

## GT-MHR Core Modeling: From Reference Modeling Definition in Monte-Carlo Code to Calculation Scheme Validation

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### Abstract

In High Temperature Gas-Cooled reactor, the fuel is in form of coated fuel particles dispersed in a graphite matrix. The use of Monte-Carlo method for the core modeling may question the principle of the absolutely unbreakable reference that constitutes the Monte-Carlo methods. Indeed, assumptions must be done for the geometrical description of the stochastic medium in Monte-Carlo codes. In this paper, different stochastic medium modeling are analysed in the Monte-Carlo code TRIPOLI4. The analysis is done for different configurations (from fuel cell geometry to simplified core configuration) and shows that in the case of an uranium based fuel and a volumic filling fraction of 26% in the fuel compact, the results are not dependant to the coated fuel particles modeling (coated particles described with an hexagonal lattice or randomly distributed). Taking advantages of these results, the Monte-Carlo modeling is used as a reference in order to validate a two steps Transport-Diffusion calculation scheme based on the APOLLO2-CRONOS2 codes and developed for the GT-MHR core modeling. The calculations are performed on a simplified 2D core modeling which is representative of all the physical effects generally encountered in this type of core (annular core configuration with a strong coupling between fuel element and reflector). Furthermore, the core calculations are also performed in transport theory (99 or 172 gr) using the characteristics methods in APOLLO2. In both cases (Diffusion calculation in CRONOS2 or Transport calculation in APOLLO2), the results obtained are in good agreement with Monte-Carlo calculations for both  $k_{\text{effective}}$  (maximum of 250 pcm) and fuel element power map (discrepancies in the range of  $\pm 2,5\%$ ).

### Keywords

*High Temperature Gas-Cooled Reactor, Stochastic medium modeling, Calculation Scheme validation*

## 1. Introduction

Today, the HTGR (High Temperature Gas cooled Reactor) appears as a promising reactor concept for the next generation of nuclear power applications. The CEA, in collaboration with FRAMATOME, is developing a core modeling dedicated to the prismatic block-type reactor. This calculation scheme is based on a usual two-steps Transport – Diffusion approach [1]. It will have to serve for design studies and industrial calculations as well as for best estimate and reference calculations.

Due to the lack of usable experimental results, the reliability of the code system used for the design studies is essentially based on results obtained with reference calculations. Such reference calculations are usually obtained with Monte-Carlo codes. These codes allow modeling the core geometry and its characteristics without any physical assumptions. However, firstly the Monte-Carlo method cannot be considered today as a reference for validating core burnup calculation and secondly, in HTGR, the fuel is in a form of dispersed particles (coated fuel particles<sup>1</sup>, embedded in a graphite matrix). It imposes the treatment of stochastic geometries in Monte-Carlo calculations and may question the principle of

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<sup>1</sup> In the paper, “coated fuel particles” will be replaced by “cfp”

the absolutely unbreakable reference that constitutes the Monte-Carlo methods. Indeed, assumptions must be done for the geometrical description of the stochastic medium in Monte-Carlo codes.

The purpose of the paper is to evaluate the physical impact of these assumptions in the CEA-FRAMATOME framework that consists in qualifying and validating the deterministic modeling of the GT-MHR [2] loaded with uranium fuel. Mastering the uncertainties of the modeling in Monte-Carlo codes allows us to use these calculations for the validation of the computational tools used for conceptual studies. This is the purpose of the second part of the paper which is dedicated to the validation of the computational tools in a simplified geometry. This simplified geometry is a 2D core modeling which is representative of all the physical effects generally encountered in this type of core (annular core configuration with a strong coupling between fuel element and reflector).

## 2. Computational methods and nuclear data

For the calculations, the CEA reactor physics code system SAPHYR is used. SAPHYR gathers several CEA codes like 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, 6] is also used for the analysis. The calculation processes used in all cases are described in Figure 1.

