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FAST REACTOR CORE-REFLECTOR INTERFACE EFFECTS REVISITED

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ABSTRACT

Recently, a simple calculation benchmark of a fast reflected reactor was performed in the frame of the MUSE program. This benchmark was calculated with different Monte Carlo and deterministic codes, all using libraries based on the same JEF2.2 nuclear data file. Apart from conclusions concerning nuclear data, it was observed that reactivity calculations performed with the ERANOS deterministic code system show a high sensitivity to the treatment of the steel reflector, where broad resonances and complex flux variations with space, energy and angle variables require sophisticated models.

We report here further investigations that we have performed with the deterministic code system ERANOS2.0 and with the continuous energy Monte Carlo code TRIPOLI-4, in

order to understand these effects and converge to a satisfactory and practical calculation scheme for steel-reflected fast-reactor cores.

Since there are practical limits to the number of groups that can be used in full core calculations, we have investigated a way to ameliorate the ERANOS calculations by improving the determination of the flux used in the ECCO cross section condensation; we expect that this approach could reduce the biases appearing in the collapsing procedure and capture the spectrum transient effects with a limited number of groups.

1. INTRODUCTION

Over the past ten years, there has been a growing interest for the operation of fast reactors as plutonium burners rather than Pu-breeders. In such Pu-burner concepts, the traditional fertile blankets are replaced by stainless steel reflectors. In this context, core-reflector interface effects have become an important issue. Indeed, while deterministic neutron transport codes can deal satisfactorily with highly absorbing blanket materials, the same codes or calculation procedures cannot easily model the complex interplay of energy and angle dependent phenomena which take place at the core-reflector interfaces.

This long standing problem [1] has recently been studied with modern deterministic codes such as ERANOS [2], but it has not been solved satisfactorily since no recommendations in terms of a calculation procedure have been given. This issue recently reappeared in the context of a calculation benchmark performed in the frame of the MUSE program [3], whose goal is to study subcritical fast reactors in the MASURCA experimental facility at CEA Cadarache. This simple benchmark was calculated with different Monte Carlo and deterministic codes, all using libraries based on the same JEF2.2 nuclear data file: TRIPOLI-4, MCNP-4B/4C, ECCO/ERANOS and KAPROS/KARBUS.

In this framework, two series of investigations have been initiated :

- concerning nuclear data, the conclusions of this benchmark [3] were that there is a reasonable agreement among all codes, as long as the exact same version of the nuclear data file is used. The importance of data evaluation and processing has been emphasized.

- concerning methodological biases in deterministic codes, either to obtain multigroup self-shielded cross sections or solve the transport equation.

Calculations performed with the ERANOS deterministic code system have shown a high sensitivity of the calculated reactivity to the treatment of the reflector.

We report here further investigations that were performed with the deterministic code system ERANOS2.0 and with the continuous energy Monte Carlo code TRIPOLI-4, in order

to understand these effects and converge to a satisfactory calculation scheme: the final objective of this work is to define a recommended deterministic calculation procedure for an accurate and computationally-efficient treatment of fast reactor neutron balance in the presence of steel reflectors.

2. CALCULATION BENCHMARK DEFINITION AND RESULTS

The geometry and composition of the benchmark are shown in Figure 1 and in Table 1. It is important to note that this is a very simplified two-zone homogeneous configuration.

Table 1: Isotopic compositions

Region	**Isotope**	**Density $\times 10^{+24}$ at/cm^3**
Zone1- Fuel	Pu239	1.5×10^{-3}
	U238	5.0×10^{-3}
	Fe56	7.0×10^{-3}
	Cr52	1.5×10^{-3}
	Na23	1.0×10^{-2}
	O16	1.5×10^{-2}
Zone2 - Reflector	Fe56	5.0×10^{-2}
	Cr52	1.5×10^{-2}
	Na23	5.0×10^{-3}

A first comparison of k_{eff} and k_∞ calculated with TRIPOLI-4 and ERANOS gives the following results:

Table 2: TRIPOLI versus ERANOS (standard calculation route) comparison

	TRIPOLI-4	ERANOS2.0
k_∞	1.67502 ± 0.00060	1.67508
k_{eff}	1.01300 ± 0.00060	0.99957

TRIPOLI is used with cross sections including probability tables in the unresolved energy range, which allow to take into account self shielding effects properly. On the other hand the ECCO infinite reflector cell calculations are performed with a 1968-group structure where the neutron source is provided by leakage from the core; the P1 order cross sections are then condensed into a 175 group structure which is used for the core transport calculation performed with the BISTRO Sn module of ERANOS. The subgroup method is used by ECCO to treat self-shielding effects.

