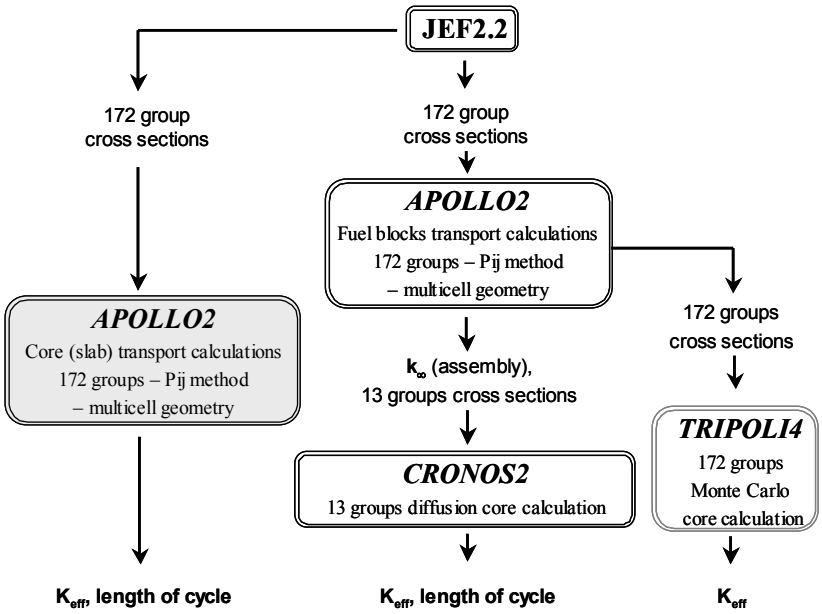


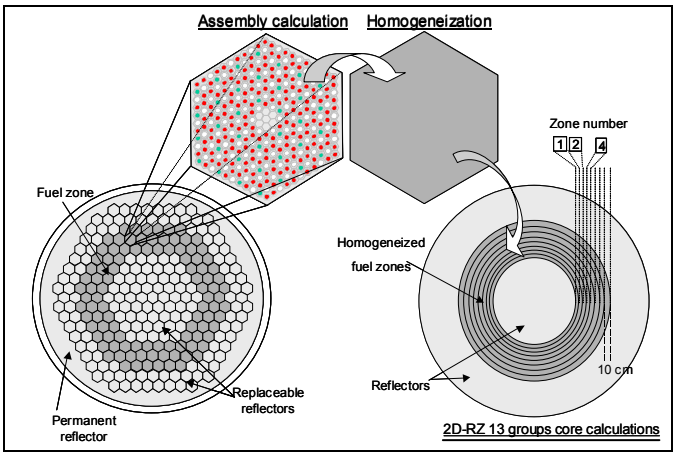

***Figure 3: Description of the different calculation processes***

Geometry descriptions are shown in Figure 4. In all cases, control rods cavities are not represented, and the core thickness is fitted in order to preserve mass balancing. The thickness of the internal reflector is 148 cm, followed by the annular fuel zone of 83,6 cm in thickness, and completed by an external reflector of 70 cm. The hexagonal assembly is made of graphite, containing 180 driver compacts, 36 transmuter compacts and 108 helium channels. The composition of the driver and transmuter fuel is given in Table 1. Each coated particle consists of a spherical kernel surrounded by triple protective coatings from pyrocarbon and SiC (so called TRISO coating). The temperatures of the fuel and graphite were respectively set to 900°C and 500°C.

In case a), the height of the active core is 800 cm, and the top and bottom reflector are 130 cm thick. Core calculations are carried out with the diffusion theory using finite elements.

