

Methodologies for Treatment of Spectral Effects at Core-Reflector Interfaces in Fast Neutron Systems

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The existence of space, angle and energy neutron flux distribution transients is a well known phenomenon which makes the calculation of fast reactors difficult when the core is surrounded by reflectors, particularly steel reflectors. The current interest for fast neutron reactors as TRU burners of relatively low power and small core size (high leakage) motivates the search for an accurate deterministic treatment of neutron reflection. Indeed, without due care taken, the treatment of reflector effects can introduce significant uncertainties in K_{eff} and power distribution calculated values.

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 calculation scheme for ERANOS: our final objective is to define a recommended deterministic calculation procedure for an accurate treatment of fast reactors neutron balance in the presence of reflectors.

Our work shows that satisfactory results can be achieved by optimization of the macrocell option already implemented in the ECCO cell code of ERANOS, the agreement with the Monte Carlo calculation becoming satisfactory even when using a reduced number of energy groups.

KEYWORDS: fast neutron reactor, ERANOS, steel reflector

1. Introduction

The existence of spectral effects at core-reflector interfaces is a well-known phenomenon which affects calculations of fast reactors when using a deterministic code system [1,2]. Indeed, the neutrons escaping from the core at high energies enter the reflector where they are slowed down by scattering. Some of these neutrons escape capture and return to the core with lower energies. Consequently, important transients arise at the interface of the two regions.

Recent results [3,4] show that conventional procedures for cross-sections condensation over a small number of energy groups (e.g. the standard 33 energy group structure) are not suitable for accurately describing the slowing-down of the neutrons reflected in the core, yielding results in poor agreement with reference continuous energy Monte Carlo solutions and very sensitive to the value of the buckling required by the cell code in the core and reflector regions.

On the contrary, satisfactory results can be achieved with a detailed multigroup energy treatment (number of energy groups ~ 300). However, such fine-group calculations are very demanding in terms of computing resources. Consequently, our goal is to find new procedures for

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condensing cross-sections over a relatively small number of energy groups while preserving the results of fine-group calculations.

2. Standard calculation procedures

For the present investigation, the ERANOS-2.0 code system [5,6] has been used. In particular the reactivity and flux (or reaction rates traverses) have been calculated with the BISTRO module [7] in the S_4P_1 approximation. The cross sections (and probability tables) are condensed with the ECCO lattice code [8] of ERANOS starting from its 1968-group library based on the JEF2.2 evaluations [9].

The ECCO standard procedures provide separately the cross sections for the core and the reflector regions which are assumed to be infinite. In this case, the calculation related to the reflector region is performed with a user-specified buckling value. This (single) value is given by a semi-empirical formula: $B^2 = 5(\pi/h)^2/8$, where h is the thickness of the reflector zone. In principle, this formula is not readily applicable to steel reflectors as it has been developed for the treatment of fertile blankets. Indeed, conventional fast reactor analysis code systems such as ERANOS are optimized for highly absorbing media like blankets, but not for reflector cell calculations. 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. The latter option has been used here. For the fuel cell calculations, an iterative procedure is used to determine a buckling giving $K_{eff} = 1$. To obtain a broad group library for the spatial calculations (e.g. the BISTRO code), a 1968-group neutron spectrum is first calculated in ECCO and used to collapse the cross-sections over the broad structure (e.g. 33 energy groups). The collapsing procedures are based on the classical formulas of condensation, using the cell fluxes as the weighting functions.

In a preliminary study of the core/reflector interface effects in a fast reactor, a simplified 1D model has been investigated. Geometry and compositions are presented in Table 1. To simulate an axial dimension, a buckling value of $2.75E-4 \text{ cm}^{-2}$ has been adopted.

Table 1: Simplified Geometry and Isotopic Compositions for 1D Model (R in cm)

		Region	Isotope	Density $\times 10^{24} \text{ at/cm}^3$
Core	Reflector	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}

The spectral effects at the core/reflector interface were quantified by computing spectral index traverses. Figures 1 and 2 confirm that there is a severe spectral transition zone at the interface that extends from 10 cm inside the core to 10 cm in the reflector.