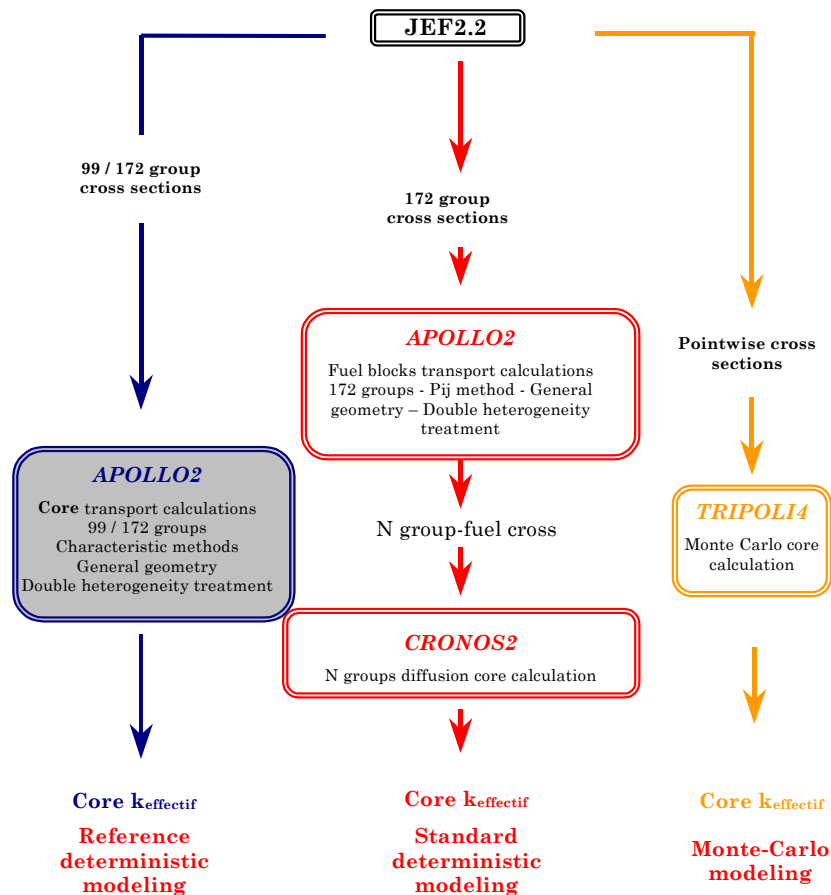


Figure 1: Description of the three different calculation processes

On the one hand, the core calculations are performed in 2D geometry, with diffusion theory (8 gr), using the CRONOS2 code. In these core calculations, the fuel element is homogenised and the flux is calculated considering 37 points in the prismatic block (linear flux interpolation). The fuel element cross-sections used in CRONOS2 are calculated by APOLLO2 in transport theory, using the probability collision method in a general geometry. This APOLLO2 calculation allows to treat simultaneously the self-shielding of the heavy nuclides and the double heterogeneity problem in the fuel compacts. On the other hand, the core calculations are also performed in transport theory (99 or

172 gr) using the characteristics methods in APOLLO2 [7, 8]. In these calculations, the core heterogeneous structure, i.e. coated fuel particles embedded in a fuel compact and fuel compacts loaded in the prismatic block, is also explicitly taken into account by using the double heterogeneity formalism. The reference calculations are performed using the Monte-Carlo code TRIPOLI4. In this last modeling, all the materials in the core are represented using pointwise cross-sections. All the data used for the calculations are issued from JEF2.2.