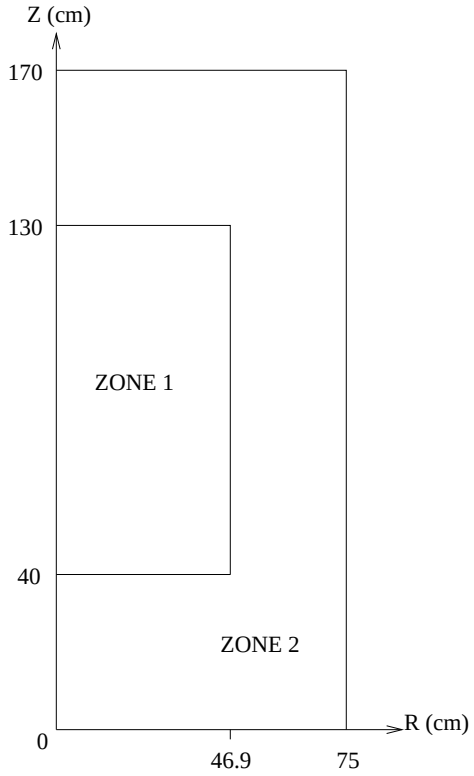

Figure1: Geometry of the Benchmark

The perfect agreement on k_∞ clearly shows that nuclear data are not responsible for the 1300 pcm discrepancy in k_{eff}. When the calculation route is modified, the resulting k_{eff} shows a large sensitivity to the various possibilities offered to the ECCO/ERANOS user [4]:

- The source term appearing in reflector cell calculations can either be provided by introducing traces of fissile material (emitting fission neutrons), or by computing neutron leakage from the core (with a softer spectrum) by a separate fuel cell calculation; in this case the source term is DB^2, where D is the diffusion coefficient and B the value of the Buckling driving the leakage. This buckling is given by a semi-empirical formula in the conventional ECCO calculation route:

$$B^2 = \frac{5}{8}\left(\frac{\pi}{h}\right)^2 \qquad (1)$$

  where h is the thickness of the reflector zone. This formula has been historically developed for the treatment of fertile blankets but is inappropriate in the case of a steel reflector. Indeed, conventional fast reactor analysis code systems such as ERANOS are clearly optimised for highly absorbing media like blankets, but not for reflector cell calculations

- The cross sections can be obtained with the ECCO code in two different ways:

  - A standard ECCO calculation provides separately the cross sections for the core and the reflector regions which are assumed to be infinite. In this case the calculations related to the reflector region are performed with a user-specified value for the buckling. This value is assumed to be constant in each energy group.

  - A Macrocell ECCO calculation allows to take into account the core coupled with the reflector: the cross sections for each region are weighted with the corresponding flux calculated in each one. In this way, the processing of the cross sections takes better account of the spatial effects at the core/reflector interface. At the present time this option in the ECCO code is available just for mono-dimensional geometries and P1 order cross sections, the same buckling being applied to each region and assumed to be constant in each energy group.

  In either option, the cross sections are condensed over the fine structure consisting of 1968 groups.

Table 3 shows the results obtained with the calculation options described above:

Table 3: Reactivity Obtained by a Core Calculation Performed with Different Conventional Reflector Cell Calculation Methods

Type of Cell Calculation	Neutron Source	Buckling	Reactivity ρ (pcm)*
Infinite	Leakage from core	$B^2 = \frac{5}{8}\left(\frac{\pi}{h}\right)^2$	-43
Infinite	Traces of fissile material	$B^2 = \frac{5}{8}\left(\frac{\pi}{h}\right)^2$	-240
Macrocell	Fuel in (macro)cell	$B^2 = \frac{\left(\frac{\pi}{h}\right)^2}{\left(\frac{\pi}{h}\right)^2 + \left(\frac{J_0}{r}\right)^2}$	-423

* 1 pcm = $10^{-5} \times \left(\Delta k / k\right)$

Table 3 shows **the considerable impact of the ECCO cross section processing route in the reflector on a key integral parameter like k_{eff}**. In the next sections we investigate in detail a number of calculation options that are important for a correct treatment of reflector effects.

3. SENSITIVITY TO CALCULATION OPTIONS

A sensitivity analysis to different ERANOS code options (Sn and Pn approximations, buckling) was performed. The ECCO cell calculations were performed under the assumption of infinite cell models. Cross sections were collapsed into 33 energy groups from the 1968-group fine energy structure. Transport calculations were carried out by the BISTRO spatial Sn module.

In order to evaluate the sensitivity to the Sn and Pn approximations, k_{eff} transport calculations were performed with different Sn (S4, S4_Symmetric, S8_Symmetric, S16_Symmetric) and Pn (P0, P1, P3) approximations. Concerning the Sn approximation (Tab. 4), assuming S4 calculation as a reference, a negligible difference is observed with the S4_Symmetric calculation, while a difference of about 120 pcm is found with the S16_Symmetric and S8_Symmetric calculations.