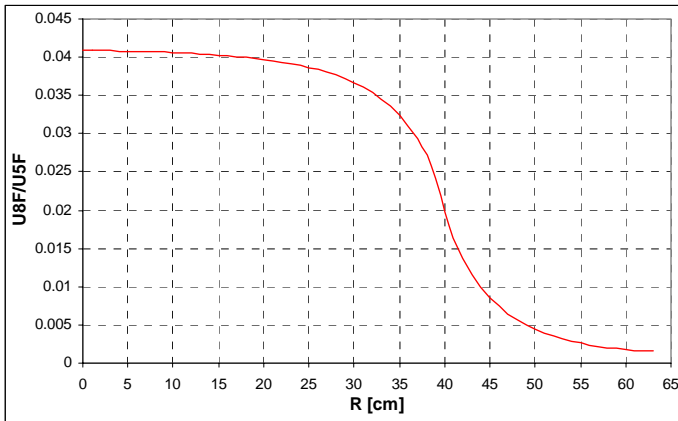


Figure 1: $\Sigma_{f,U238}/\Sigma_{f,U235}$ Traverse

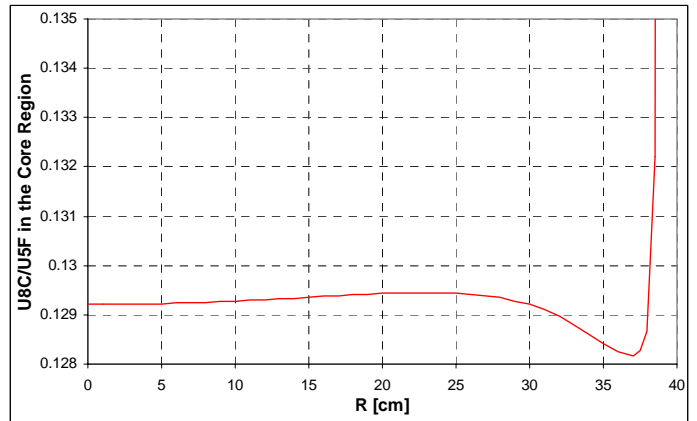


Figure 2: $\Sigma_{C,U238}/\Sigma_{f,U235}$ Traverse in the Core

The observed interface effects will certainly affect the results of a deterministic calculation if the cross-sections are not accurately collapsed in energy and space (and angle).

In the following, the analysis is focused on the results of the multiplication factor, K_{eff} , and on selected reaction rate distributions: the U235 fission, the Pu239 fission and the U238 capture rate. The results obtained with the ECCO standard procedures of cross-section processing are presented. The energy dependence is shown by increasing the number of energy groups.

In Figures 3 to 6, each traverse has been normalized to 1 at the core center. The effects on K_{eff} and reaction rate distributions through the number of energy groups NG are shown.

It can be noticed that the effects on K_{eff} are very large: a reactivity change of about 2500 pcm is found when going from NG=33 to NG=1968. As demonstrated in previous studies [3], the fine-group calculation gives results in good agreement with Monte-Carlo simulations, consequently it is taken as the reference case here. Regarding the reaction rate distributions, the case with NG=299 can be considered as representative of the reference solution.

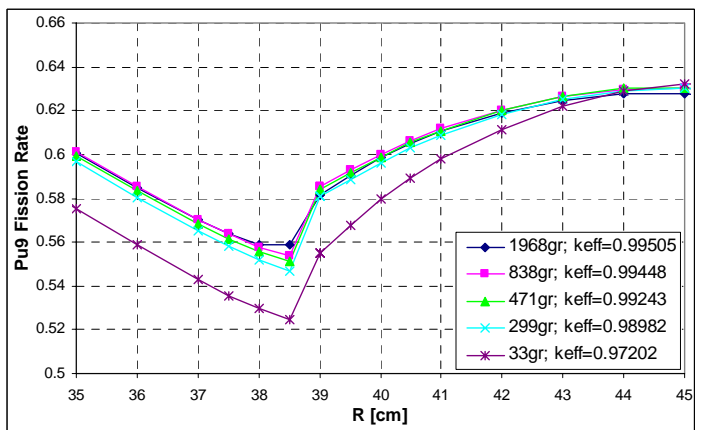
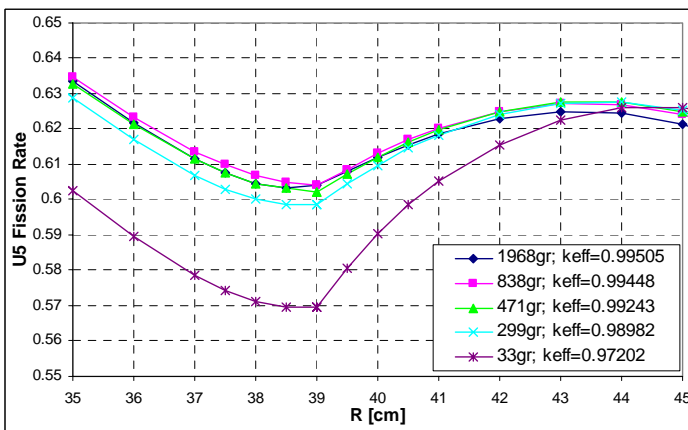


Figure 3: U235 Fission Rate Traverse at the Interface Figure 4: Pu239 Fission Rate Traverse at the Interface