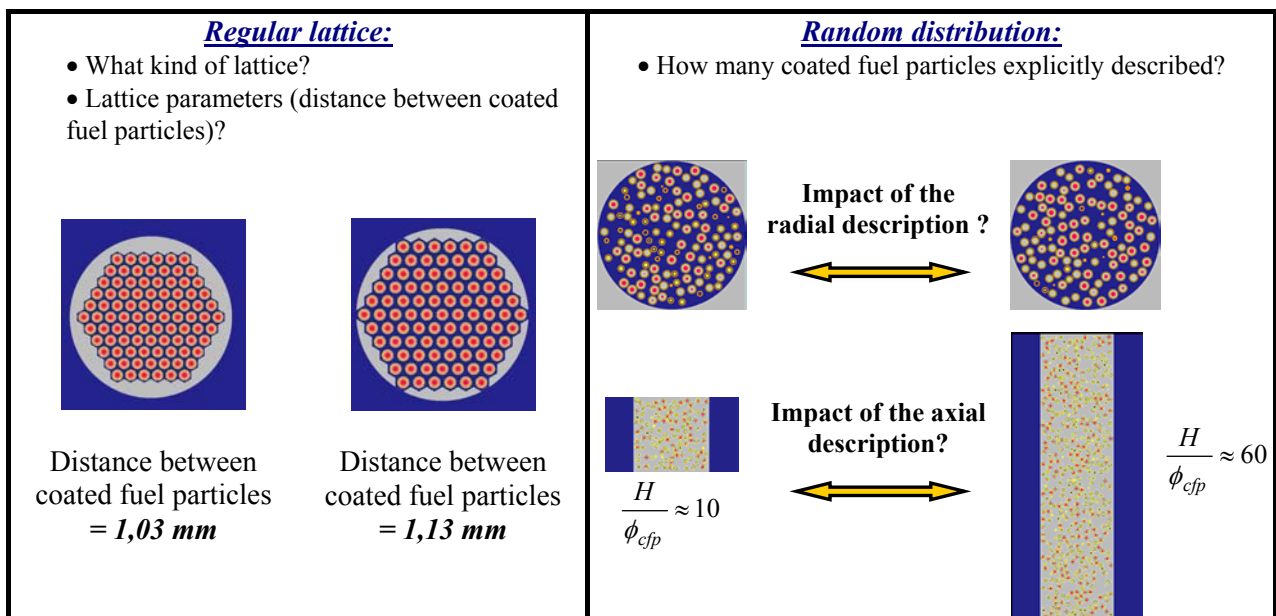
The results obtained in both deterministic calculations (results such as  $k_{\text{effective}}$  and power map) are compared to the reference calculations performed with the Monte-Carlo code TRIPOLI4. The aim of this work is not only to validate the core calculation in CRONOS2 code (diffusion) but also to validate the core calculation in APOLLO2 (transport) in order to use this modeling as a reference (core depletion analysis).

### 3. Analysis of the stochastic medium modeling in Monte-Carlo code

#### 3.1. Description of the problem

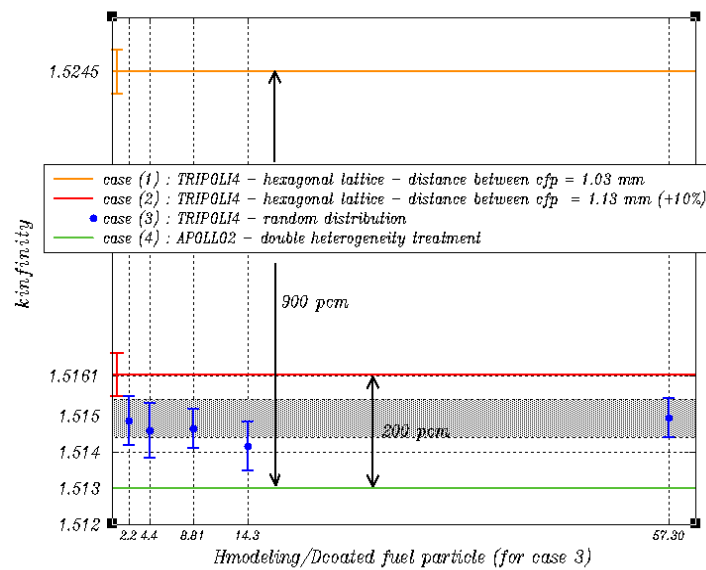
The use of the Monte-Carlo method as a reference for the HTR calculations underscores the problem of the stochastic medium modeling in such a code. Indeed, in the core modeling, it is necessary to describe the coated fuel particles in the fuel compact. Different methods were investigated and they are gathered in Table 1. 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 core but only a small amount (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.

Table 1: Description of the different modeling investigated in Monte-Carlo simulation



#### 3.2. Analysis on a simplified geometry

The analysis is performed on a fuel cell geometry representative of the fuel element lattice. The results are gathered in Figure 2.



**Figure 2: Monte-Carlo modeling impact on fuel cell  $k_{\infty}$**

As far as the random distribution is concerned, we showed that in this configuration (i.e. a volumic filling fraction of 0.26 in the fuel compact and fuel particles loaded with uranium based fuel), the results do not depend of the number of coated fuel particles explicitly described in the fuel compact. By modeling 900 particles randomly distributed (ratio  $H_{\text{modeling}}/\phi_{\text{cfp}} \approx 10$ ), we obtained the same results as in reference calculation (about 5000 particles described with a ratio  $H_{\text{modeling}}/\phi_{\text{cfp}} \approx 60$ ). Furthermore, we also found that all the repeated random calculations performed with the same number of particles but with different random distributions were consistent between each other (discrepancies lower than 1 sigma).