In case b) the core is described in a 2-dimensional XY geometry, with $n_X$ = 161 square cells along X-axis, and $n_Y$ = 2 square cells along y-axis. The cell dimension (1,862 cm) is sized in order to respect the graphite volume. The driver/transmuter/helium ratio is fully respected. Top and bottom reflective conditions were set on y-axis as well as on the left side of x-axis.

a)



b)

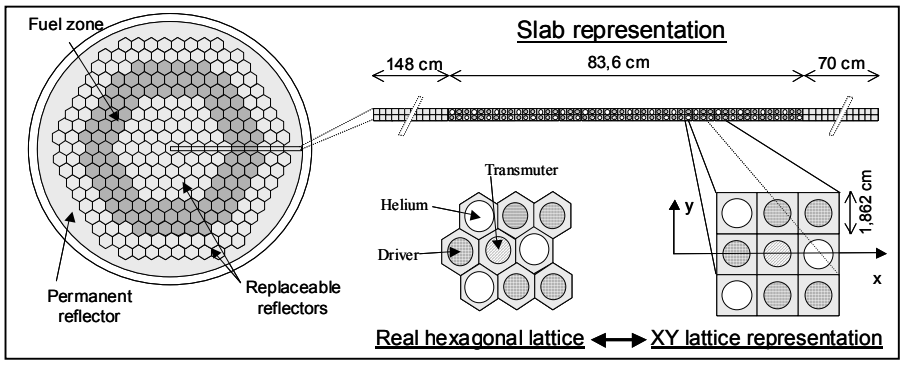



***Figure 4: Cross sectional view of core modeling in a) 2D-RZ core calculations, b) slab calculations***

Three kinds of results will be compared in the following:

- Single assembly calculations in infinite medium, performed with APOLLO2, and named "assembly.",

- 2D-RZ core calculations with diffusion theory, , named "2D-RZ", performed with CRONOS2 and validated with TRIPOLI4 multigroup calculations at beginning of cycle,

- Slab calculations, performed with APOLLO2, without assembly calculations, named "Slab".

## 4.2. Results and discussion

Figure 5 shows the multiplication factor obtained from core calculations, in cases a) and b), and compared with assembly calculations in infinite medium. Concerning slab calculations, a corrective factor of $\Delta k_{eff}$ = -0,03 is applied on $k_{eff}$ to take into account effects of axial leakages and cartesian geometry. This corrective factor was estimated at beginning of cycle comparing slab calculations with Monte Carlo results.

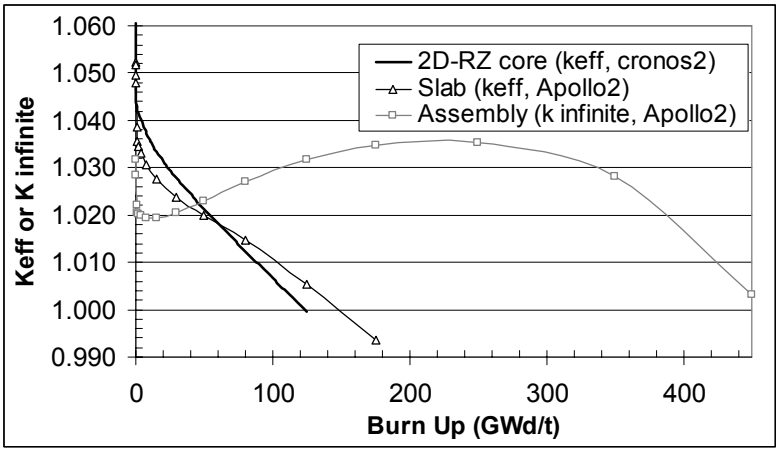



***Figure 5: multiplication factor versus burn up as a function of the method***

Assuming that the CRONOS2 calculations stops as soon as $k_{eff} < 1$, the burn up reaches approximately 120 GWd/t. Figure 5 shows the large influence of the graphite reflector on the core reactivity. In fact, due to a large migration area of 410 $cm^2$, many neutrons escape the active core and are slowed in the reflector, before going back to the core. The neutron balance in the core is largely modified because of the reflectors, and finally $k_{eff}$ is greater than the $k_{infinity}$ calculated in infinite medium (when passing from assembly calculations to core calculations, the reactivity increase due to a better thermal utility

factor and larger resonance escape probability factor is not compensated by leakages). This is also of first importance on the $^{240}$Pu transmutation into $^{241}$Pu, because the probability for neutrons to escape the large 1 eV resonance of $^{240}$Pu is greater when reflectors are described. Figure 6 gives an overview of how far neutron flux in the active core is disturbed by reflectors. Neutron fluxes at different locations (as shown on Figure 4) in the core are compared to APOLLO2 single assembly calculations in infinite medium.