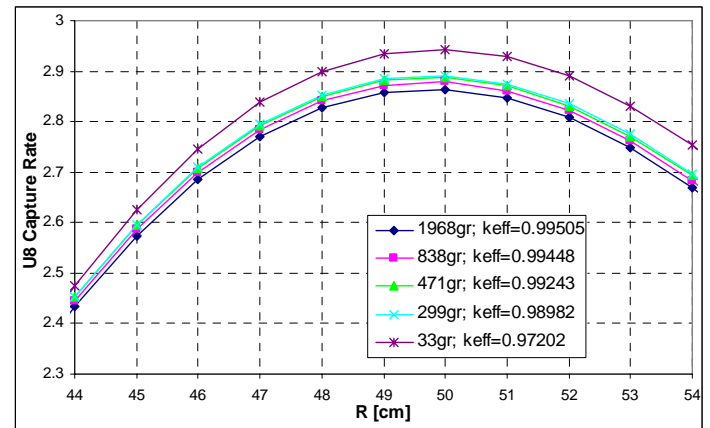
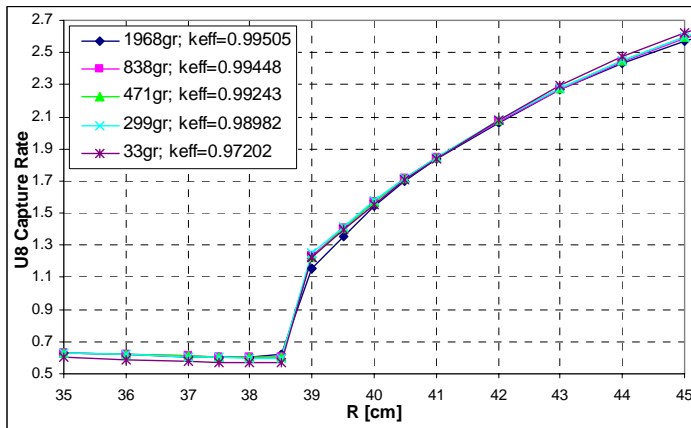


Figure 5: U238 Capture Rate Traverse at the Interface Figure 6: U238 Capture Rate Traverse in the Reflector

Using the ECCO standard procedures, a dependence has also been noticed on the buckling provided in the cell calculation to process the core and the reflector cross-sections. Figure 7 shows that the reference calculation (NG=1968) is not affected by a different choice of the buckling, the impact on K_{eff} and on the reaction rate distributions (in the following figure represented just by the U235 fission rate) being negligible. In the case of the fine reference calculation (NG=1968), no cross-section condensation is performed, consequently the results are insensitive to the buckling value. On the contrary, with NG=33 the buckling produces a significant change of the weighting function and therefore, of the collapsed cross-sections. Figure 8 shows the effects due to a change of the buckling value in the reflector.

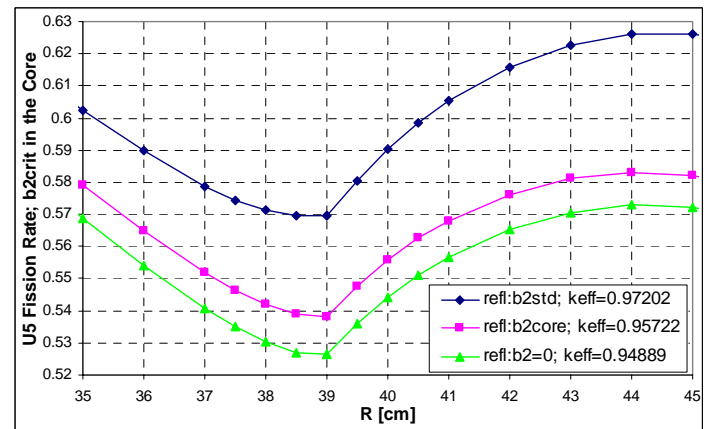
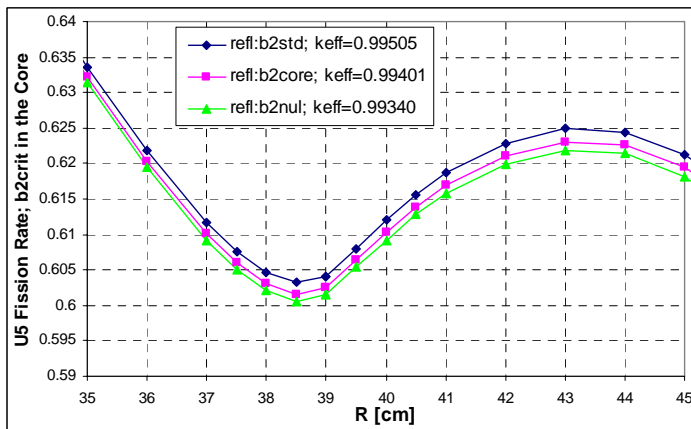


Figure 7: Impact of the Buckling Value Provided in the Reflector on the Fine Reference Calculation

Figure 8: Impact of the Buckling Value Provided in the Reflector on the Calculation with NG=33

3. Improved procedure

It has already been established that a detailed multigroup energy treatment (number of energy groups NG of the order of 300) is needed in order to accurately account for spectral transients at interfaces. Based on these results, one concludes that attention must be paid to the determination of the weighting function to be used for the cross-section condensation from the fine energy structure to a broad one.