Furthermore, we showed that calculations performed with a regular lattice distribution were strongly dependent on the lattice parameter. Finally, in our case, we found that the results obtained with an hexagonal lattice (distance between coated fuel particles = 1,13 mm) are in good accordance with all the results obtained with random distributions (discrepancies lower than 200 pcm). Due to the gain on calculation time, this hexagonal lattice is chosen as the reference coated fuel particles description in the 2D core modeling described in the next chapter.

#### 4. Analysis on a 2D core configuration

The calculations were performed on a 2D core configuration representative of the GT-MHR. In this configuration, the core was fully loaded with standard fuel element. The analysis was done for a core loaded with a fresh uranium fuel (15 % in  $U^{235}$  – about 26% for the volumic filling fraction in the fuel compact) but also with a depleted fuel. In the last case, the fuel composition for different burnup is described by using 24 heavy nuclides and 77 fission products.

##### 4.1. Analysis of an homogeneous core configuration

###### 4.1.1. Characteristics of the core modeling

In this first part, the calculations were done considering a  $1/12^{\text{th}}$  symmetry for the core. We compared the integral values such as core  $k_{\text{effective}}$ , the ratio between production and absorption in the annular zone of the core and the averaged fuel element power map. The modelings used in both transport calculation (APOLLO2) and diffusion calculation (CRONOS2) are presented in Figure 3. In the APOLLO2 core modeling, the flux calculation was performed with the methods of characteristic by considering more than 40000 points for the flux calculation in the core.

