APOLLO2 : A NEW TWO-LEVEL CALCULATION SCHEME APPLIED TO PWR ASSEMBLY DEPLETION COMPUTATION.

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1. ABSTRACT

A new method to improve the representation of the flux gradient in PWR assemblies during depletion calculations is presented herein.

This original two-level scheme calculation consists in performing the depletion computation with two subsequent flux calculations based first on the Pij method with a general interface current formalism and then on the S_N method.

Several validations based on three different PWR configurations are presented : the absorption rate and the k_∞ obtained with the new scheme are compared with the values issued from some fine Pij calculations.

2. INTRODUCTION

APOLLO2 is a modular transport code (Ref. 1,2) developed at the French "Commissariat à l'Energie Atomique" in a joint development effort with EDF and FRAMATOME. APOLLO2 has been adapted, industrialized and qualified by FRAMATOME for its own needs. The code has been packaged into SCIENCE code package in 1994 (Ref. 3) and is also used by CEA and EDF for their own neutronic applications. APOLLO2 solves the multigroup Boltzmann transport equation using a collision probability or a S_N methods. The code also supports a top level self-shielding model and a predictor/corrector method for isotopic depletion of the fuel. In addition, APOLLO2 includes all relevant modules needed for critical buckling computations, transport/transport equivalence and space and energy collapses.

The collision probability method (or Pij method) is routinely used for calculating PWR fuel assemblies. The main disadvantage of this method is the flat flux hypothesis in each calculation mesh. In order to calculate the flux gradients correctly, it is essential to divide the cells into a large number of calculation meshes. The number of meshes necessary could make calculation times prohibitive for developing an industrial calculation system.

This work was carried out to improve the representation of the flux gradient in PWR assemblies during depletion. With this aim in view, a new and original method has been proposed which consists in performing the flux with two subsequent complementary calculations.

In this new scheme, the first level is devoted to the self-shielding and the leakage calculation with fine energy and spatial meshes. At this stage, the self-shielding calculation is performed exactly as in the classical “one-level” calculation scheme. A first flux and leakage calculation is performed by using the Pij method with multicell approximation (combination of general interface current formalism with a cylindrization technique).

The second level is dedicated to the flux calculation with the nodal S_N method. To prepare the cross section sets for the S_N calculation, each cell is homogenized in order to obtain the equivalent cross sections on the defined output low-group energy and spatial meshes.

3. FLUX CALCULATION METHODS IN APOLLO2

Thanks to its modularity, the code allows the implementation of different calculation schemes. Two methods are used in APOLLO2 to solve the multigroup transport equation. The first is the collision probability method (or Pij method) which is routinely used to calculate PWR fuel assemblies. It solves the transport equation in its integral form.

The second method is the S_N method, also known as the discrete ordinate method. It solves the integral-differential form of the multigroup transport equation taking into account the breakdown into discrete angular and spatial elements. It makes it possible to calculate the anisotropic scattering correctly.

3.1. COLLISION PROBABILITIES METHODS.

Nowadays, recommended neutronic design calculations for pressurized water reactors (PWRs) are usually based on a one level scheme calculation in which multigroup flux computations are performed using the Pij solution of the integral transport equation with the interface current method. In this formalism, a unit PWR assembly is sub-divided into cells and collision probabilities matrices are computed for each uncoupled cell. The detailed flux can then be reconstructed from the knowledge of interface current surrounding each cell. In each point of the surface surrounding a cell, the outgoing angular flux can be expressed in two usual interface current approximations respectively identified as UP0 and UP1. In both cases, the outgoing flux is spatially uniform along each side of the cell. With the UP1 and the UP0 approximation, the outgoing angular flux is represented respectively with a linear angular and an isotropic approximation.

For reference calculation, the 2D Pij direct formalism can be used. This method uses a double numerical integration over ρ (line) and ϕ (angle). The integration mesh consists of sets of parallel neutron trajectories with different orientations (Figure 1).

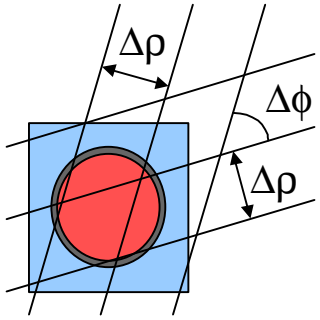

Figure 1. 2D Pij direct formalism – Integration mesh.

It is obvious that the accuracy of the calculation depends on the numeric integration formula defined by the parameters $\Delta\rho$ and $\Delta\phi$ ($\Delta\rho$ and $\Delta\phi$ represents respectively the interval between two discretes values of ρ and ϕ). With this method, it is possible to use in the APOLLO2 code a sectorized spatial mesh (defined by the α variable) in each cell of the lattice (Figure 2).

