

## Neutronic modeling for a Gas-Cooled Fast Reactor assuming coated fuel particles

H.Golfier<sup>1</sup>, L.Buiron, C. Poinot, B. Pothet, J-F Salavy, E. Studer

*CEA Saclay, DEN/DM2S/SERMA, F-91191 Gif-sur-Yvette Cedex, France*

**Abstract** – This paper focuses on the modeling of Gas Cooled Fast Reactor with the SAPHYR system and in particular the APOLLO2 code. It aims to estimate the APOLLO2 code accuracy, solving the neutron transport equation in range of fast neutron reactors. One important step for the qualification is to compare the neutronic code system used for design studies with reference Monte-Carlo calculations. The first part of the study consists in the comparison of cell calculations obtained with 2 different schemes: one based on the APOLLO2 code, and the other on one TRIPOLI4 Monte Carlo code. The second section presents the core calculations performed with an APOLLO2 two-level scheme and TRIPOLI4 code. For each part of the study, several cases have been explored. It is pointed out that the calculation times are more interesting with the deterministic code.

A two level PIJ/SN APOLLO2 scheme is proposed. In this scheme, the first level is devoted to the self-shielding and the leakage calculation on a cell configuration. At this stage, PIJ method is performed with a 172 energy mesh. To prepare the cross section sets for SN calculation, each fissile cell is homogenized in order to obtain the equivalent cross sections on defined energy and spatial meshes. The second level is dedicated to the flux calculation with the nodal SN method in RZ core configuration.

The cell and core calculations present keff discrepancies in the range from 120 pcm to 600 pcm. In this paper, the efficiency of a new treatment of absorption and scattering rates in the self-shielding module of the multigroup transport code APOLLO2 has been evaluated. This new method consists in treating the resonant mixture as a unique entity, and in taking into account the scattering resonance. The treatment of resonant mixture can lead to reduce discrepancies (versus reference calculations) of several percents on the resonant absorption reaction rates.

The Two-Level Scheme provides promising results with 172-group cross section libraries. These results confirm the APOLLO2 scheme as a tool for design studies in a great range of reactors. It indicates a low residual reactivity discrepancy within the range of 300 to 625 pcm between TRIPOLI4 and APOLLO2.

### 1. Introduction

Gas Cooled Fast Reactors (GFR) draw interest from the nuclear cycle (higher conversion factor than thermal reactors, higher burn-up...). They appear as relevant candidates for several Generation IV goals on economics, safety, reliability, sustainability and proliferation resistance. First exploratory studies have been carried out and showed interesting features [1,2]. All these considerations drove the CEA to investigate on a GFR core with high power. This study is based on a 3000MWth GFR design with a carbide or oxide fissile fuel and ZrC or SiC inert matrix support.

This study aims to evaluate, on the one hand, the deterministic calculation code APOLLO2 [5,6,7] capability to be applied in conceptual studies on Gas Cooled Fast Reactors. It drove to consider a similar scheme as the one assumed in PWR calculation (a two-level scheme with the same cross section libraries) [13]. The reliability of the neutronic code system used for design studies is essentially based on results obtained with reference calculations, usually carried out with Monte-Carlo code.

<sup>1</sup> Corresponding author :

Phone: (33) 1 69 08 32 87  
Fax: (33) 1 69 08 99 35  
e-mail: hgolfier@cea.fr

## 2. GFR overview and context

CEA's R&D program on a Gas Cooled Reactors technology pathway relies on the study of a long term Gas Cooled Fast Reactor (GFR) with integral cycling of minor actinides including optimized management of fuel and waste. First exploratory studies have been concentrated on small size GFR cores of 600 MWth power and have shown interesting features [2,3,4].

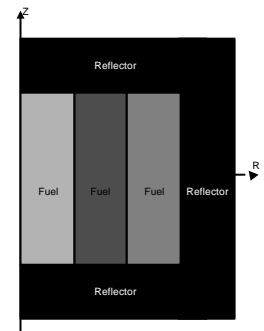
In order to increase GFR performances, it was also decided to investigate large power reactors. In GFR, one option for the fuel is to consider a dispersed particles fuel (coated fuel particles embedded in a matrix). GFR with oxide or carbide fissile fuel presents interesting core performances, breeding ratio, and provides up to 3000 MWth.