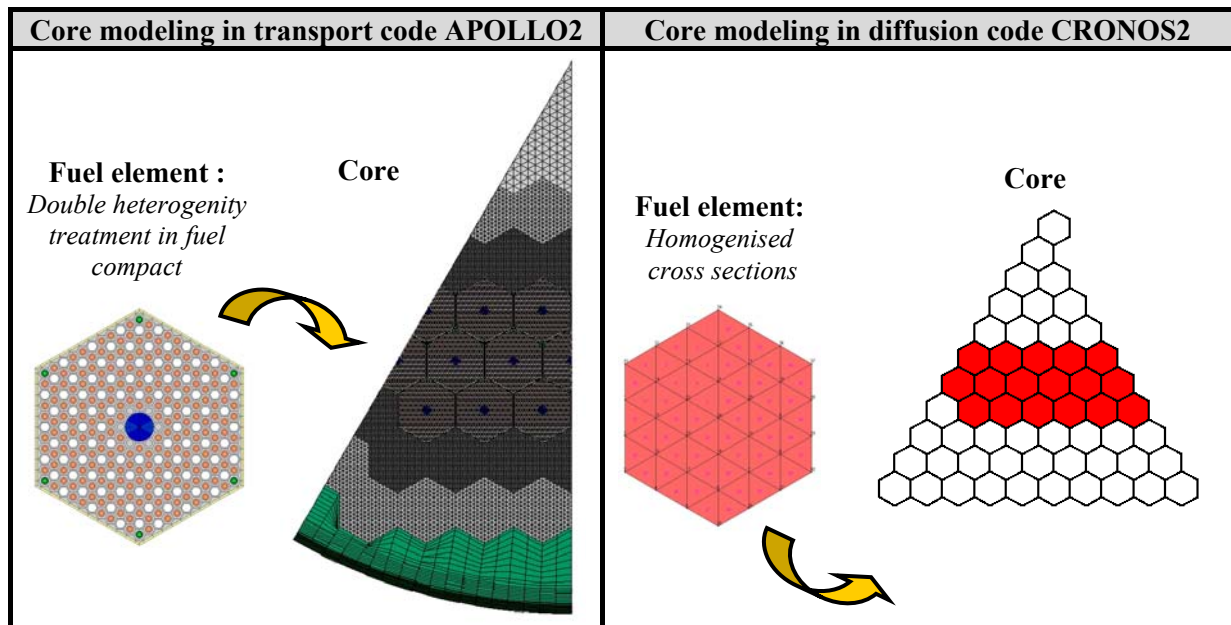


Figure 3: Characteristics of the core modeling in APOLLO2 and CRONOS2

#### 4.1.2. Analysis of the integral parameters

The results are gathered in Table 2 and Table 3. In both core configurations (core fully loaded with fresh or depleted fuel), it can be noticed that all the results are in good accordance. The core calculation in CRONOS2 (diffusion theory – 8 gr) allows to obtain very good results on both  $k_{\text{effective}}$  value and ratio between production and absorption in the annular zone containing the fuel element. In any cases, the discrepancies observed between CRONOS2 and TRIPOLI4 are lower than 250 pcm<sup>2</sup>. As far as the transport calculation in APOLLO2 is concerned, it can be stressed that the energy group structure and the cross sections anisotropy (P0 corrected or P1) do not have a significant impact in the case of the core loaded with uranium based fuel. In any cases, the discrepancies do not exceed 300 pcm. Moreover, it can be stressed that in both deterministic calculations, the fuel element composition does not have a significant impact on the discrepancies.

Table 2:  $k_{\text{effective}}$  and P/A in annular zone for a core uniformly loaded with fresh fuel (0 GWd/t)

CORE FULLY LOADED WITH FRESH FUEL (0 GWd/t)	Core $k_{\text{effective}}$ ( $\sigma$ in pcm)	P/A <sup>(3)</sup> in annular zone ( $\sigma$ in pcm)	Vol. Leakage [pcm]
<b>TRIPOLI4</b> CFP place in a regular lattice in the fuel compact	1,4316 ± 32 pcm	1,5753 ± 45 pcm	9560
<b>TRIPOLI4</b> CFP randomly distributed in the fuel compact	1,4312 ± 32 pcm (-30) <sup>4</sup>	1,5760 ± 65 pcm (+40)	9640
<b>CRONOS2</b> Diffusion 8 gr - Homogeneous fuel element	1,43268 (+75)	1,57913 (+240)	9732
<b>APOLLO2</b> Transport 172 gr - Cross Sections P1	1,42945 (-150)	1,57670 (+50)	9804
<b>APOLLO2</b>	1,43037	1,57666	9737

<sup>2</sup> pcm: per cent mili =  $10^5 \cdot \ln\left(\frac{k_1}{k_2}\right)$

<sup>3</sup> P/A = Production vs. Absorption in the annular zone of the core containing the fuel elements

<sup>4</sup> ( ) Discrepancy in pcm. The reference calculation is given by TRIPOLI4 with coated fuel particles described in a regular lattice

Transport 99 gr - Cross Sections P0 corrected	(-80)	(+86)	
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The last remark concerns the coated fuel particles modeling in the Monte-Carlo code TRIPOLI4. In the 2D core configuration and as far as the integral parameters are concerned, the different modelings (random or regular distribution) gave results in good accordance (the discrepancies calculated on both  $k_{\text{effective}}$  and P/A ratio are lower than  $\sigma$ ).

Table 3:  $k_{\text{effective}}$  and P/A in annular zone for a core uniformly loaded with depleted fuel (100 GWd/t)

CORE FULLY LOADED WITH DEPLETED FUEL (100 GWd/t)	Core $k_{\text{effective}}$ ( $\sigma$ in pcm)	P/A in annular zone ( $\sigma$ in pcm)	Vol. Leakage [pcm]
<b>TRIPOLI4</b> CFP place in a regular lattice in the fuel compact	1,0936 ± 33 pcm	1,2110 ± 45	10200
<b>CRONOS2</b> Diffusion 8 gr - Homogeneous fuel element	1,09406 (+40)	1,21012 (-70)	10080
<b>APOLLO2</b> Transport 99 gr - Cross Sections P0 corrected	1,09037 (-290)	1,20936 (-135)	10357

#### 4.1.3. Analysis of the average fuel element power map

The discrepancies observed on the fuel element power map are given on Figure 4 and Figure 5. Whatever the calculation is (transport calculation in APOLLO2 or diffusion calculation in CRONOS2), we observed a little overestimation of the power in the inner ring of the core and a little underestimation in the outer ring compare to TRIPOLI4. However, all the discrepancies observed are in the range of  $\pm 1,5\%$ .