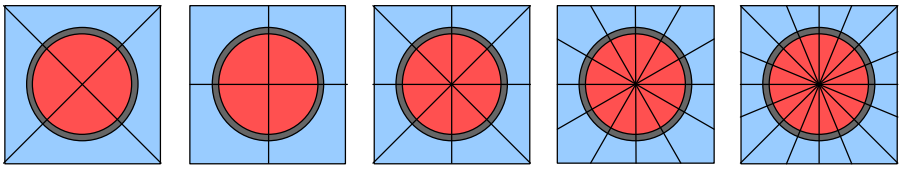

Figure 2 : Examples of sectorized spatial meshes for the direct Pij method.

The collision probabilities method makes it possible to accurately describe the cell (fuel pins, cladding, moderator etc.). For this reason, the method is used in all fuel assembly calculations,

particularly to cover self-shielding. It has two limitations : first of all, the Pij method developed in APOLLO2 only takes into account the transfer anisotropy using a transport correction of order 0. The effects on the fuel assembly calculation are only noticeable in the presence of an absorber and remain slight. As said before, the main disadvantage of the Pij method is the flat flux hypothesis in each of the calculation regions. In order to calculate the flux gradients correctly, the cells must be describe with a very fine mesh.

3.2. S_N METHOD.

Thi method is also known as the discrete ordinate method. It solves the integral-differential form of the multigroup transport equation taking into account the breakdown into discrete angular and spatial elements. It makes it possible to calculate the transfer anisotropy correctly. Furthermore, the nodal method, designated LL, implies a linear variation of the flux alongside and inside the mesh. The SN method is therefore an effective and inexpensive method for calculating steep flux gradients while maintaining a limited number of calculation regions. However, the resolution methods (finite or nodal differences) can only be used to calculate simplified geometries composed of homogeneous blocks and in which the pins cannot be explicitly described.

APOLLO2 includes some modules which permit the use of the S_N method. This method has been recently applied with success for C/M comparisons, obtained by CEA (Ref. 4), in MISTRAL and EPICURE experimental programs. In particular, improved results on pin by pin power around heterogeneities and near reflector have been obtained.

4. TWO LEVEL CALCULATION SCHEME

The two-level calculation scheme (TLS) is based on the following principles : the self-shielding calculation requires a fine energy mesh and a precise description of the geometry in each cell. However, the flux calculation can be made using a smaller number of energy groups and a homogenized geometry. The proposed calculation scheme therefore consists in breaking down the calculation into two levels.

4.1. FIRST LEVEL

The first level is dedicated to the self-shielding and the leakage calculation. At this stage, the self-shielding calculation is performed exactly as in the classical “one-level” calculation scheme. A first flux and leakage calculation is performed. Reactor leakage is incorporated in the flux calculation through a B1 leakage coefficient computed in a homogenized, infinite medium.

In the APOLLO2 assembly depletion calculation, the fuel pellets are divided into several rings, where each ring defines a self-shielding zone. Thanks to the modular structure of the code, self-shielding and flux calculation for depletion can be performed in the same and simplified geometry.

Self-shielding calculations are performed on a simplified geometry where fuel cells are gathered in a few classes, from 1 to 45 (number of classes x number of rings self-shielded cross-sections sets). Usually, about 20 classes of cells are used in the depletion calculation geometry (the total number of cells in a one-eighth assembly is 45, but only 39 cells contain fuel pins and therefore undergo depletion).
Then, low-cost two-dimensional calculations can be performed by combining the general interface current formalism with a cylindrization technique (using a Wigner-Askew model) and with the here above defined classes.

4.2. SECOND LEVEL

The second level is dedicated to the flux calculation with the nodal S_N method. To prepare the cross section sets for the S_N calculation, an homogenization method is used, based on an equivalence principle, in which the homogenized cross sections, corrected by the equivalence factors, are defined so that the reaction rates from the first level calculation are preserved. Each cell is homogenized in order to obtain the equivalent cross-sections on the defined output low-group energy and spatial meshes : less than 20 groups for the energy mesh and only one mesh per cell for the spatial mesh. The nodal spatial approximation requires only a 1x1 mesh, whereas the diamond spatial approximation necessitates more than a 2x2 meshes in the homogeneous cells to obtain an accurate spatial convergence.

Since recent developments in the APOLLO2 code, it is now feasible to compute the depletion by combining the homogeneous flux performed by the S_N calculation with the heterogeneous microscopic cross sections assessed in the self-shielding stage of the 1st level calculation. To take into account the homogenization effect, the microscopic cross sections are multiplied by the equivalence factors. In this way, the "ring-by-ring" depletion effect is preserved for each fuel pellet despite the fact that homogeneous cells are used for the flux computation. This new model gives complete satisfaction, especially for the gadolinium depletion.