Table 4: 33 Energy Group Calculations: Sn Effect

SN APPROXIMATION	k_{eff} (33, P1)	Sn effect (pcm)
S4	0.97941	-
S4_Symmetric	0.97958	+17
S8_Symmetric	0.97826	-117
S16_Symmetric	0.97818	-126

Concerning the Pn approximation (Tab. 5), taking the P0-corrected calculation as a reference, differences of about 320 pcm (P1 calculation) and 460 pcm (P3 calculation) are observed.

Table 5: 33 Energy Group Calculations: Pn effect

PN APPROXIMATION	k_{eff} (33, S4)	Pn effect (pcm)
P0-corrected	0.98261	-
P1	0.97941	-326
P3	0.98721	+468

In order to study the k_{eff} sensitivity to the buckling, 33-energy group transport calculations were performed using cross sections pre-processed with different buckling values in the reflector cell calculations, using the semi-empirical formula; two buckling values were adopted after substituting h = 23.8 cm ($B^2=1.086\cdot10^{-2}$ cm^{-2}) and h = 40.0 cm ($B^2=3.855\cdot10^{-3}$ cm^{-2}) in the semi-empirical formula (1).

The results are summarized in Table 6. A large difference (about 1600 pcm) is observed. In order to evaluate the buckling effect in a more realistic configuration, the simplified reflector composition was replaced by a reflector composition closer to the actual MASURCA/MUSE reflector (including Fe, Ni, Cr, Si, V, Mn, Co, Cu, Mo,…); results show that the B^2 effect decreases as one approaches a realistic reflector composition (from 1590 pcm to 289 pcm). Then, transport calculations were performed after adding a radial and an axial steel shield past the reflectors: no difference was observed with respect to the previous case (same 270 pcm discrepancy). We therefore concluded that the B^2 effect was not caused by the limited reflector thickness.

Table 6: 33 Energy Group Calculations: B^2 effect

	Simplified Reflector Composition	MUSE Reflector Composition	MUSE Reflector and Shielding Composition
k_{eff} (33 groups , S4-Symmetric, $B^2=1.086\cdot10^{-2}$ cm^{-2})	0.99546	1.04665	1.05785
k_{eff} (33 groups , S4-Symmetric, $B^2=3.855\cdot10^{-3}$ cm^{-2})	0.97958	1.04376	1.05495
B^2 effect (pcm)	-1595	-276	-274

Upon analyzing the macroscopic scattering cross sections in the reflector, we observed that the $5.5\cdot10^3$ - $2.6\cdot10^4$ eV energy range is significantly different in the two reflector models (compositions). We therefore suspect that the cross section difference in that range is responsible for the reactivity difference. Sensitivity calculations will be performed to investigate this further.

4. INVESTIGATION CONCERNING THE MACROCELL STRUCTURE

To study the importance of the Macrocell structure on the calculated core parameters, we have performed 175-energy group macrocell ECCO calculations based on an 8-zone (4 in the fuel and 4 in the reflector) 1D cylindrical geometrical description of the whole reactor for the radial and axial directions. 175-energy group cross sections were collapsed from a 1968 fine energy structure and transport calculations were carried out with the BISTRO spatial module.

The strategy consisted of an iterative procedure with the aim to evaluate the buckling values such that the one dimensional transport calculation for the radial and axial directions and the two-dimensional transport calculation would yield the same k_{eff} results. Starting from a guess buckling value (B^2=0 was assumed in the calculation route), a macrocell calculation and a two dimensional transport calculation were carried out; a one dimensional transport calculation was performed for each direction with the guess buckling value. Different one-dimensional transport calculations by the BISTRO spatial module were performed for each direction with different buckling values, in order to find the B^2 value making the one-dimensional transport k_{eff} equal to the two-dimensional transport k_{eff}. The calculated radial and axial buckling values represent the starting B^2 values for another calculation. The convergence is reached when the two dimensional transport k_{eff} do not show any meaningful difference from the previous iteration two-dimensional transport calculation result.

Table 7: Iterative Route for 175-Energy Group Macrocell Calculation

Iteration 1:

Macrocell	Buckling	k_cell (1968g)	k_cell (175g)	k_BISTRO_R (175,P0,S4)	k_BISTRO_RZ (175,P0,S4)
Axial	0 (Guess)	1.04755	1.04274	1.16947	1.00261
Radial	0 (Guess)	1.05872	1.05212	1.16557	

Buckling search from 1D transport calculation by BISTRO spatial module giving
k_BISTRO_R (175,P0,S4)= k_BISTRO_RZ (175,P0,S4):
B^2(radial)=$5.26828\cdot10^{-4}$ cm^{-2} B^2(axial)=$5.45734\cdot10^{-4}$ cm^{-2}

Iteration 2:

Macrocell	Buckling	k_cell (1968g)	k_cell (175g)	k_BISTRO_R (175,P0,S4)	k_BISTRO_RZ (175,P0,S4)
Axial	$5.2682\cdot10^{-4}$	0.89139	0.88520	1.00287	1.00288
Radial	$5.4573\cdot10^{-4}$	0.90797	0.90147	1.00281	

Results show that only two iterations are sufficient in order to reach convergence and obtain values of the axial and radial buckling in a rigorous way (without the inadequate semi-empirical formula (1)); moreover, by using this iterative procedure no meaningful dependence of transport calculation results on the buckling was observed.