A recent study [4] has demonstrated that an improved set of broad-group cross sections can be obtained by an iterative method. Recall that the broad group cross-sections are generally defined so as to preserve the reaction rates, i.e. $\sigma_I \Phi_I = \sum_{i \in I} \sigma_i \phi_i$, where I and i are the broad and fine-group structure indices, respectively. The broad-group flux Φ_I being unknown, the following (classical) iterative procedure can be used to improve the broad-group cross-sections:

$$\sigma_I^{(0)} = \frac{\sum_{i \in I} \sigma_i \phi_i}{\Phi_I^{(0)} \left(= \sum_{i \in I} \phi_i \right)}, \quad \sigma_I^{(1)} = \frac{\sum_{i \in I} \sigma_i \phi_i}{\Phi_I^{(1)}}, \quad \dots, \quad \sigma_I^{(K)} = \frac{\sum_{i \in I} \sigma_i \phi_i}{\Phi_I^{(K)}} \quad \text{Eq.1}$$

where the $\Phi_I^{(K)}$ are calculated with the $\sigma_i^{(K-1)}$ and K is the iteration index.

This procedure is easily implemented, since only one fine-group calculation is needed, the iterative $\Phi_I^{(K)}$ calculation being performed at the broad-group level, and it produces just one set of cross sections for the core and another one for the reflector. Figure 9 compares the reference results with the 33-group calculation obtained with the ECCO standard procedures and this iterative method.

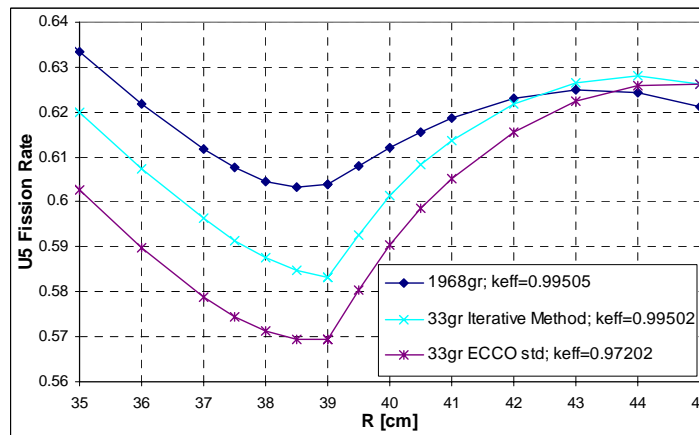


Figure 9: Reference / Standard Procedure / Iterative Method Results Comparison

It can be observed that the application of such an iterative procedure is very satisfactory for the reactivity determination, the agreement between the 33 and the fine-group calculation becoming very good and the convergence being reached rather rapidly. However, some difficulties still remain as evidenced by the reaction rate distributions (see Figure 9), even if the results are better than the standard calculation. Indeed, the iterative method leads to a 33-group cross-section set giving balance terms (leakage included) identical to the fine-group calculation, but the partial currents at the interface core/reflector are not reproduced. This is the reason for the discrepancies observed in the reaction rate distributions.

4. Macrocell options

In order to describe the macrocell method, we first consider the transport equations in the P_1 approximation:

$$\Delta \Phi_1(\vec{r}, E, \vec{\Omega}) + \Sigma_t(E) \Phi_0(\vec{r}, E, \vec{\Omega}) = S_0(\vec{r}, E, \vec{\Omega}) + \iint \Sigma_s^0(E', \vec{\Omega}' \rightarrow E, \vec{\Omega}) \Phi_0(\vec{r}, E', \vec{\Omega}') dE' d\vec{\Omega}' \quad \text{Eq.2}$$

$$\frac{1}{3} \Delta \Phi_0(\vec{r}, E, \vec{\Omega}) + \Sigma_t(E) \Phi_1(\vec{r}, E, \vec{\Omega}) = S_1(\vec{r}, E, \vec{\Omega}) + \iint \Sigma_s^1(E', \vec{\Omega}' \rightarrow E, \vec{\Omega}) \Phi_1(\vec{r}, E', \vec{\Omega}') dE' d\vec{\Omega}' \quad \text{Eq.3}$$

where the moments Φ_0 and Φ_1 are respectively the flux and the current characterising the system under study. The solution over a broad-group structure with a deterministic code requires the use of the following formulas of condensation:

$$\Phi_n^g(\vec{r}, \vec{\Omega}) = \int_{\Delta E_g} \Phi_n(\vec{r}, E, \vec{\Omega}) dE \quad n = 0, 1, \quad \Sigma_{t,g}^n(\vec{r}, \vec{\Omega}) = \frac{\int \Sigma_t(E) \Phi_n(\vec{r}, E, \vec{\Omega}) dE}{\Phi_n^g(\vec{r}, \vec{\Omega})}, \quad \text{Eq.4}$$

$$\Sigma_{s,g' \rightarrow g}^n(\vec{r}, \vec{\Omega}' \rightarrow \vec{\Omega}) = \frac{\int dE \int \Sigma_s^n(\vec{\Omega}', E' \rightarrow \vec{\Omega}, E) \Phi_n(\vec{r}, E', \vec{\Omega}') dE'}{\Phi_n^g(\vec{r}, \vec{\Omega})} \quad \text{Eq.5}$$

From Eqs. 4 and 5, it can be observed that the weighting function used in the collapsing procedure corresponds to the real solution (flux and current) of the system. Its position dependence leads to broad-group cross-sections which become space dependent too, even in regions where the continuous-energy cross-sections are spatially flat. This situation, typical of systems with strong transition zones such as at core/reflector interfaces, requires that several collapsing sub-regions be distinguished, leading to the preparation of multiple sets of broad-group cross-sections.