The S_N method has been selected because this formalism permits to take into account anisotropy of neutrons and, in addition, nodal approximation is used because it allows, with the same accuracy, to reduce the number of spatial meshes in comparison with the standard diamond spatial approximation method. Furthermore, the nodal method, designated LL, implies a linear variation of the flux alongside and inside the mesh. The S_N model gives very good satisfaction in the computation of assemblies with pin heterogeneities (BP, water holes, absorbers,…). However, the resolution methods (finite or nodal differences) can only be used to calculate simplified geometries composed of homogeneous blocks and in which the pins cannot be explicitly described.

5. ASSEMBLIES AND LATTICE GEOMETRIES

In this paper, we present the first depletion calculations applied to PWR assemblies with this two-level calculation scheme and their validation. The following lattices have been computed in reflected boundaries conditions :

- 5x5 cells lattice including four gadolinium poison cells , especially chosen to maximize the effect of a steep flux gradient (Figure 3) ;

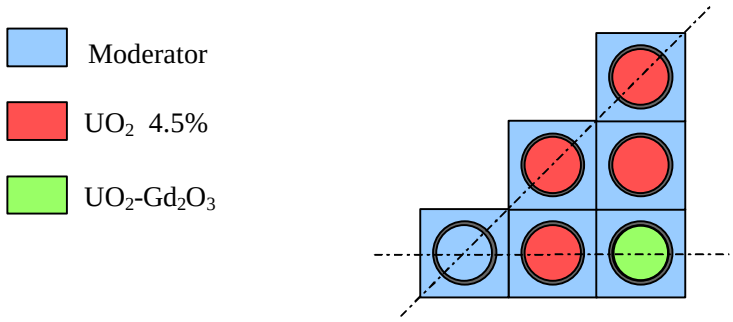

Figure 3. One eighth of the PWR UOX 5x5 lattice with 4 gadolinium cells.

- a typical 17x17 PWR assembly with 16 gadolinium poison cells, called UOX+GD assembly (Figure 4);

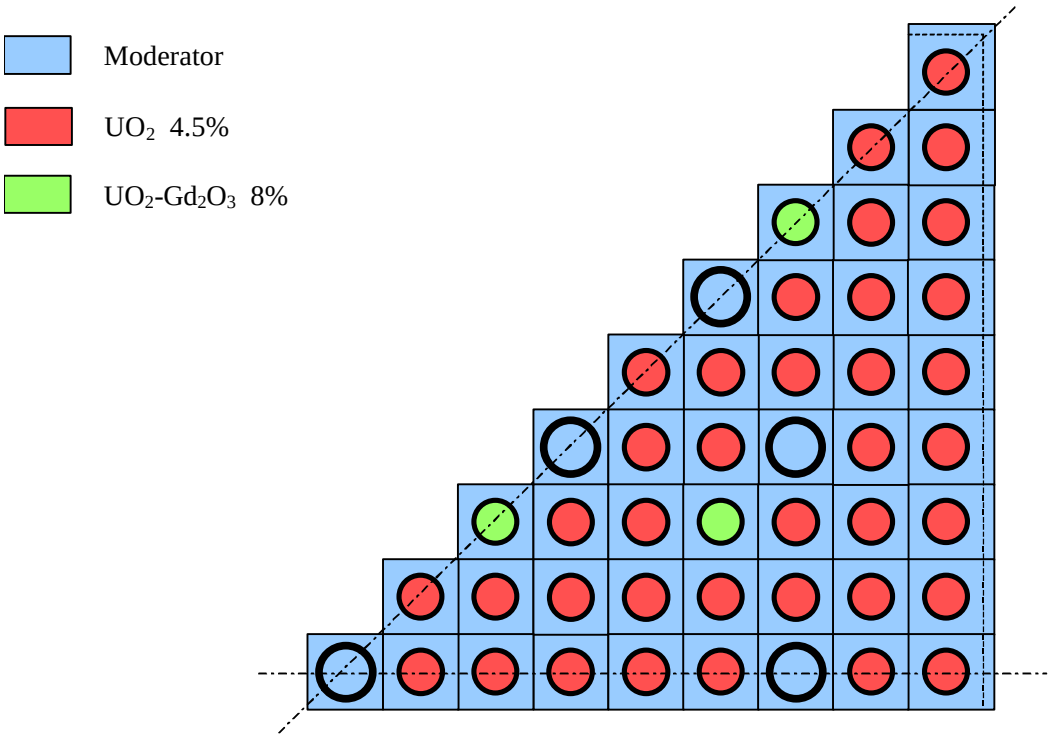

Figure 4. One eighth of the PWR UOX 17x17 assembly with 16 gadolinium cells.

- 17x17 MOX PWR assembly, called MOX assembly (Figure 5).