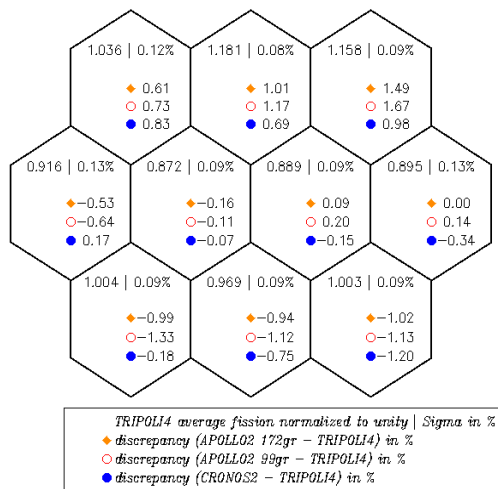


Figure 4: Averaged fuel element power map and discrepancies vs TRIPOLI4 – 0GWd/t

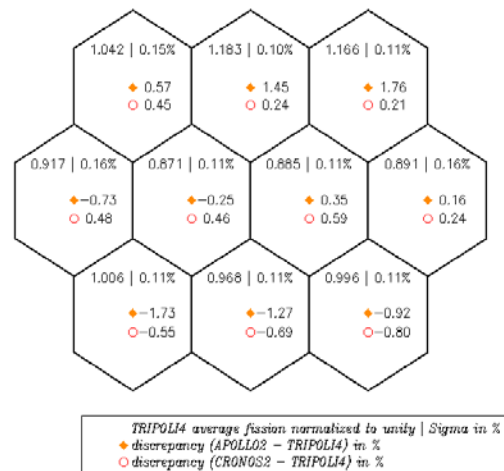


Figure 5: Averaged fuel element power map and discrepancies vs TRIPOLI4 – 100GWd/

#### 4.1.4. Analysis of the pin-by-pin power map

The last analysis concerned the fine power map in selected fuel assembly. The comparison is done between TRIPOLI4 and APOLLO2 by comparing the pin-by-pin power map of the three fuel elements shown in Figure 6. The comparison is done on more than 600 fuel compacts and showed that the discrepancies between APOLLO2 and TRIPOLI4 results were in any cases lower than 3,80%. Examples of fission rate profiles in fixed directions are given in Figure 8 and Figure 9. These results showed the reliability of the Transport code APOLLO2 to calculate core configuration and to be used as a reference modeling for core depletion analysis.



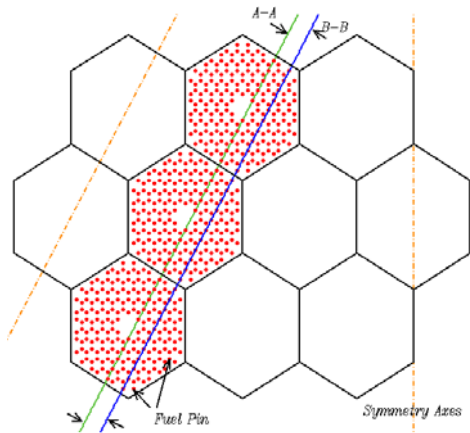


Figure 6: Description of the three analysed fuel elements

Table 4: Observed discrepancies on the pin-by-pin power map

Number of analysed pins	630
Peak power in TRIPOLI4	$2,14 \pm 0,27\%$
Peak power in APOLLO2 99 gr	2,13 (same location as in TRIPOLI4)
Max discrepancy between APOLLO2 and TRIPOLI4[%]	$3,80\% \pm 0,31\%$