In the ECCO standard procedures previously discussed, where a cell calculation is performed separately for each region assumed to be infinite, the accuracy of the results depends on how good this weighting function approximates the real solution of the system.

In the ECCO code, a more sophisticated macrocell option is implemented, which allows a representation of the core coupled with the reflector and produces broad-group cross-sections by condensation with the corresponding flux and current calculated in each region or sub-regions.

Surprisingly, it has been found that the use of this ECCO macrocell option does not improve the results obtained with the standard procedures when a broad number of energy groups is used in the deterministic calculation, even if the cross-sections are processed for several core and reflector sub-regions.

In order to understand this unexpected result, a detailed analysis was performed, supported by perturbation studies, leading to the conclusion that the ECCO macrocell option needed improvements. It is believed that the difficulties encountered by ECCO have to be attributed to the anisotropic treatment of the collision probability flux solution.

Pending these improvements, a pseudo-macrocell calculation was performed outside the usual ERANOS procedures. The fine-group cross-sections were used as inputs to a fine spatial 1D BISTRO S_n calculation, which then provided the flux and current to be used in the collapsing procedure. The results of this pseudo-macrocell calculation were found to be very satisfactory, as shown in Figures 10 to 13, especially if the reflector is sub-divided into 2 sub-regions (“refl:5+35” in the legend refers to a calculation where the reflector cross-sections were prepared for two sub-regions of 5 and 35 cm).