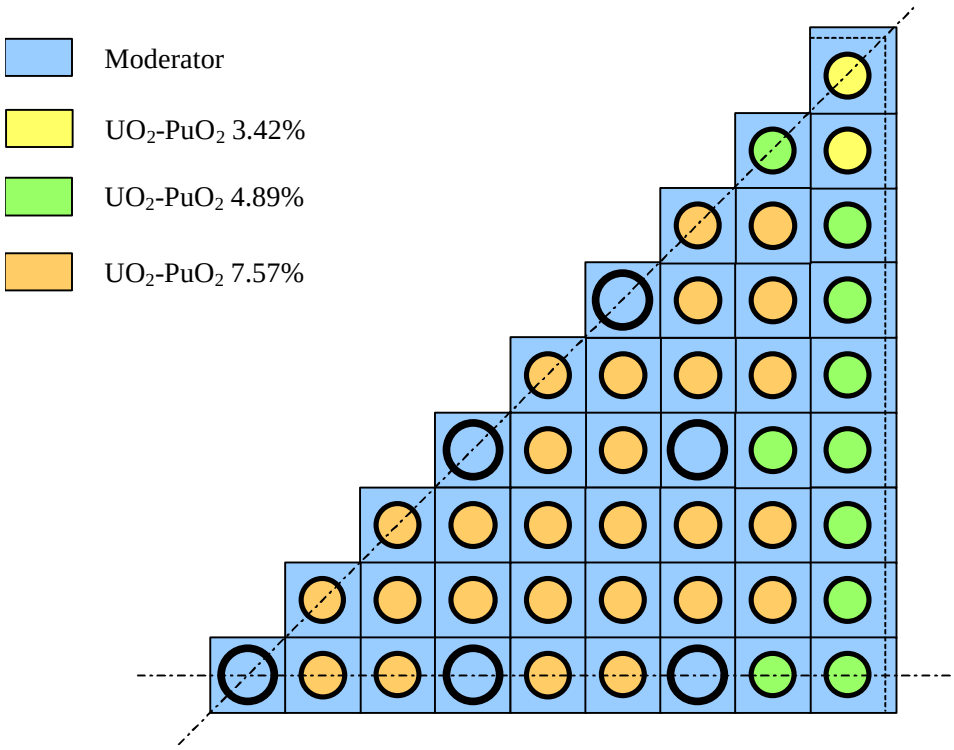

Figure 5. One eighth of the PWR MOX 17x17 assembly.

6. CALCULATIONS CONDITIONS.

Three types of depletion calculations are presented for each PWR configurations describe here above :

- a reference depletion calculation using the 2D direct Pij formalism with 45 classes of cells for self-shielding and depletion calculations ;
- a depletion calculation using UP1 multicell Pij formalism with 45 classes of cells for self-shielding and depletion calculations ;
- a TLS (two-level scheme) depletion calculation with a simplified geometry for the first level (8 classes for UOX+GD assembly and 12 classes for MOX assembly) and 45 cells for the second level (so for the depletion calculations) ;

The calculation conditions used in APOLLO2 are defined as follows :

- library : CEA93 version 4 with a 99 groups energy mesh (ranging from 0 eV to 10 MeV) ; the isotopes come from the JEF 2.2 evaluation ;
- depletion chain : 20 isotopes for the heavy nucleus and 77 fission products ;
- number of points in the fuel pins for the multicell and direct Pij calculations :
  - four points in the UOX and in the MOX fuel pin ;
  - six points in the UOX+GD pin ;

- self-shielding : calculated using the standard APOLLO2 model (with the energy cut-off between the ST and WR moderation models defined in Ref. 5) for the following isotopes : ^{238}U, ^{235}U, ^{239}Pu, ^{240}Pu, ^{241}Pu, ^{242}Pu, ^{154}Gd, ^{155}Gd, ^{156}Gd, ^{157}Gd and Zirconium.

Due to the memory and the calculation time, the reference direct Pij depletion calculations have been computed with the following options :

[α = 4 ; $\Delta\rho$ = 0.02 cm ; $\Delta\phi = \pi/48$ radians] for the 5x5 lattice

[α = 2 ; $\Delta\rho$ = 0.02 cm ; $\Delta\phi = \pi/48$ radians] for the assemblies.

The reference 2 groups power distributions at 0 MWd/t for the assemblies have been computed by a direct Pij formalism with the following more accurate options :

[α = 3 ; $\Delta\rho$ = 0.02 cm ; $\Delta\phi = \pi/48$ radians].

After some parametric studies, the following set of options (Table 1) have been defined for the three PWR configurations.

Table I. Two-level calculation scheme options.