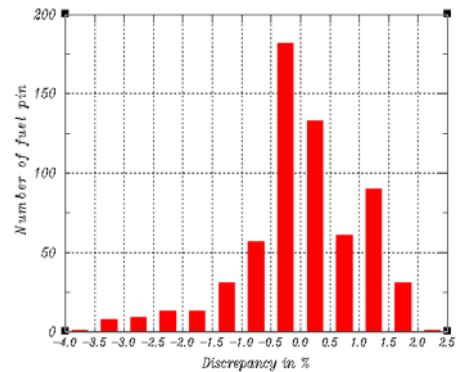


Figure 7: Statistic distribution of the pin-by-pin discrepancies

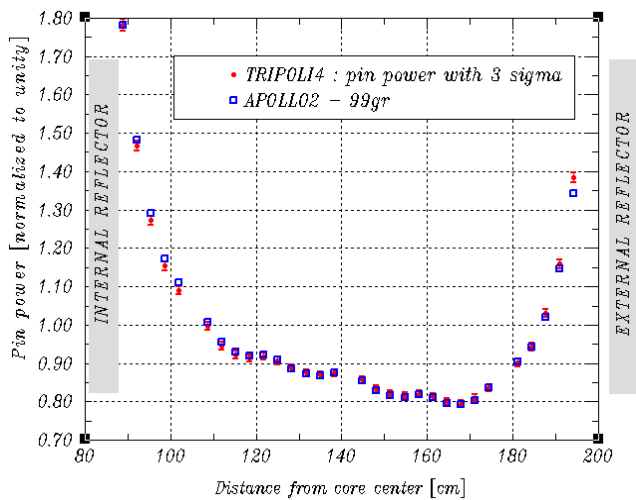


Figure 8: Comparison between the pin power across the A-A direction

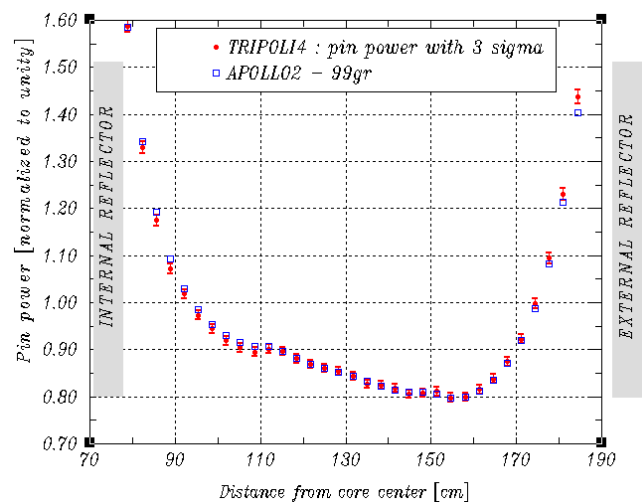


Figure 9: Comparison between the pin power across the B-B direction

## 4.2. Analysis of an heterogeneous core configuration

### 4.2.1. Characteristics of the core modeling

The last configuration concerned the 2D core loaded with three different types of fuel element as shown in Figure 10. The fuel compositions are issued from the fuel element depletion calculation in APOLLO2 and are representative of burnup rates of 0, 50 and 100 GWd/t. The geometry of the 1/6<sup>th</sup> core described in APOLLO2 is given in Figure 11.

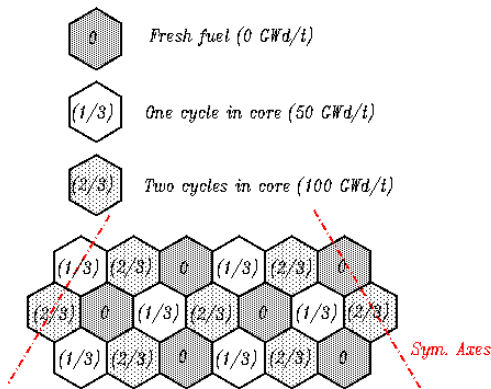


Figure 10: Location of the different fuel elements in the core

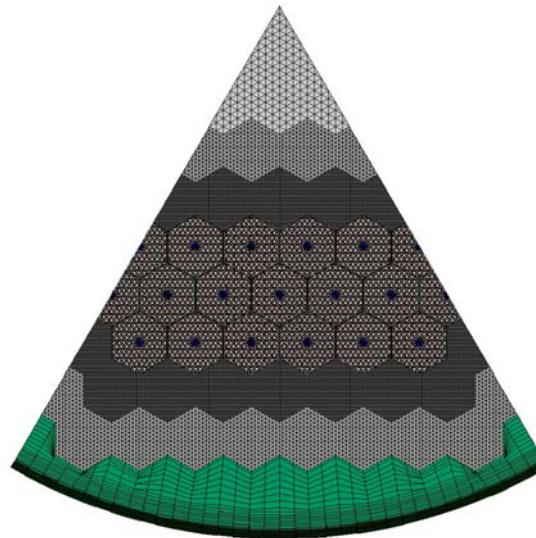


Figure 11: Core geometry in APOLLO2 code

#### 4.2.2. Results and discussion

As in the previous configuration, the  $k_{\text{effective}}$  and production versus absorption ratio calculated in transport and diffusion theory are in good agreement with TRIPOLI4 results. The maximum discrepancy is 370 pcm ( $\sigma$  equal to 47 pcm). The total leakage (leakage from the annular zone of the core) is well calculated by both deterministic calculations.