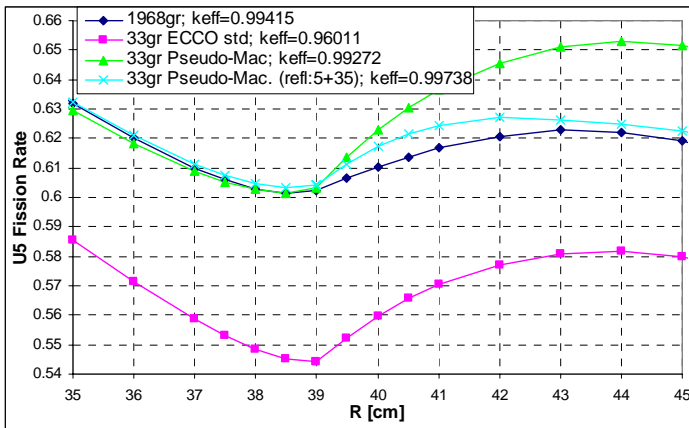


Figure 10: U235 Fission Rate Trav. at the Interface

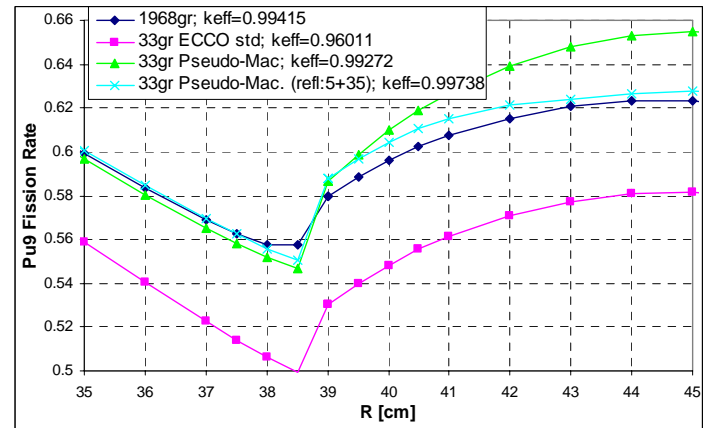


Figure 11: Pu239 Fission Rate Trav. at the Interface

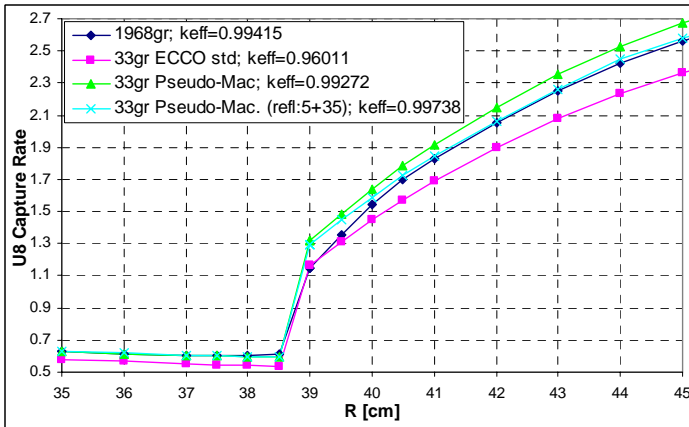


Figure 12: U238 Capture Rate Trav. in the Reflector

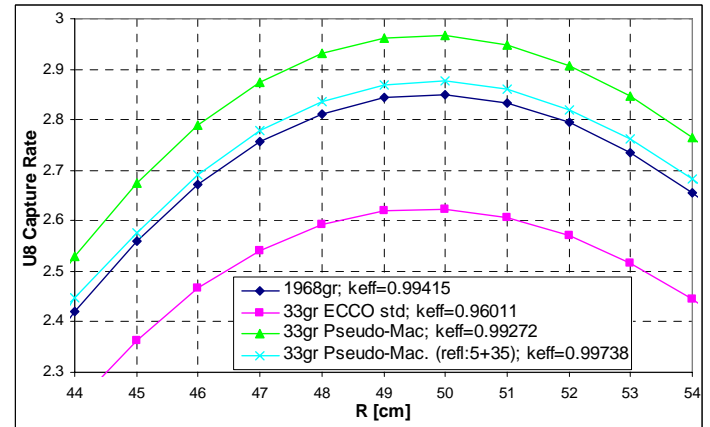


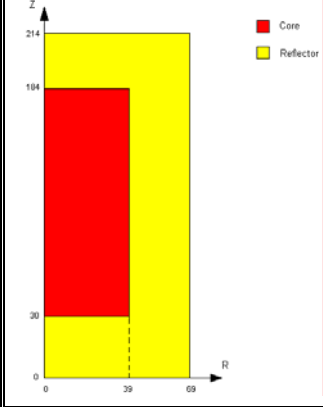
Figure 13: U238 Capture Rate Trav. in the Reflector

5. Application of the pseudo macrocell option to a 2D model

The pseudo-macrocell calculation of the previous section has been shown to be capable of accurately treating the core/reflector interface in the case of a simple 1D model. In the following, the analysis is applied to 2D RZ models, these examples showing how the method can be extended to multi-dimensional problems.

Two RZ models have been analyzed. Table 2 shows the geometry and composition of the first one.

Table 2: Geometry and Isotopic Compositions for a 2D Model



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}

As in the case of the 1D model, it has been demonstrated that the use of the ECCO standard procedures is not suitable here to process the cross-sections over a broad energy structure, the results (K_{eff} and reaction rates distributions) giving significant discrepancies compared to the fine-group calculation. As an example, the U235 fission rate traverses are presented in Figures 14 and 15; the change in K_{eff} vs. NG is also reported. In particular, Figure 14 shows the radial traverses, calculated at $Z=103$ cm and normalized to 1 at the core center ($R=0$); while Figure 15 shows the axial traverses, calculated along the radial position $R=10$ cm and normalized to 1 at $Z=97$ cm.

As expected, it can be observed that the effects on K_{eff} are very large: a reactivity change of about 4000 pcm is observed when going from NG=33 to NG=1968.

The K_{eff} value calculated with JEF2.2 and the TRIPOLI-4 continuous-energy Monte Carlo code is 0.99891 ± 0.00015 , which is in good agreement with the fine-group calculation.

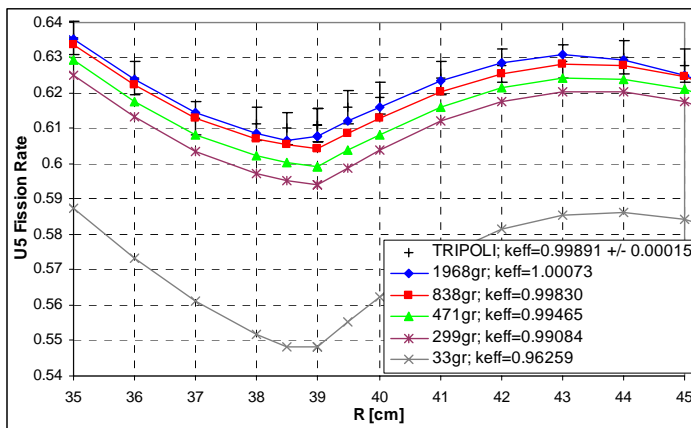


Figure 14: U235 Fission Rate Radial ($Z=103$ cm) Traverse at the Interface

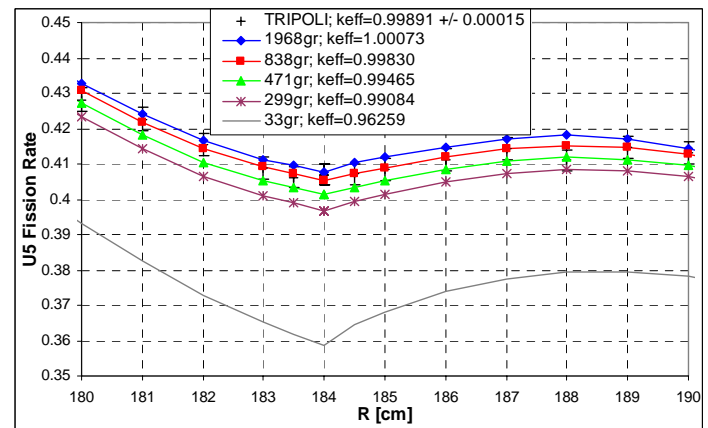


Figure 15: U235 Fission Rate Axial ($R=10$ cm) Traverse at the Interface

In an attempt to get improved few-group cross-sections, the pseudo-macrocell option of Section 4 was applied in the following way.