Geometry	First level		Second level		
	Multicell option	Number of classes for self-shielding and flux calculation	S_N	Energy mesh	Number of classes for flux calculation and depletion
5x5 lattice	UP1	6	S_{16}	6 groups	6
UOX+GD	UP1	8	S_4	6 groups	45
MOX	UP1	12	S_4	6 groups	45

For all the two groups power distributions, the normalization condition used is :

$$\sum_{i=1}^{Ncell}\left(T^1_{abs,i} + T^2_{abs,i}\right) = 100$$

$T^1_{abs,i}$: absorption rate in the fast group [10 MeV – 0.625 eV]

$T^2_{abs,i}$: absorption rate in the thermal group [0.625 MeV – 0. eV]

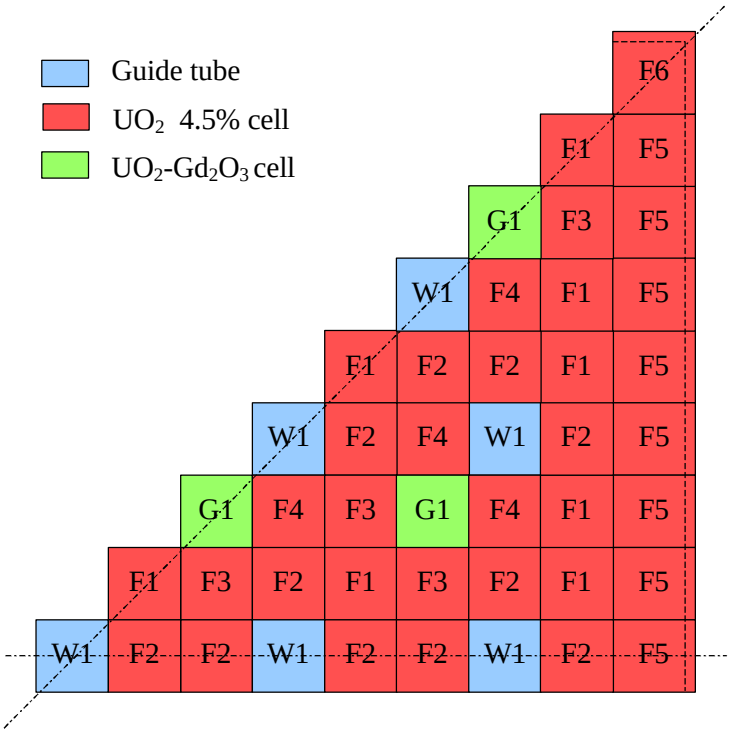

Figure 6. UOX+GD assembly - 8 classes of cell used.

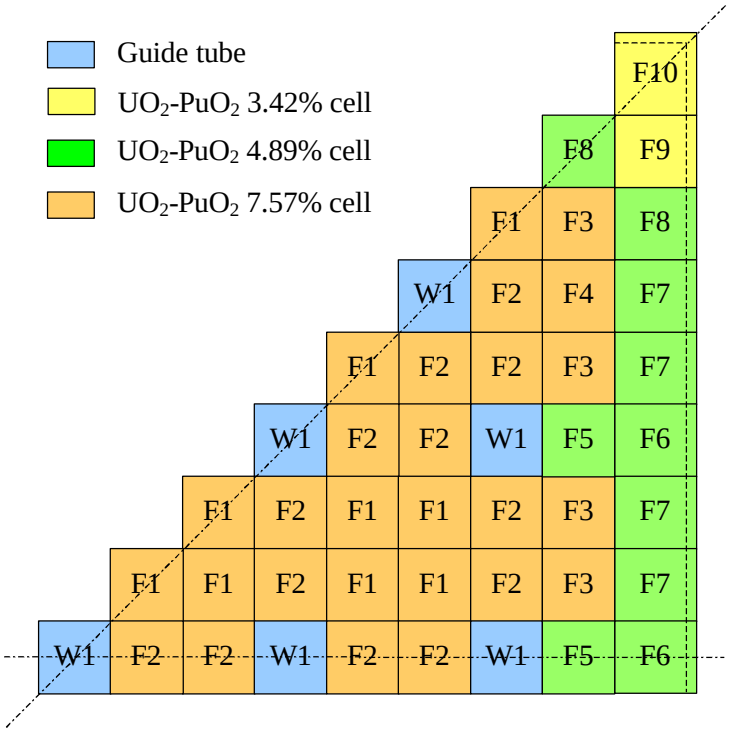

Figure 7. MOX assembly - 12 classes of cell used.

7. RESULTS

The results show an improvement on cell by cell powers around heterogeneities and k_∞ during depletion have been obtained. In terms of reactivity, the following results have been obtained :

- From 0 to 40 GWd/t on the 5x5 cells lattice, k_∞ discrepancies between one-level scheme calculations (UP1 Pij-Multicell method) and the reference ranged from -600 pcm to +240 pcm : this error is now cut to [-40 pcm ; +60 pcm] with the TLS calculation (Figure 8).
- For the UOX+Gd lattice calculations using the one-level scheme with depletion ranging from 0 to 12 GWd/t, the k_∞ discrepancies were included in [-250 pcm ; +100 pcm] against [+80 pcm ; 0 pcm] with the two-level scheme (Figure 9).
- For the MOX assembly, the two schemes give similar results : from 0 to 40 GWd/t, the k_∞ discrepancies were included within [-40 pcm ; +60 pcm] (Figure 10).