Realistic core configurations (see Figure 1) have been set up to compare the deterministic calculation and the Monte Carlo one. The main characteristics are listed in Table 1. Several power densities, fissile compounds and matrices have been considered in order to account for a wide range of GFR configurations. Further studies pointed out that the most efficient reflector is  $Zr_3Si_2$ .

Table 1: Main characteristics of core configurations

Core	3600 MWth (GBR4)	3000 MWth	3000 MWth	3000 MWth	3000 MWth	600 MWth
Case	3600MWth_OXY GBR4	3000MWth_OXY SiC	3000MWth_OXY SiC	3000PWth_CAR ZrC Zr3Si2	3000PWth_CAR ZrC Zr3Si2	600MWth_CAR SiC
fuel	Oxide	Oxide	Oxide	Carbide	Carbide	Carbide
matrix	-	SiC	SiC	ZrC	ZrC	SiC
reflector	steel	steel	steel	$Zr_3Si_2$	$Zr_3Si_2$	$Zr_3Si_2$
Volumic fraction	16.97% structure/55.9% Gas/27.13% comb	5% structure/ 40% Gas / 55% fuel+matr	5% structure/ 40% Gas / 55% fuel+matr	5% structure/ 40% Gas / 55% fuel+matr	5% structure/ 40% Gas / 55% fuel+matr	10% structure/ 40% Gas / 50% fuel+matr
Core volume	17 m <sup>3</sup>	75 m <sup>3</sup>	75 m <sup>3</sup>	75 m <sup>3</sup>	75 m <sup>3</sup>	10 m <sup>3</sup>
Power density	212 KW/l	40 KW/l	40 KW/l	40 KW/l	40 KW/l	80 KW/l
Fuel Weight density	9.33g/cm <sup>3</sup>	11.03g/cm <sup>3</sup>	11.03g/cm <sup>3</sup>	9.33g/cm <sup>3</sup>	9.33g/cm <sup>3</sup>	9.33g/cm <sup>3</sup>
Pu fraction	19%	25%	25%	25%	25%	18%

Figure 1 : RZ core description



## 3. General overview of the APOLLO2 code and data system

### 3.1 The Data system

The 172-group cross section libraries required for APOLLO2 calculations are derived from the JEF2.2 evaluated nuclear data files. This library is already assumed for PWR calculations.

### 3.2 The APOLLO2 code

APOLLO2 [9,10,11,12,13] is a French modular code which solves the neutron transport equation in a wide range of lattice configurations. It has been developed by the "Commissariat à l'Energie Atomique" with the support of Framatome ANP and EdF.

Beyond the neutronic flux calculation methods, APOLLO2 contains a modern self-shielding model, models for critical buckling treatment and for transport/transport equivalence. Moreover, various types of geometry can be described. As far as flux calculation is concerned, various methods are available in APOLLO2: the collision probability ( $P_{ij}$ ) method is commonly used in industrial applications.

A SN solver is also accessible in APOLLO2. The flux variation in angle is treated explicitly and the anisotropic scattering can be taken into account. The number of spatial and energetic meshes may be strongly reduced allowing the use of the SN solver after homogenization. This way permits a better treatment of the flux gradient. The SN solver of APOLLO2 is based on a nodal method, treating one point per spatial mesh.

### 3.3 Description of the Two-Level Scheme calculation

The Two-Level core Scheme (TLS) is derived from PWR scheme described in [12,13,14] and in Figure 2. The first part of the calculation is a full  $P_{ij}$  multicell calculation as described previously. The  $P_{ij}$  solution of the transport equation is therefore used to condense the 172 energy group cross sections into 33 or 8 energy groups only. Condensation and homogenization are performed through an equivalence procedure. The 33 energy group mesh is derived from ERANOS code and data studies [2,3,4].