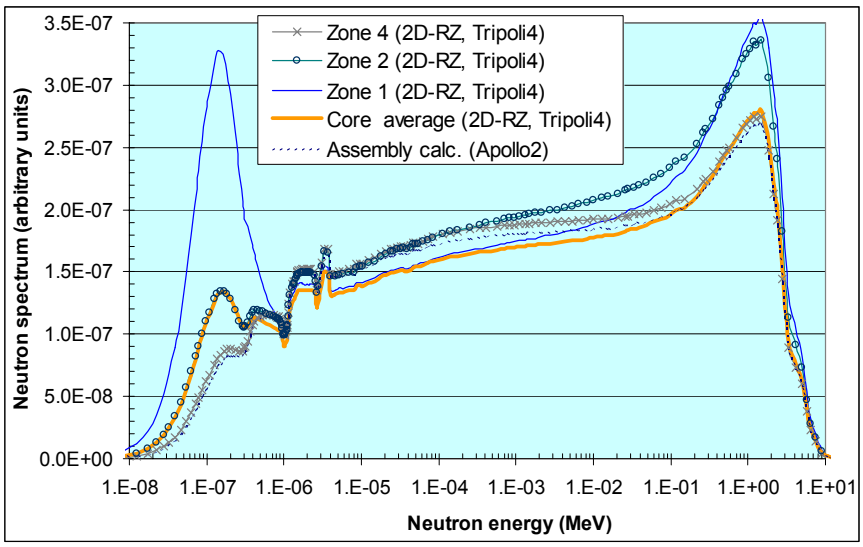



***Figure 6: Neutron spectrum in different core zones compared to assembly calculations***

For the sake of simplicity, only a few regions are plotted. In zone 1 close to the reflector, the thermal component (< 1eV) reach 19% of the total flux, whereas it is 11% in case of the average core and only 8,3% in infinite medium. In zone 2, deeper in the core, the neutron spectrum behaves as the core average. In the center part of the core (plotted as zone 4), the neutron spectrum follows the fundamental zone very well. In fact, for an annular core of 80 cm in thickness, the 40 cm inner part of fuel is well represented by the fundamental mode.

The transmutation rate of isotope depends on the fuel location in the core due to the difference between neutron spectra. Figure 7 shows the core average concentration of $^{241}$Pu, but also results for zone 1 and zone 4.