For the absorption reaction rates, we present only the highest discrepancies. These always refer to the 0 MWd/t absorption distribution. In the fast energy range (group 1) we do not observe significant discrepancies (Figures 11, 13, 15, 17, 19, 21). In the thermal energy range [0 eV ; 0.625 eV] (group 2), discrepancies between one-level scheme calculations and the reference are about 3% at 0 GWd/t in the gadolinium poison cells for the 5x5 lattice (Figure 12) and the UOX+Gd assembly (Figure 16) and in the corner cell for the MOX assembly (Figure 20). With the two-level scheme, the discrepancies are now less than 0.5% (Figures 14, 18, 22).

On the same very accurate depletion calculation geometry with 45 cells (depletion calculation without classes) and fuel pellets divided into several rings, one flux calculation for a step with the one-level scheme is time consuming and the two-level scheme allows to reduce the computation time by a factor of 8 to 10.

Compared to the one level scheme, the TLS always improves the treatment of assemblies with steep flux gradient.

CONCLUSIONS.

The objective of this study was to validate a new two-level scheme.

The first level is devoted to the self-shielding and the leakage calculation with fine energy and spatial meshes. At this stage, the self-shielding calculation is performed exactly as in the classical “one-level” calculation scheme. A first flux and leakage calculation is performed by using the Pij method with multicell approximation.
The second level is dedicated to the flux calculation with the nodal S_N method. To prepare the cross section sets for the S_N calculation, each cell is homogenized in order to obtain the equivalent cross sections on the defined output low-group energy (6 groups) and spatial meshes. The depletion is performed by combining the homogeneous S_N flux with the heterogeneous microscopic cross sections assessed in the first level.

Three different PWR configurations have been computed:

- 5x5 cells lattice including four gadolinium poison cells , especially chosen to maximize the effect of a steep flux gradient;
- 17x17 UOX PWR assembly with 16 gadolinium poison cells, called UOX+GD assembly;
- 17x17 MOX PWR assembly, called MOX assembly.

Three types of depletion calculations have been compared :

- a 2D direct Pij reference calculation;
- a classical “one-level” calculation with the UP1 multicell Pij formalism;
- a two-level scheme calculation.

Concerning the k_∞, we observe an improvement for the discrepancies essentially for lattices with gadolinium poison cells. For the MOX assembly, the one-level UP1 calculation and the two-level calculation give equivalent results.
Comparisons of absorption reaction rates point out better results with the two-level scheme (discrepancies divided by about 3).

Concerning cost calculation, the new two-level scheme is very efficient and allows to reduce the calculation time by a factor about 8 to 10 compared to the one-level scheme.

ACKNOWLEDGEMENTS

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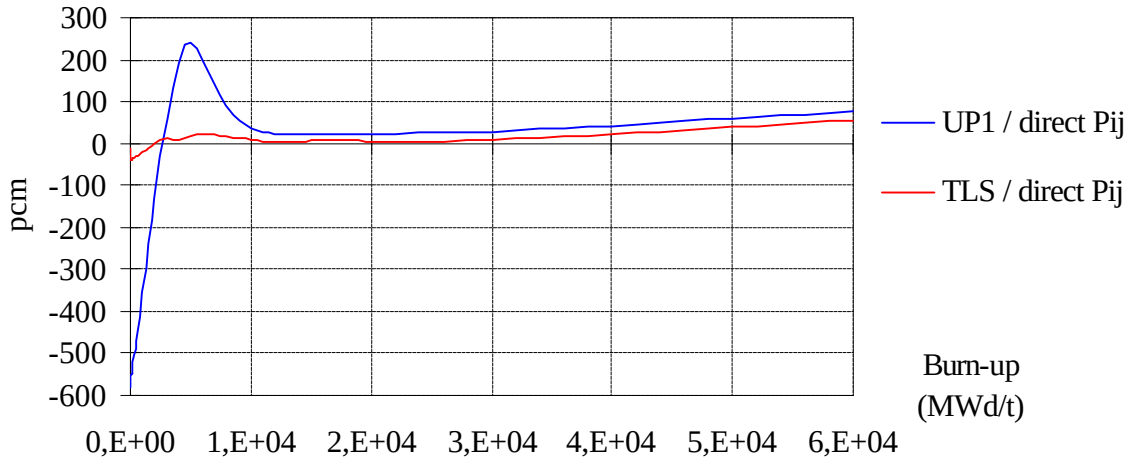

Figure 8. 5x5 lattice - k_∞ discrepancies during depletion.