The Two-Level PIJ/SN (TLS) APOLLO2 scheme described in is used for the core calculation, and consists on:

- the first level devoted to the self-shielding and a leakage calculation on heterogeneous cell configurations with 172-group cross section libraries. At this stage, the self-shielding, the flux and the leakage calculations are performed by using PIJ method;
- a flux calculation run on a 1-dimension geometry which includes the reflector's cells, in order to determine the reflector's cells capture sections;
- to prepare the cross section sets for SN calculation, each fissile cell is homogenized in order to obtain the equivalent cross sections on the defined energy and spatial meshes. The second level dedicated to the flux calculation with the nodal SN method in RZ core configuration (see Figure 1).

In order to reduce this computation time, this SN method has been replaced by a diffusion method (DIF). However, the algorithm remained identical to the one presented previously.

Figure 2: PIJ scheme and adaptations for the Two-level SN scheme

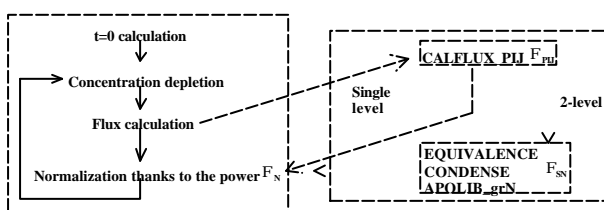
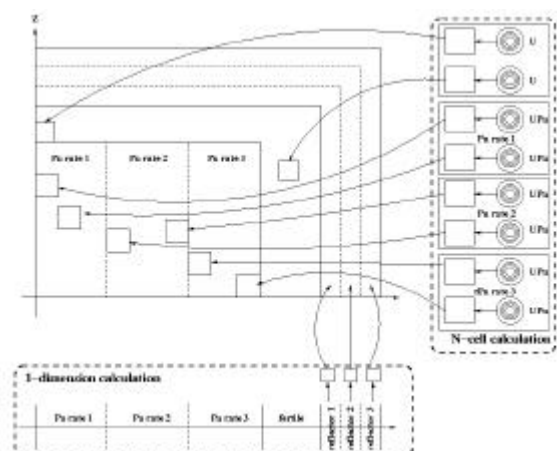


Figure 3: Extended two-level SN core scheme



#### 4. Element of validation of the TLS APOLLO2 scheme

The reliability of the neutronic code system used for design studies is essentially based on comparisons to reference calculations. Such reference calculations are usually obtained with Monte-Carlo codes. These methods allow modeling the core geometry without any additional physical assumptions. Our calculation scheme will be compared to a reference Monte Carlo simulation provided by the TRIPOLI4 code [8], especially dedicated to the transport of neutrons and the electromagnetic radiation. It is able to provide a  $k$  infinite as well as reaction rates. The cross sections are taken from the JEF2.2 evaluation and the TRIPOLI4 calculations performed on point wise energy mesh. The TRIPOLI's set of data are picked up in the APOLLO2 data, to make sure of the agreement between the two calculations.

In order to validate the Two-Level Scheme, various calculations have been carried out; in order to identify discrepancies, the reactivity decomposition adopted is:

$$\frac{dk}{k} = \underbrace{\sum_{isot,g} \frac{T_{isot,g}^{ProdAP2} - T_{isot,g}^{ProdT4}}{T_{tot}^{ProdT4}}}_{\text{production}} - \underbrace{\sum_{isot,g} \frac{T_{isot,g}^{AbsAP2} - T_{isot,g}^{AbsT4}}{T_{tot}^{AbsT4}}}_{\text{absorption}} ; \text{ where Prod and Abs refer to the production rate and absorption rate respectively, isot refers to isotope, tot refers to total and g refers to energy group. Notice that the absorption rate and the production rate are renormalized to the fission rate.}$$

rate respectively, isot refers to isotope, tot refers to total and g refers to energy group. Notice that the absorption rate and the production rate are renormalized to the fission rate.