Table 5: Comparison of the  $k_{\text{effective}}$  and P/A in annular zone for a core loaded with three different types of fuel (0, 50 and 100 GWd/t)

CORE LOADED WITH THREE DIFFERENT TYPES OF FUEL	Core $k_{\text{effective}}$ ( $\sigma$ in pcm)	P/A in annular zone ( $\sigma$ in pcm)	Vol. Leakage [pcm]
<b>TRIPOLI4</b> CFP in a regular lattice	1,2725 ± 45 pcm	1,4076 ± 47 pcm	10080
<b>CRONOS2</b> Diffusion 8 gr - Homogeneous fuel element	1,27235 (- 10)	1,40240 (- 370)	9731
<b>APOLLO2</b> Transport 99 gr - Cross Sections P0 corrected	1,27056 (- 150)	1,40773 (- 10)	10250

As far as the average fuel power distribution is concerned, we obtained very good results with discrepancies observed in the range of  $\pm 2,5\%$  for diffusion calculations and  $\pm 1,6\%$  for transport calculations (99 gr).



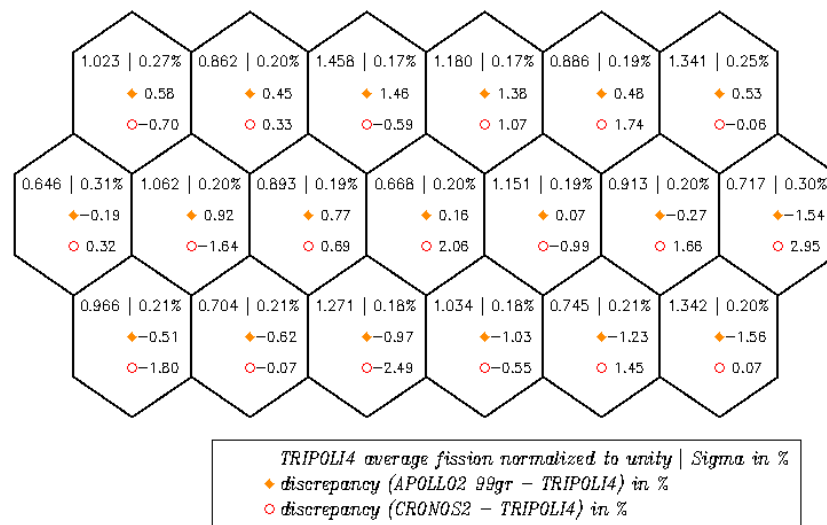


Figure 12: Averaged fuel element power map and discrepancies vs TRIPOLI4  
Core loaded with three different types of fuel elements

## 5. Conclusion

The aim of the analysis was to evaluate the reliability of the core modeling developed at CEA in collaboration with FRAMATOME and dedicated to the prismatic block-type reactor. This modeling is based on a two steps Transport-Diffusion calculation scheme.

The Monte-Carlo code TRIPOLI4 was used as a reference in order to evaluate the discrepancies on integral parameter such as  $k_{\text{effective}}$  but also on fuel element power map. A preliminary analysis showed that, in the case of the GT-MHR core loaded with uranium based fuel and for a filling fraction of approximatively 26% in the fuel compact, the results are independent to the coated fuel particles modeling (random or regular distribution) in the Monte-Carlo code. As a consequence, the Monte-Carlo modeling is used as a reference for 2D core analysis.

Whatever the 2D core configurations are (homogeneous or heterogeneous configuration), the results obtained with CRONOS2 in diffusion-8gr are in good agreement with the reference one. The  $k_{\text{effective}}$  and the ratio between production and absorption in the annular zone are calculated in any cases with a discrepancy lower than 250 pcm. As far as the fuel element power map is concerned, the discrepancies observed are in the range of  $\pm 2,5\%$ . Besides, this analysis showed that the transport code APOLLO2 was well adapted to calculate complex 2D core configuration. We obtained good results on both integral parameters and fine distribution such as the pin-by-pin power map. Therefore, the APOLLO2 core model can be envisaged with a high level of confidence for further analysis such as core depletion.

## 6. Acknowledgements

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## 7. References

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