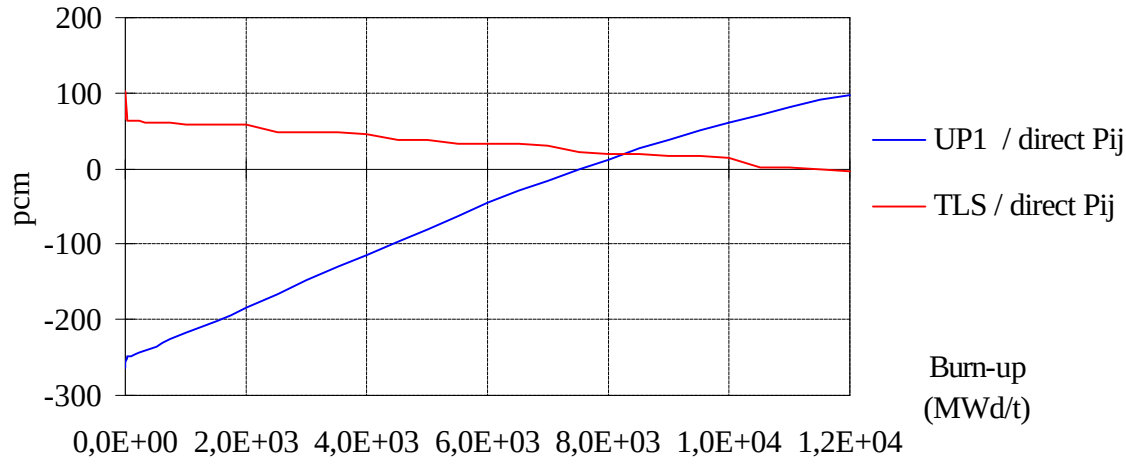

Figure 9. UOX+GD assembly - k_∞ discrepancies during depletion.

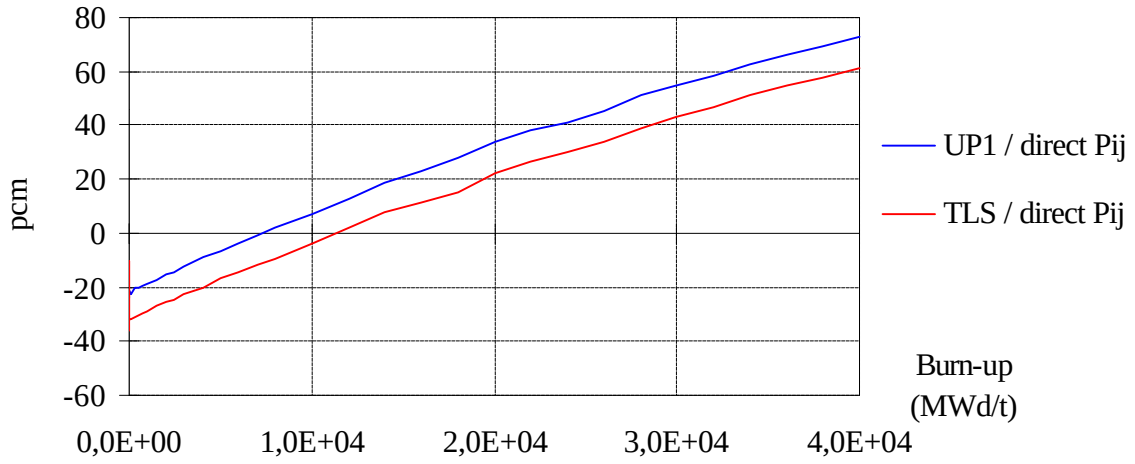

Figure 10. MOX assembly - k_∞ discrepancies during depletion.

		-0,09
	-0,24	-0,11
-0,20	0,03	-0,04

Figure 11. 5x5 lattice – Absorption rate group 1 – 0 GWd/t – Relative error (%) between UP1 and direct Pij calculation.

		-1,38
	-0,81	0,47
-5,38	-2,54	2,34

Figure 12. 5x5 lattice – Absorption rate group 2 – 0 GWd/t – Relative error (%) between UP1 and direct Pij calculation.

		-0,21
	-0,33	-0,22
0,10	0,03	-0,04

Figure 13. 5x5 lattice – Absorption rate group 1 – 0 GWd/t – Relative error (%) between TLS and direct Pij calculation.

		0,17
	0,10	0,43
-0,42	-0,44	0,23

Figure 14. 5x5 lattice – Absorption rate group 2 – 0 GWd/t – Relative error (%) between TLS and direct Pij calculation.

								-0,42
							-0,09	-0,32
						-0,24	-0,24	-0,34
					-0,14	0,07	0,06	-0,18
				-0,23	0,00	-0,06	-0,28	-0,27
			0,16	0,50	0,33	-0,12	0,08	-0,14
		-0,06	0,41	-0,07	-0,15	0,15	-0,33	-0,27
	0,24	0,04	0,68	0,21	-0,13	0,39	-0,23	-0,22
0,06	0,58	0,42	0,10	0,47	0,24	-0,15	0,02	-0,14

Figure 15. UOX+GD assembly – Absorption rate group 1 – 0 GWd/t – Relative error (%) between UP1 and direct Pij calculation.