#### 4.1 Simulations of cell configurations

##### *Description of cell configurations*

The main characteristics of the cell configurations are derived of Table 1 : triangular pattern, 6 rings in the cell, gas volume ratio equal to 40%, Pu ratio equal to 25%, rate of particles in the matrix equal to 60%, T/D ratio equal to 0.15 (where D is the diameter of the fuel kernel, and T is the coating thickness). By the way, several fissile compounds and matrix materials have been considered: Oxyde and carbide fuel, Steel, SiC and ZrC matrices.

The Table 2 reports the discrepancies of reactivity between APOLLO2 and TRIPOLI4 (AP2/T4). With the absorption and production rates, it is possible to obtain the decomposition of the reactivity by energy group and for each fissile isotopes. These APOLLO2 calculations were performed with a 172 energy groups.

##### *Analysis of cell configuration*

With regard to the reactivity, all PIJ or SN methods provide the same results thanks to the use of an equivalence process. The discrepancy between the Monte Carlo method (T4) and the deterministic calculation method (AP2) is lower than 220 pcm. Furthermore, we noticed that the APOLLO2 scheme presents a slight lower-reactivity.

The reactivity decomposition for the CAR\_SIC case (CUPu + SiC matrix) is plotted in Figure 4. The main contributions are located in the energy range from 50 eV to 1.48 keV, and from 15 keV to 100 keV. The most important gaps are located in groups whose energy is lower than 1 keV where large resonances of isotopes are located. The absorption rate decomposition (in pcm) is illustrated in Figure 5. The maximal discrepancy between APOLLO2 and TRIPOLI (AP2/T4) doesn't exceed 220 pcm close an energy ranging from 40.2 eV to 100 eV. Otherwise, the groups of energy presenting the strongest discrepancies are those of the uranium 238 and plutonium 239 resonances. A particular tendency can be

noticed with a positive contribution in the fast spectrum (6.07 MeV , 204 keV) and with a negative contribution under 1 keV.

An isotopic decomposition was performed in order to obtain more details (see Figure 6 and Figure 7). This study pointed out that a mixture of isotopes with resonances in the same energy interval may degrade the self-shielding process. Investigations have been carried out to assess a new development in self-shielding. Up to now, the self-shielding module of the multigroup transport code APOLLO2 [15] could treat one resonant isotope mixed with moderator isotopes. Consequently, the self-shielding treatment on resonant mixture was an iterative one. Each resonant isotope of the mixture is treated separately, the other resonant isotopes of the mixture being then considered as moderator isotopes. This approximation can lead to discrepancies of several percents on the resonant absorption reaction rates.

Two more sophisticated models [16] have been considered. The first consists in treating the resonant mixture as a unique entity (mixture self-shielding). The second model takes into account the transfer self shielding. The first model mitigates the problem of resonance overlapping in the slowing down range: the new treatment was applied between the groups 64 and 92 [204eV - 4eV]. The second method permits to correct the transfers to high energy in case of weak moderation by the present light isotopes in the cell (Si, C). It permits to test the contributions in the fast part of the spectrum.

The two methods of self-shielding have been tested separately. With regard to reactivity, the results presented in Table 3 show that each of these self-shielding options permits to decrease reactivity discrepancies.

The transfer self-shielding of  $^{238}\text{U}$  has an important effect since it permits to recover about 150 pcm on reactivity. The self-shielding of the other isotopes has a smaller effect.

The analysis of the absorption rate for  $^{238}\text{U}$  and  $^{239}\text{Pu}$ , the major contributors puts in evidence two zones of gaps (see Figure 6 and Figure 7) :

- In the [1keV-1MeV] energy groups, two groups have meaningful contributions (of the order of - 70 pcm each) for the  $^{238}\text{U}$ , corresponding to [16-24 keV] and [11-15 keV];
- In the slowing down domain, a set of resonances contributes in an important way (maximum 70 pcm). For the  $^{239}\text{Pu}$ , the major groups are [122-183 keV], [470-650 eV] and [59-69 eV]. One can suspect the treatment of the self-shielding in the unresolved resonance range;
- Two remarks can be highlighted from this analysis:
  - With regard to  $^{238}\text{U}$ , the treatment of transfer self-shielding accentuates the discrepancies in the unresolved resonance range. This implies a compensation of reactivity;
  - The treatment of mixture resonance particularly for  $^{239}\text{Pu}$  has a good impact and reduces reactivity discrepancy. The treatment of resonant mixture can lead to reduce discrepancies (versus reference calculations) of several percents on the resonant absorption reaction rates.