5. INVESTIGATION CONCERNING THE NUMBER OF GROUPS

To study the importance of the energy structure of the calculation performed, we have investigated a simplified 1D model as presented in Fig.2 (the fuel and reflector compositions are those given in Table 1).

For this model the TRIPOLI Monte Carlo code gives k_{eff} = 1.07116 (ρ = + 6643.3 pcm). We have compared the results with ERANOS in terms of reactivity value, U^{235} and Pu^{239} fission rate distribution. The ERANOS results were obtained with different numbers of groups NG.

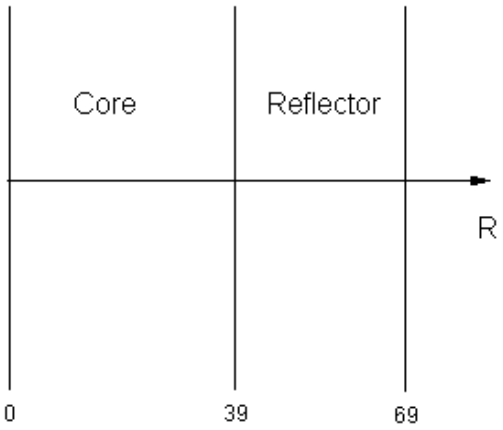

Figure2: Simplified Geometry for 1D model

The reactivity calculations were performed by the BISTRO Sn code with the following approximations: S16 for the angular quadrature, P1 for the anisotropic scattering treatment and with different numbers of groups NG = 33, 172, 299, 471, 838. The results of this approach are summarised in the following tables. They are differentiated with respect to the option used for the ECCO calculation and the number of energy groups for the reactivity calculation.

Table 8: Standard ECCO Calculation
(buckling provided in the reflector region: B^2=7.867988E-03 cm^{-2})

NG	ρ [pcm]
33	4693.4
172	5298.0
299	6344.0
471	6602.7
838	6806.8

Table 9: Standard ECCO Calculation
(buckling provided in the reflector region: $B^2=0$)

NG	ρ [pcm]
33	1986.7
172	3550.7
299	5565.7
471	6059.3
838	6461.5

Table 10: Macrocell ECCO Option (buckling provided: $B^2=0$)

NG	ρ [pcm]
33	4234.2
172	4962.4
299	6147.5
471	6440.7
838	6680.9

We observe a significant change in reactivity with NG. The dependence is very strong for low values of NG. A convergence of the results seems to be reached by increasing the number of energy groups.

The results shown above suggests to extrapolate the results up to NG=1968 (such a large calculation could not be done with the available computer resources). See Fig.3-5:

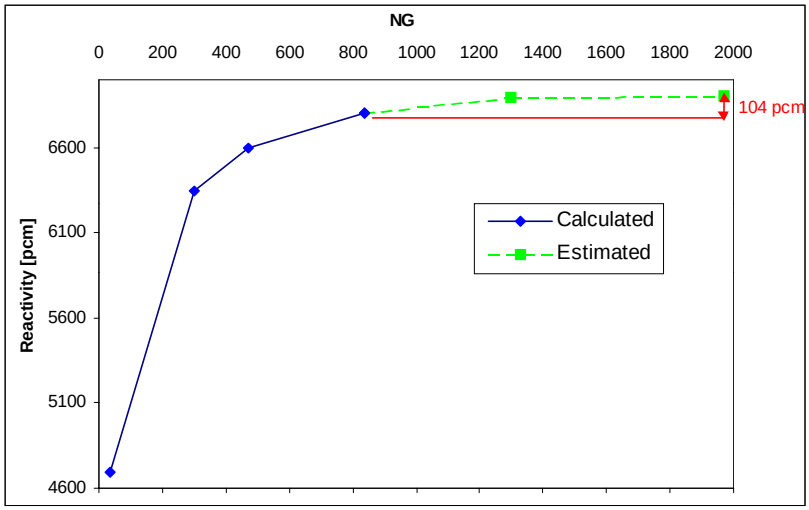

Figure 3: Standard ECCO – B^2(reflector)=7.867988E-03 cm^{-2}

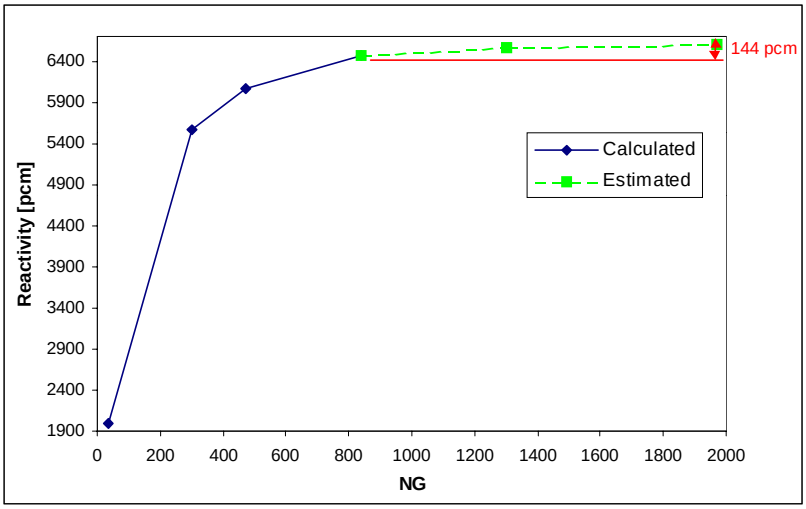

Figure 4: Standard ECCO – B²(reflector)=0

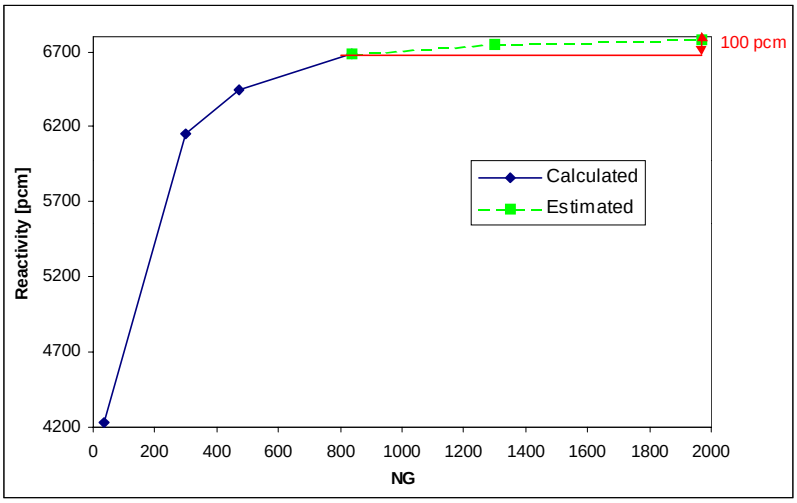

Figure 5: Macrocell ECCO option – B²=0

Finally we conclude that a fine treatment (NG=1968) would provide the following results:

Table 11: extrapolation for NG=1968

Case	ρ [pcm] (ERANOS)	Δρ (ERANOS – TRIPOLI)
Standard ECCO - B2=7.867988E-03 cm^{-2}	6910	-266.7
Standard ECCO - B2=0	6604	-39.3
Macrocell ECCO option - B2=0	6780	136.7

We can observe **that the agreement with TRIPOLI is satisfactory**, within about 250 pcm for each case.

We also observe that a good agreement is found for the different ECCO options. This was not expected looking at the results obtained for low NG. Referring to Tables 8 and 9, for example for NG=33, we can notice that changing the buckling in the reflector region (0 instead of 7.867988E-03 cm^{-2}) affects the reactivity by about 2700 pcm. This discrepancy decreases to just 300 pcm (Table 11) when NG=1968. This is likely due to the spectral effect of the leakage term DB^2. Because the buckling introduced in the ECCO code has no energy dependence, the leakage term varies in energy like the diffusion coefficient. Condensing to 33 groups, the energy dependence of the other terms in the balance equation is already approximate with respect to a fine treatment. In this situation, a rough spectrum distribution in the leakage term could have a significant effect. Instead, if we keep the ultrafine structure, the energy dependence of all the terms in the balance equation is well reproduced: in this case the spectral distribution of the leakage term is expected to have a modest impact. This is most likely the reason why the effect of a different choice of B^2 values decreases with increasing NG.

The ERANOS – TRIPOLI comparison was also done for the fission rate distributions. In Figures 6 to 9 we show the change in the U^{235} and Pu^{239} fission rate distribution for the Standard ECCO – B^2(reflector)=0 and Macrocell ECCO option – B^2=0 case vs. radial position. Finally in Figures 10-11 the fission rate calculated for the two cases with NG=838 are compared with the TRIPOLI results.