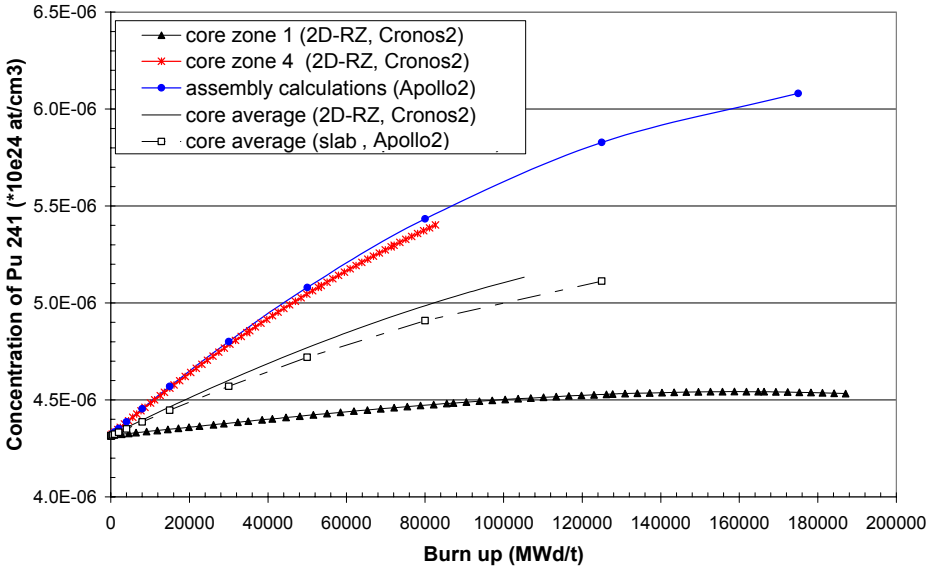



***Figure 7: 241Pu concentration as a function of burn-up***

These results indicate that the change of the keff and the isotopic concentration with the burnup cannot be calculated accurately using assembly calculations. More precise results are obtained from the slab model. The production of $^{241}$Pu in assembly calculations is overestimated because the neutron spectrum is harder and $^{240}$Pu captures are increased. Furthermore, $^{240}$Pu decreases faster than reality and contributes also to the global overestimation of the reactivity (see Figure 5). Table IV shows the main isotopes in term of absorptions and fissions in the fuel.

| Isotope | $^{239}$Pu | $^{240}$Pu | $^{241}$Pu |
|---|---|---|---|
| **2D-RZ core (Cronos2)** | 1.27e-5 | 8.54e-6 | 5.03e-6 |
| **Slab calc. (Apollo2)** | 1.27e-5 | 8.64e-6<br>+ 1% | 4.91e-6<br>- 2% |
| **Assembly calc. (Apollo2)** | 1.28e-5 | 8.07e-6<br>- 6% | 5.45e-6<br>+ 8% |
| ***Reactivity effect Δk*** | | *-0,012* | *- 0,013* |

***Table 3: Concentration of main contributing isotopes (*1e24 at.cm$^{-3}$) at 80 000 MWd/t***

$^{239}$Pu, $^{240}$Pu and $^{241}$Pu represents respectively 97,5% and 80% of fissions and absorptions in the active core, and the differences in the estimation of $^{240}$Pu and $^{241}$Pu concentrations reach respectively 6% and 8% (2D-RZ core and slab comparison). In this case, the cumulated reactivity effect due to the discrepancies in $^{240}$Pu and $^{241}$Pu concentrations is $\Delta k = 0{,}025$, which is very important worth compared to the small excess reactivity of the core. Figure 5 shows that once xenon and samarium poisoning is stabilized (~500 MWd/t), $k_{eff}$ is about 1,03 , which is only 3% above the end of cycle criteria. So, the reactivity range during operation is very limited, and slight perturbations of the reactivity have large influence on lifetime. Isotopic concentrations must be determined with accuracy but leakages have also an important role. One can note that (according to Figure 5) if $\Delta k_{eff} = + 0{,}005$, the burn-up is extended for 25 000 MWd/t, corresponding to 54 days.

## 5. Conclusion

Destruction of transuranic waste discharged from LWR is the subject of a significant analysis effort. Following a GENERAL ATOMICS proposal for a deep burn concept, CEA has defined a specific modeling in order to evaluate in a proper way the performances. To address this issue, different MC and deterministic based models have been developed and set up for both pebble-type and bloc-type reactors. At the CEA a deterministic approach has been developed for the uranium-based GT-MHR, associated with intensive and rigorous validation phases [4]. However, the quite good results obtained on these ongoing validation phases may back in to question for the GT-MHR fully loaded with transuranic fuel. This paper presented preliminary comparisons between MC and deterministic calculations on a fuel element containing high amounts of transuranic isotopes. The results showed discrepancies a little bit larger than for a uranium fuel at high burnup in the GT-MHR.
In term of performances, preliminary results show sensitivity of the maximum BU to the reactivity balance. Moreover, fuel back end cycle studies in PWR are usually tackled on the basis of a fuel assembly model. These calculations performed in infinite medium and based on the fundamental mode hypothesis, allow reaching rapidly the fuel mass balance avoiding core calculations. In this paper, information is provided with regard to the precautions that must be taken in transuranic cycle studies carried out on annular core configurations as the one encountered in the GT-MHR. It turns out that the transuranic mass balances in a GT-MHR cannot be estimated easily from fuel element calculations but rather need the use of a core modeling approach taking into account the presence of the graphite reflectors.

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