And to conclude, these analysis showed that the use of a more sophisticated model for self-shielding permits to decrease the discrepancies between APOLLO2 and TRIPOLI4, additional investigation are underway to mitigate the effects.

Table 2: Reactivity discrepancies between AP2/T4 on various cell configurations

TYPE	kinf A2	kinf T4	sigma T4	AP2/T4 disp.
Units			pcm	pcm
CAR_SiC	1,27315	1,27583	43,1	-210
CAR_ZrC	1,18923	1,19075	41,5	-128
OXY_SiC	1,21985	1,22139	41,3	-126
OXY_ZrC	1,11970	1,12006	41	-32

Table 3: Sensitivity to self-shielding option for CAR\_SiC cell

Case : CAR_SiC	AP2/T4 pcm
T4 (reference)	-
AP2 standard	<b>-211</b>
U238 : scattering self_shielding (trss)	-64
U238+Pu239 : trss	<b>-86</b>
U238+Pu239+Pu240 : trss	-73
U238+Pu239+Pu240 : mixture self-shielding	<b>-87</b>

Figure 4: Decomposition of the  $\frac{dk}{k}$  discrepancies between AP2/T4 for CAR\_SiC cell

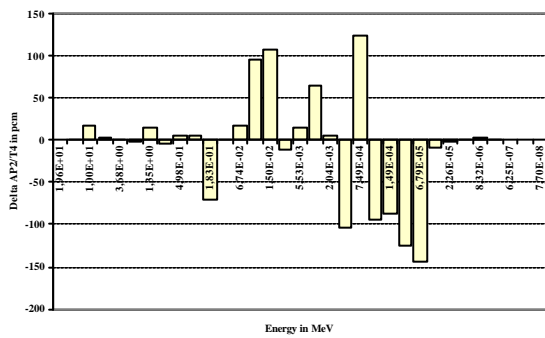


Figure 5: Decomposition of the absorption rate discrepancies between AP2/T4 for CAR\_SiC cell

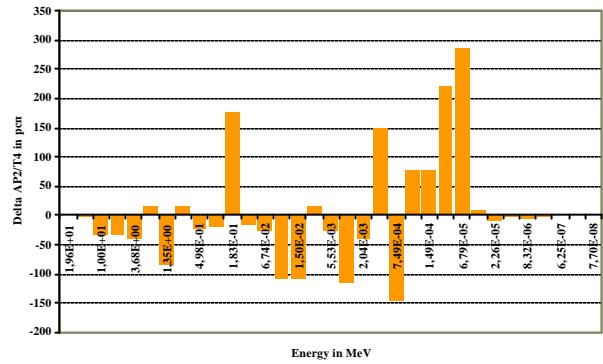


Figure 6: Sensitivity to the self-shielding options (standard, transfert, mixture) between AP2/T4 on the  $^{239}\text{Pu}$  absorption rate for CAR\_SiC cell

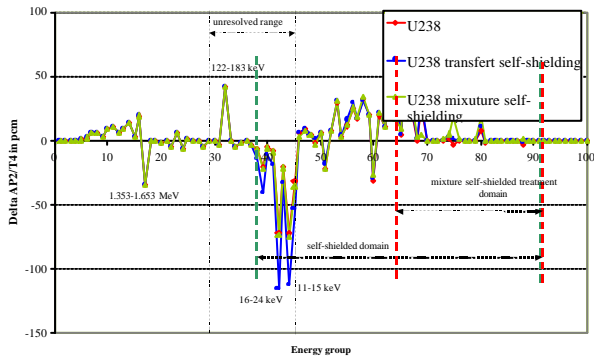
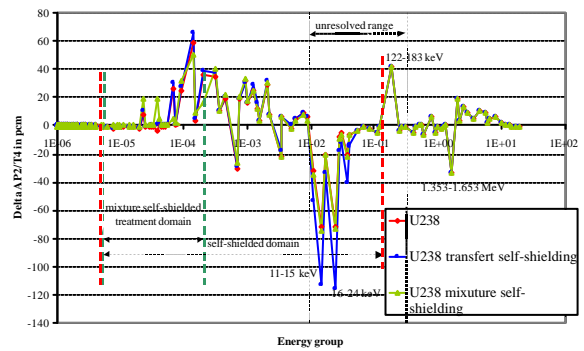