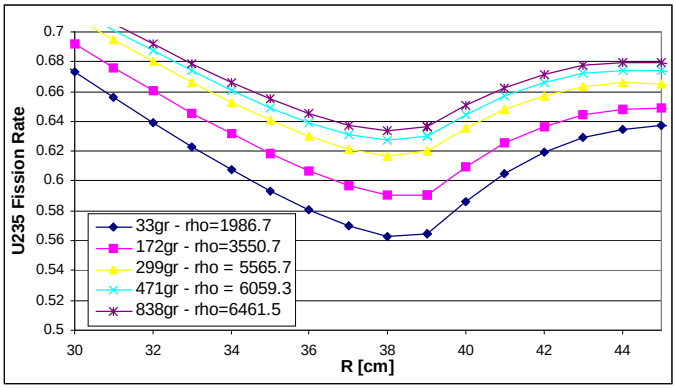

Figure 6: ^{235}U Radial Fission Traverse (Standard ECCO – B2=0)

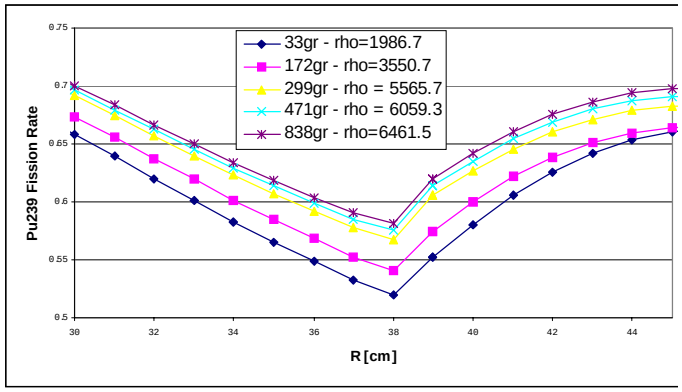

Figure 7: ^{239}Pu Radial Fission Traverse (Standard ECCO – B2=0)

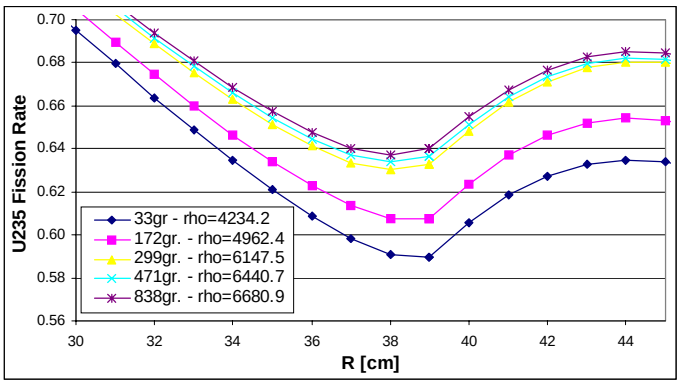

Figure 8: ^{235}U Radial Fission Traverse (ECCO Macrocell – B2=0)

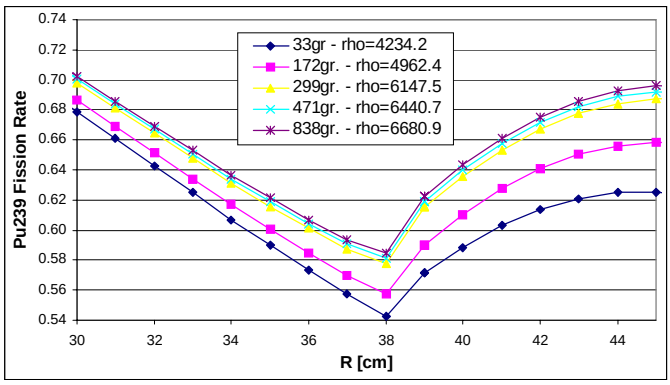

Figure 9: ^{239}Pu Radial Fission Traverse (ECCO Macrocell – B2=0)