A 1D model, with a 39-cm thick core and a 30-cm thick reflector, was obtained from the radial direction of the 2D problem. In the flux calculation, an axial buckling was provided, accurately determined in order to give the same multiplication factor as the corresponding 2D

1968-group calculation. The cross-sections were collapsed from NG=1968 to NG=33 using as weighting functions the flux solution of this 1D model. The cross-sections so obtained were then used in the original 2D system. The results are reported in the following figures.

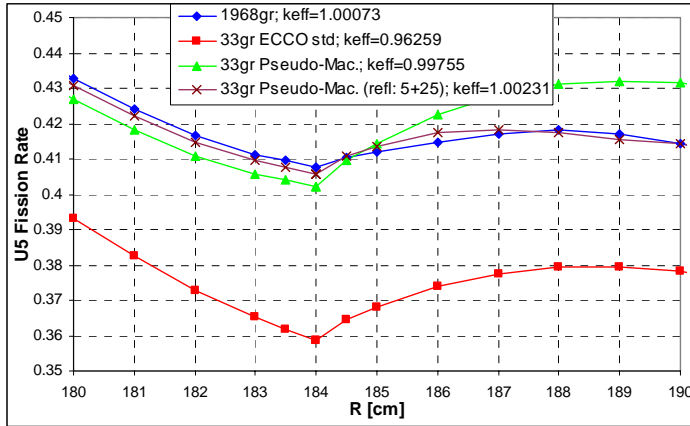


Figure 16: U235 Fiss. Rate Radial (Z=103 cm) Trav. at the Interface via the Pseudo-Macrocell Scheme

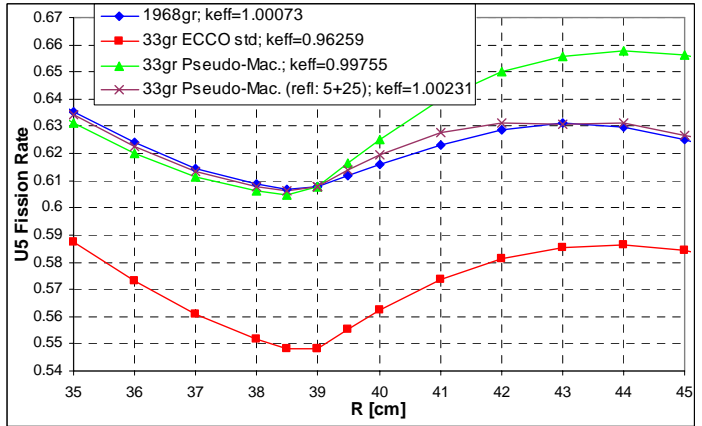


Figure 17: U235 Fiss. Rate Axial (R=10 cm) Trav. at the Interface Using the Pseudo-Macrocell Scheme

It can be seen that the case where the reflector is divided into two sub-regions yields very satisfactory results: in the comparison NG=1968 vs. NG=33, the discrepancy in the reactivity is reduced from 4000 to 150 pcm and the traverses (both radial and axial) agree within a margin of less than 1%.

A second 2D model was investigated with a smaller core height in order to increase neutron leakage from the core into the axial reflector. Table 3 shows the geometry and compositions of this second 2D model.

The K_{eff} value calculated with JEF2.2/TRIPOLI-4 is 1.00128 ± 0.00013 , which is in good agreement with the fine-group calculation.

Table 3: Geometry and Isotopic Compositions for a 2D Model

	Region	Isotope	Density $\times 10^{+24}$ at/cm ³
	Zone1- Fuel		Pu239
		U238	6.25×10^{-3}
		Fe56	7.0×10^{-3}
		Cr52	1.5×10^{-3}
		Na23	1.0×10^{-2}
Zone2 - Reflector		O16	1.5×10^{-2}
		Fe56	5.0×10^{-2}
		Cr52	1.5×10^{-2}
	Na23	5.0×10^{-3}	

In order to obtain the 33-group cross-sections able to reproduce the 1968-group calculation, we used the same procedure as in the previous case.

The U235 radial traverse (see Figure 18) is normalized to 1 at the core center (R=0) and the axial one (see Figure 19) at Z=59 cm.