Figure 7: Sensitivity to the self-shielding options (standard, transfert, mixture) between AP2/T4 on the  $^{238}\text{U}$  absorption rate for CAR\_SiC cell



## 4.2 Simulation of core configurations

The APOLLO2 scheme applied to core calculation uses the extended Two-Level Scheme. The flux calculation performed in the second step, has been carried out either with the SN method or the diffusion method in order to reduce the computation time. Several cases have been considered:

- Carbure SiC, steel reflector, 600MWth,
- Oxyde SiC,  $Zr_3Si_2$  reflector, 3000MWth,
- Oxyde SiC, steel reflector, 3000MWth,
- Carbure ZrC,  $Zr_3Si_2$  reflector, 3000MWth,
- Carbure ZrC, steel reflector, 3000MWth.

The more interesting cases are the two cores with  $Zr_3Si_2$  reflectors. Several calculation options have been performed with different energy meshes and calculation methods:

- 8-group diffusion calculation hereafter named Dif\_8g,
- 33-group diffusion calculation hereafter named Dif\_33g, the 33 energy group mesh is taken from [3],
- 33-group transport calculation hereafter named Tr\_33g,
- 172-group transport calculation hereafter named Tr\_172g,
- Monte-Carlo code calculation hereafter named T4.

The T4 calculation serves as reference calculation and the results are compared to the various APOLLO2 methods (see Table 4).

## 4.3 Analyses of core configurations results

With regard to reactivity, the discrepancies between the Monte Carlo method (T4) and the deterministic calculation method (AP2) range from 235 to 723 pcm. Furthermore, it is to be noticed that the APOLLO2 scheme presents a higher difference for the cases with steel in matrix or reflector due to the lack of self-shielding treatment for  $^{56}\text{Fe}$  isotope (see Table 5). The calculation with 8 energy groups is less accurate: one notes compensations between calculation with 8 energy groups and the calculation with 33 energy groups. A calculation with the SN method with a 33 energy groups overestimates the reactivity by 600 pcm, whereas the diffusion calculation with 8 groups overestimates the reactivity by 700 pcm.

For the further analyses, only the Oxyde SiC core (3000MWth\_OXY\_SIC\_ZR3SI2) will be presented. Moreover, it is not foreseeable to achieve the calculations with 172 energy groups for the conceptual studies (see Table 4). Using the decomposition formula for the cell configurations, the reactivity discrepancies and the absorption rate discrepancies are plotted in Figure 8 and Figure 9. One can notice that the errors on the production and absorption rates can reach 15% to 20% in the range of energy where the neutron density is negligible. With regard to the reactivity, the discrepancy between APOLLO2 and TRIPOLI4 schemes does not exceed 465 pcm. However, the same phenomenon as for the cell is to be noticed: compensation appears, which reduces the global discrepancies result.

The reactivity decomposition gives a maximum value of 125 pcm in the energy range from 677 to 67.9 eV. In order to determine the cause of this effect, an isotopic analysis with a 172 energy mesh was performed. It appears that 3 major isotopes which have resonance at the same energy ranges, contribute to the discrepancy:  $^{238}\text{U}$ ,  $^{239}\text{Pu}$ ,  $^{241}\text{Pu}$  (see Table 7). The impact of  $^{238}\text{U}$  on the macroscopic absorption

discrepancy reaches  $-612$  pcm, which corresponds approximately to the global macroscopic discrepancy. The impact of  $^{239}\text{Pu}$  on the macroscopic absorption discrepancy is smaller. However, we note such compensation towards the different energy groups.