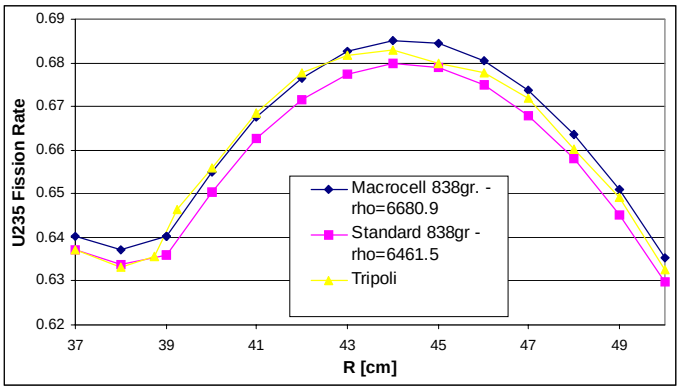

Figure 10: ERANOS vs. Tripoli U5 Fission Rate

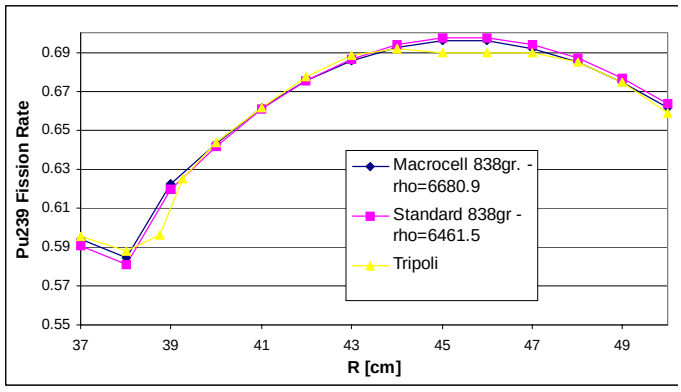

Figure 11: ERANOS vs. Tripoli U5 Fission Rate

Figures 6 to 9 show that the fission rate distribution could be reproduced rather well with NG equal to at least 299. Figures 10 and 11 show that **the ERANOS – TRIPOLI agreement is very satisfactory: the discrepancies are less than 1%** which is within the uncertainties associated to both the deterministic and Monte Carlo codes.

6. INVESTIGATION CONCERNING THE GROUP STRUCTURE OPTIMISATION

We see from the previous analysis that an increase of the number of groups allows a much better agreement between ERANOS and TRIPOLI, this agreement being almost perfect when the full core calculation is performed in 1968 groups. A large number of groups also reduces the impact of the other calculation options (choice of B^2 value, macrocell structure, …).

Nevertheless, calculation time and memory requirements necessary for ERANOS calculations increase as the square of NG and, today, it is not realistic to perform 1968 groups calculations for a full 3D core with a complex geometry and full composition. Therefore it would be desirable to reduce the energy group structure to a more reasonable number of groups.

In this context we have performed TRIPOLI calculations to evaluate the energy domain where the dominant core-reflector interface phenomena take place. Figure 12 shows the spectral distribution (in the ERANOS 175g structure, group 1 being the highest energy group) of the net neutron currents between volumes located in the core and in the reflector:

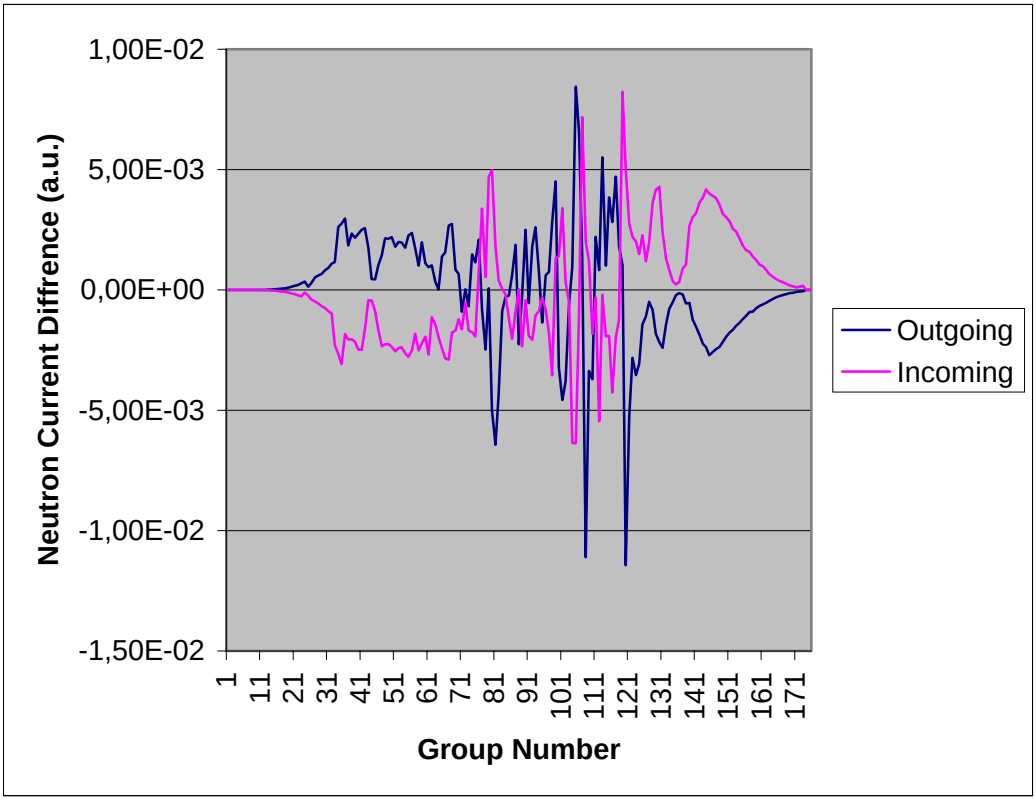

Figure 12: Spectral Variation of the Neutron Current at the Core –Reflector Interface

We see that a large energy range is covered, which makes it difficult to focus on a precise domain for a group structure refinement; Figure 13 shows the macroscopic scattering cross sections in the reflector.