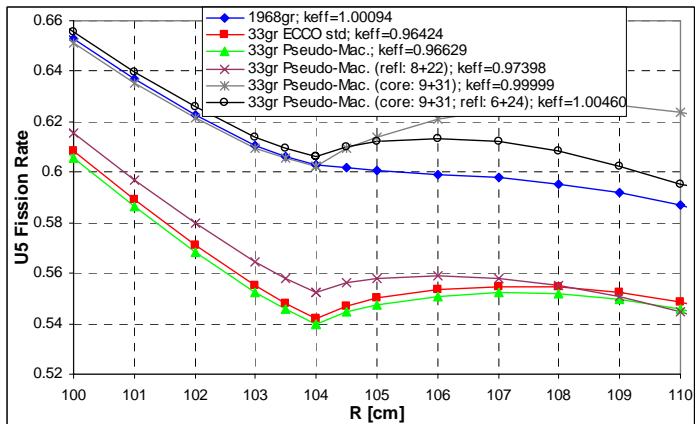
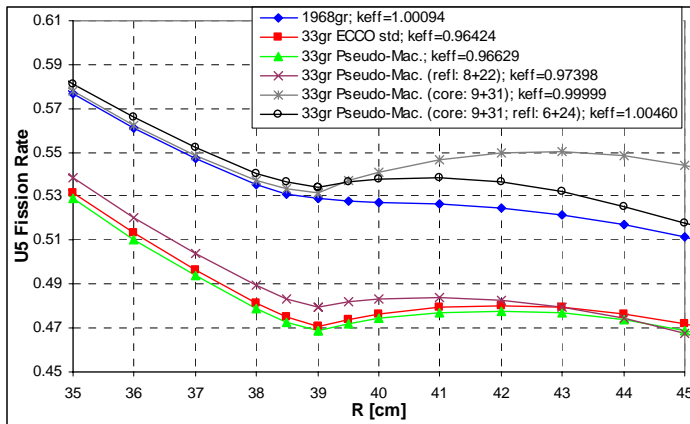


Figure 18: U235 Fission Rate Radial (Z=65 cm) Trav. at the Interface Using the Pseudo-Macrocell Scheme
 Figure 19: U235 Fission Rate Axial (R=10 cm) Trav. at the Interface Using the Pseudo-Macrocell Scheme

In this more severe situation, it was necessary to sub-divide both the core and the reflector into two sub-regions to obtain good results. Indeed, we observe that the calculation labeled “33gr Pseudo-Mac.”, corresponding to the case of a pseudo-macrocell calculation without subdivision of the reflector and the core, recovers just 200 pcm of the 3800 pcm reactivity discrepancy between the 33-group standard and the reference calculation. By dividing the reflector into two sub-regions (case “33gr Pseudo-Mac. (refl:8+22)”), about 1100 pcm of the discrepancy is recovered. By dividing the core into two sub-regions (case “33gr Pseudo-Mac. (core:9+31)”), an important gain is obtained. Finally, if both the core and the reflector are divided into two sub-regions, the discrepancy in the rate distribution is dramatically reduced.

Presumably, these results could be further improved by optimizing the size of the sub-regions or by further sub-dividing the core and reflector regions.

6. Conclusions

In this paper, we have presented the latest results of our on-going investigation of core-reflector interface effects in fast reactors. Our ultimate goal is to define a recommended procedure within the ERANOS deterministic code system for an accurate and efficient treatment of fast reactors with steel reflectors.

Recent studies have demonstrated that the use of the standard cross-section calculation and condensation procedures implemented in the cell code ECCO of ERANOS required a detailed multigroup energy treatment (number of energy groups NG on the order of 300, rather than just 33) to account for spectrum transient effects at the core-reflector interfaces, the agreement with respect to a reference continuous energy Monte Carlo calculation being then strongly improved.

In an attempt to define a new calculation procedure that would be sufficiently accurate while not too demanding in terms of computing resources, we have established that improved sets of 33-group cross-sections can be obtained by simply iterating in the condensation process. This is helpful for preserving reactivity. However, some difficulties still remain with the reaction rate distributions. With respect to this aspect, other solutions have been investigated.

In particular, we have tested a sophisticated macrocell option implemented in the ECCO cell code, which allows a representation of the core coupled with the reflector. This option produces broad-group cross-sections from the fine-group flux and current calculated in each region or sub-regions. However, contrary to our expectations, this ECCO macrocell option gave results which were still dependent on the number of energy groups used in the deterministic calculation. In addition, no improvements were observed when the cross-sections were produced for more core and reflector sub-regions. A detailed analysis, supported by perturbation studies, lead to the conclusion that the ECCO macrocell needed improvements, in particular with respect to the anisotropic treatment of the collision probability flux solution.

A pseudo-macrocell calculation has been performed outside the usual ERANOS procedures. The fine-group cross-sections were used as inputs to a fine spatial 1D BISTRO S_n calculation, which then provided the flux and current to be used in the collapsing procedure. When tested on small 1D and 2D reactor models, this pseudo-macrocell calculation was found to yield very satisfactory results, especially if the reflector and the core were sub-divided into 2 sub-regions.

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