The groups in which the strongest discrepancies are observed are in the range of large resonance. The modification of APOLLO2 self-shielding for the mixture resonance treatment has been applied as previously [16] between the groups 64 and 92 [204-4eV]. In the Table 6, we note that this treatment increases the discrepancy on the reactivity around 100 pcm. However, as seen in Figure 11, it mitigates the problem of the resonance recovery in the slowing down range and limits dramatically compensations.

Figure 8: decomposition of reactivity discrepancy for OXY\_SIC\_ZR3SI2 configuration

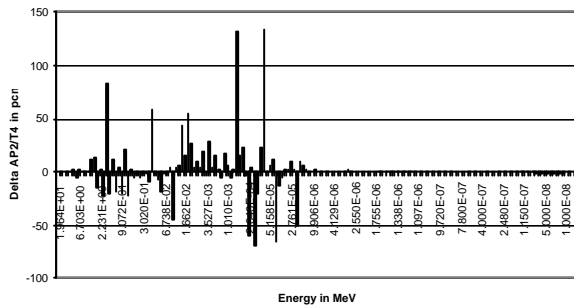


Figure 9: decomposition of absorption rate discrepancy for OXY\_SIC\_ZR3SI2 configuration with Tr\_172g calculation

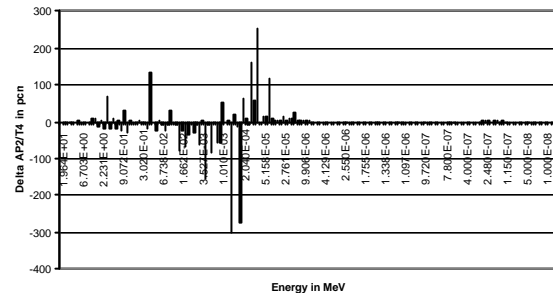


Figure 10: 238 uranium energy group contributions to the absorption rate discrepancy for OXY\_SIC\_ZR3SI2 configuration with Tr\_172g calculation

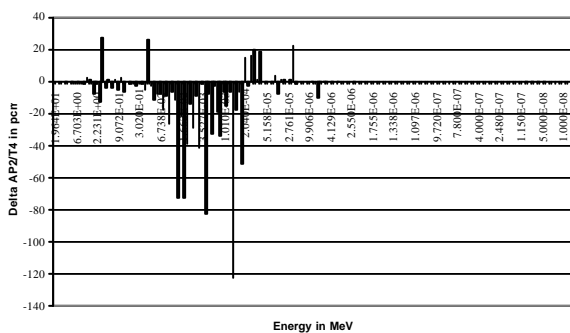


Figure 11: sensitivity to self-shielding option on absorption rate discrepancy for OXY\_SIC\_ZR3SI2 configuration with Tr\_33g calculation

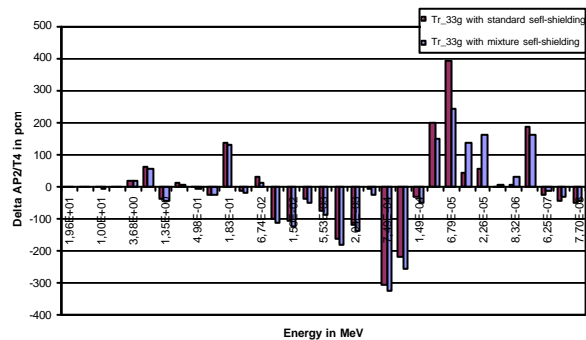




Table 4: Computation times and memory for various tested codes and methods

Case	T4	Tr_172g	Tr_33g	Dif_33g	Dif_8g
600MWth_CAR_SIC	244930 s*	X	4810 s 39.2 Mmots	84.7 s 41.3 Mmots	66.3 s 18.5 Mmots
3000MWth_OXY_SIC_ZR3SI2	179220 s*	496430 s 349.7 Mmots	14600 s 125.9 Mmots	256.5 s 115 Mmots	159 s 54.1 Mmots