The main resonances are located between groups 75-85 and 93-145. Therefore we decided to refine the 175 groups energetic structure between these limits to obtain a new 299 groups structure. We then performed ERANOS calculations with this modified 299 groups structure and we compared them to the results obtained with the 175-group and standard 299-group structure as shown in Table 12.

Table 12: Reactivity of 1D Model Calculated with Standard/Modified 299gr Structure (macrocell description of the reflector, semi-empirical Buckling)

ERANOS Energetic Structure	Reactivity ρ (pcm)
175g	+ 5240
299g Standard	+ 5831
299g modified	+ 6106

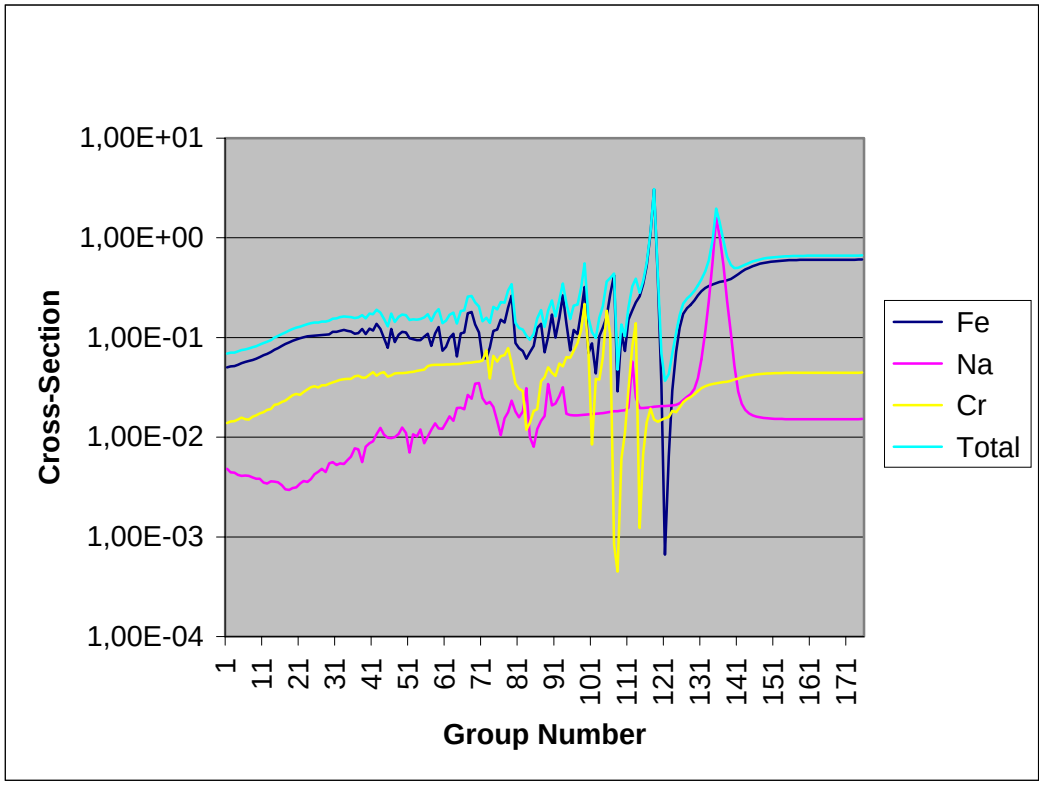

Figure 13: Macroscopic Scattering Cross Sections in the Reflector

We see that **our attempt to optimise the energetic structure improves the ERANOS-TRIPOLI agreement by 275 pcm** in the macrocell calculation; nevertheless, there is still a large discrepancy of 500 pcm. This point is still under study. As this is was a first attempt to evaluate the potential of this approach, we believe it is possible to optimise the energy structure further.

CONCLUSION

We have shown that, apart from potential problems arising from nuclear data, current deterministic methods of steel-reflected fast-reactors calculations are still responsible for errors in reactivity predictions, as was already the case some 20 years ago. This discrepancy comes from the approximations performed in the treatment of the core-reflector interface effects, which were found to be very large in benchmarks with a limited number of isotopes in the reflector. Although some improvement can be achieved by optimizing key calculation parameters (the number of different sub-zones in the cell calculations, the value of buckling in the reflector, the Sn and Pn parameters, the energetic structure) it appears at this point that a good agreement can only be achieved by increasing the number of energy groups. We estimate that about 300 groups will be required to get acceptably accurate results.

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