								-1,70
							0,73	-1,05
						2,42	0,91	-0,89
					-1,56	0,02	0,81	-0,73
				-1,43	-1,68	-1,58	-1,15	-1,03
			-0,84	0,52	-0,01	-1,47	-1,20	-0,99
		2,13	0,27	0,41	2,23	0,02	-1,29	-1,06
	0,29	0,22	0,51	0,72	0,30	0,17	-1,14	-1,01
-2,59	-0,90	-1,20	-2,17	-0,65	-1,15	-2,28	-1,38	-0,98

Figure 16. UOX+GD assembly – Absorption rate group 2 – 0 GWd/t – Relative error (%) between UP1 and direct Pij calculation.

								0,05
							0,16	-0,03
						-1,92	0,28	0,30
					-0,20	0,55	0,50	0,19
				-0,30	0,14	0,30	0,08	0,15
			-0,70	0,25	0,33	-0,22	0,41	0,09
		-0,38	0,33	-0,34	-2,14	0,52	0,14	0,15
	-0,26	-0,40	-0,91	-0,18	-0,26	0,48	0,07	0,05
-0,86	0,24	0,47	-0,66	0,25	0,58	-0,30	0,32	-0,05

Figure 17. UOX+GD assembly – Absorption rate group 1 – 0 GWd/t – Relative error (%) between TLS and direct Pij calculation.

								0,51
							-0,32	0,19
						0,18	0,15	0,67
					-0,89	-0,46	-0,48	0,06
				0,92	0,48	0,47	0,55	0,45
			-2,11	-0,72	-0,92	-1,32	-0,16	-0,08
		0,50	-0,60	0,34	0,41	-0,57	0,68	0,25
	-0,44	0,17	-1,41	-0,44	0,27	-0,96	0,38	0,02
-0,34	-0,41	0,30	-0,80	0,02	0,45	-0,89	0,34	-0,29

Figure 18. UOX+GD assembly – Absorption rate group 2 – 0 GWd/t – Relative error (%) between TLS and direct Pij calculation.

								0,08
							0,32	0,12
						-0,07	0,23	0,18
					-0,17	0,77	0,40	0,34
				-1,03	0,02	0,06	-0,40	0,00
			-0,21	0,58	0,88	-0,17	0,56	0,37
		-0,48	0,67	-0,43	-0,34	0,67	-0,41	0,07
	-0,51	-0,46	0,68	-0,43	-0,40	0,71	-0,41	0,06
-0,26	0,63	0,64	-0,25	0,66	0,72	-0,16	0,48	0,36

Figure 19. MOX assembly – Absorption rate group 1 – 0 GWd/t – Relative error (%) between UP1 and direct Pij calculation.

								-3,39
							-0,12	-2,10
						0,77	1,57	-0,47
					-3,63	1,41	2,33	0,43
				-2,72	-1,63	-1,67	-1,17	-0,50
			-3,77	0,75	1,28	-3,96	-0,85	0,05
		-0,36	0,82	-0,10	0,08	0,78	-1,19	-0,33
	-0,52	-0,39	0,72	-0,17	-0,04	0,78	-1,23	-0,34
-4,29	0,50	0,55	-4,10	0,81	0,96	-3,94	-1,07	0,05

Figure 20. MOX assembly – Absorption rate group 2 – 0 GWd/t – Relative error (%) between UP1 and direct Pij calculation.

								0,19
							0,14	0,25
						-0,58	0,22	0,18
					-0,20	0,46	0,14	0,11
				-1,19	-0,12	-0,08	-0,28	0,11
			-0,22	0,57	0,52	-0,20	0,57	0,34
		-0,53	0,80	-0,50	-0,62	0,52	-0,27	-0,05
	-0,53	-0,46	0,86	-0,48	-0,59	0,61	-0,25	-0,01
-0,45	0,85	0,87	-0,27	0,79	0,75	-0,11	0,68	0,31

Figure 21. MOX assembly – Absorption rate group 1 – 0 GWd/t – Relative error (%) between TLS and direct Pij calculation.

								-0,33
							-0,13	-0,21
						0,22	0,06	-0,15
					-2,39	-0,17	0,32	-0,39
				-0,02	-0,51	-0,22	0,04	0,05
			-2,74	-0,19	-0,32	-2,38	-0,64	-0,28
		0,01	-0,17	0,07	-0,09	-0,09	0,05	-0,41
	-0,26	-0,04	-0,13	-0,11	-0,25	-0,21	0,04	-0,39
-1,25	0,28	0,36	-1,85	0,37	0,24	-1,72	0,10	-0,37

Figure 22. MOX assembly – Absorption rate group 2 – 0 GWd/t – Relative error (%) between TLS and direct Pij calculation.