Table 5: keff discrepancies between AP2/T4 according to various methods

TYPE	AP2 Tr_33g/T4 discr	AP2 Diff_33g/T4 discr	AP2 Diff_8g/T4 discr.
Units	pcm	pcm	pcm
600MWth_CAR_SIC	503	582	706
3600MWth_OXY_GBR4	625	723	485
3000PWth_CAR_ZRC	471	524	541
3000MWth_OXY_SIC	511	545	661
3000MWth_OXY_SIC_ZR3SI2	360	415	466
3000MWth_CAR_ZRC_ZR3SI2	235	294	303

Table 6: keff discrepancies between AP2/T4 according to various methods for OXY\_SIC\_ZR3SI2 configuration

3000MWth_OXY_SIC_ZR3SI2	Tr_172g/T4	Tr_33g/T4 with standard self shielding	Tr_33g/T4 with mixture self shielding	Dif_33g/T4	Dif_8g/T4
AP2 Diff_8g/T4 discr.	360	360	460	415	465

Table 7 : isotopic contribution to absorption rate discrepancies for OXY\_SIC\_ZR3SI2 with Tr\_172g calculation

Group	Upper energy of the group in Mev	AP2_172_trans/T4 ABS Rate	Max. isotopic contribution on absorption rate			
			PU239	PU240	PU241	U238
17	1.653E+00	66	23	9	3	27
32	1.832E-01	131	80	7	13	26
42	2.479E-02	-94	-13	-3	-4	-73
44	1.503E-02	-80	-3	-2	-1	-73
49	5.005E-03	-75	-23	-6	-3	-41
51	3.355E-03	-171	-67	-9	-8	-83
53	2.035E-03	-85	-44	-4	-4	-33
55	1.434E-03	-62	-36	-5	-2	-19
56	1.234E-03	-68	-31	-5	1	-34
60	6.773E-04	-315	-155	-23	-15	-122
63	3.043E-04	-283	-176	-25	-28	-52
64	2.040E-04	58	26	-8	15	14
67	9.166E-05	154	77	34	20	19
68	7.567E-05	57	47	7	2	1
69	6.790E-05	242	198	15	16	19
73	4.552E-05	116	78	38	0	0
Sum*		-692	-59	-20	-1	-612

## 5. Conclusions

The purpose of the paper was to analyze the deterministic modeling with the APOLLO2 code, in the framework of GFR. The analysis of the APOLLO2 modeling based on the two-level scheme is led by the comparison with Monte-Carlo code TRIPOLI4. The analysis has been performed for different fuel, matrix, and volume cores.

Various calculation methods available in the APOLLO2 code have been applied. All the results were compared to reference Monte-Carlo simulation. A Two-Level Scheme has been developed, and it provides promising results. A residual discrepancy on the reactivity between TRIPOLI and APOLLO2 has been pointed out : within the range of 300 and 625 pcm depending on the presence of steel.

Up to now, the self-shielding module of the multigroup transport code APOLLO2.v6 could treat one resonant isotope mixed with moderator isotopes. Consequently, the self-shielding treatment is an iterative one and can lead to discrepancies of several percents on the resonant absorption reaction rates on resonant mixtures. Two new methods have been investigated. The first one consists in treating the resonant mixture as a unique entity (mixture self-shielding) and the second one takes into account the scattering self shielding effect. The first treatment is devoted to the problem of the resonance overlapping in the slowing down range. It was applied between the groups 64 and 92 [204eV - 4eV], where there is a resonance overlapping between the resonance of  $^{238}\text{U}$  and  $^{239}\text{Pu}$ . The second method permits to correct the scattering to high energy and to improve the result with regard to reactivity. However, the treatment of scattering self-shielding accentuates the discrepancies in the unresolved resonance range. More sophisticated models for self-shielding are underway to suppress the counterbalances.

To conclude, the core analysis is coherent with the cell results.  $k_{\text{eff}}$  discrepancies are satisfactory enough to use this scheme for core design calculation (discrepancy less than 600 pcm), but errors remain in the self-shielding process of the 2 major isotopes ( $^{238}\text{U}$ ,  $^{239}\text{Pu}$ ). Furthermore, the 33-group diffusion calculation is a good compromise in terms of accuracy and computation time.

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