Flux reconstruction methods for assembly calculations in the code APOLLO2

Igor Zmijarevic, Emiliano Masiello and Richard Sanchez
Commissariat à l'Energie Atomique
Direction de l'Energie Nucléaire
Service d'Etudes de Réacteurs et de Mathématiques Appliquées
CEA de Saclay, DM2S/SERMA
91191 Gif-sur-Yvette cédex, France
igor.zmijarevic@cea.fr,emiliano.masiello@cea.fr,richard.sanchez@cea.fr

Abstract

A technique for flux reconstruction has been incorporated in the code APOLLO2 allowing for fast generation of accurate burnup libraries. The burnup flux is obtained as the product of a pivot flux from a large-macrogroup heterogeneous-assembly calculation times an energy shape factor based on a fine-energy flux. The latter is obtained from a fast multicell calculation for a few types of representative cells in the assembly. The reconstruction formula preserves the reaction rates predicted by the large- macrogroup, heterogeneous-assembly calculation. Analysis of a BWR MOX benchmark shows that the reactivity error for a 70 MWd/t burnup cycle did not exceed 90 pcm and the maximum error in pin powers did not exceed 1%.

KEYWORDS: flux reconstruction, generation of burnup libraries, BWR.

1. Introduction

Generation of parameterized cross section data for core depletion calculations involves a large number of two-dimensional assembly transport calculations. However, the use of approximate reconstruction techniques can help reduce the cost of the calculations. [1] The goal of the reconstruction algorithm is to approximate as well as possible a direct fine-group 2D heterogeneous calculation. This can be achieved by performing three simplified transport calculations: a 1D fine-group or simplified 2D calculation for several representative cell types of the assembly, a 2D macrogroup intermediate calculation with homogenized cells, and a final large-macrogroup 2D calculation on the real assembly geometry. The intermediary calculation is used to provide realistic collapsed cross sections for the coarse-group heterogeneous calculation. The fine energy structure and flux spatial variation over the assembly are accomplished separately by the fine-group calculation and the 2D heterogeneous calculation, respectively. Leakage corrections are also introduced in the fine-group and in the reconstructed flux to take into account leakage effects in critical conditions.

2. General reconstruction formulas

The basic idea of flux reconstruction can be illustrated with a simple example. Assume one knows a correct value for the integral of the flux over a domain and an estimation for the

variation of the flux within the domain. We reconstruct a detailed flux that respect the integral over the domain by the formula

$$\phi(x) = \phi \times \frac{\widetilde{\phi}(x)}{\int_X \widetilde{\phi}(x)dx},\ x \in X.$$

In this equation X can be a domain in energy, in space or in both variables and:

- $\phi(x) =$ reconstructed detailed flux variation in domain X,
- $\phi =$ known integral of the flux over domain X,
- $\widetilde{\phi}(x) =$ known unnormalized variation of the flux in domain X.

The previous reconstruction formula is best presented by introducing the *shape factor*,

$$f(x) = \frac{\widetilde{\phi}(x)}{\int_X \widetilde{\phi}(x)dx},$$

so that the reconstructed flux,

$$\phi(x) = \phi \times f(x),\ x \in X,$$

results from the scaling of the *pivot* flux ϕ with the shape factor $f(x)$. Notice that the shape factor is always normalized to 1,

$$\int_X f(x)dx = 1,$$

so the reconstructed flux preserves the correct value of the integral of the flux over the domain,

$$\int_X \phi(x)dx = \phi,$$

while incorporating the detailed variation over x given by $\widetilde{\phi}(x)$.

This basic idea is easily generalized for use in flux reconstruction for assembly calculation. We introduce now an explicit dependence in two phase space variables $\phi(x, E)$, where x stands for space and E for energy. As a simple example, assume that we have computed two fluxes: $\phi(\cdot, E)$ and $\phi(x, \cdot)$, where $\phi(\cdot, E)$ is coarse in space and detailed in energy, while $\phi(x, \cdot)$ is detailed in space and coarse in energy, and that we want to reconstruct the flux $\phi(x, E)$, detailed in both space and energy. We shall handle integration on a coarse (slow) variable by taking the coarse value directly, only detailed (fast) variables will get integrated. Then, we can use one of the two formulas:

$$\phi(x, E) = \phi(x, \cdot) \times f(\cdot, E), \tag{1}$$

and

$$\phi(x, E) = \phi(\cdot, E) \times f(x, \cdot), \tag{2}$$

where the dot $(\cdot)$ denotes the coarse variable so that $\phi(x, \cdot)$ and $\phi(\cdot, E)$ are integrals over the dotted variables on the respective coarse domains, E_c and X_c.

We shall concentrate in the first of these formulas. Flux reconstruction (1) improves the pivot flux $\phi(x,\cdot)$, which has a coarse energy detail, by using a shape factor based on the flux $\phi(\cdot,E)$ which has better energy resolution but poorer spatial detail,

$$f(\cdot,E)=\frac{\phi(\cdot,E)}{\int_{E_c}\phi(\cdot,E)dE}, \tag{3}$$

while preserving the detailed spatial variation given by the pivot flux:

$$\int_{E_c}\phi(x,E)dE=\phi(x,\cdot).$$

2.1 Reaction-rate conservation

Both flux-reconstruction formulas preserve the integral of the flux over a coarse mesh while managing to increase the resolution in the interior of the coarse mesh. Formula (1) over an energy mesh and formula (2) over a spatial mesh. However, the two formulas also provide a useful reaction-rate conservation property.

Here we suppose that we have a cross sections map, $\Sigma(x,E)$, detailed in space and energy. Regarding the first reconstruction formula in (1), we consider the case when the cross sections for the calculation of the spatially detailed flux $\phi(x,\cdot)$ are obtained by an energy-condensation using the energy-detailed flux $\phi(\cdot,E)$ as weighting flux:

$$\Sigma(x,\cdot)=\frac{\int_{E_c}\Sigma(x,E)\phi(\cdot,E)dE}{\int_{E_c}\phi(\cdot,E)dE}=\int_{E_c}\Sigma(x,E)f(\cdot,E)dE.$$

Then, the reconstructed flux $\phi(x,E)$ preserves the reaction rates of the spatially-detailed pivot flux $\phi(x,\cdot)$:

$$\tau_{E_c}(x)=\int_{E_c}\Sigma(x,E)\phi(x,E)dE=\Sigma(x,\cdot)\phi(x,\cdot). \tag{4}$$

Similarly, if the cross sections for the calculation of $\phi(\cdot,E)$ are obtained by spatial smearing using the space-detailed flux,

$$\Sigma(\cdot,E)=\frac{\int_{X_c}\Sigma(x,E)\phi(x,\cdot)dx}{\int_{X_c}\phi(x,\cdot)dx},$$

then the reconstructed flux preserves the reaction rates of the energy-detailed pivot flux

$$\tau_{X_c}(E)=\int_{X_c}\Sigma(x,E)\phi(x,E)dx=\Sigma(\cdot,E)\phi(\cdot,E).$$

3. General methodology

Isotopic depletion for an assembly is computed in a series of burnup or depletion steps. At each burnup step a new space-and-energy detailed assembly flux $\phi(x,E)$ is computed to provide the average reaction rates for each depletion region in the assembly. We shall denote this flux by $(\phi_i^g)_{BU}$, where g is a fine group and i is a depletion region.

We work with three transport calculations, 1D cell or simplified 2D, 2D cell-homogenized assembly and 2D heterogeneous assembly, with decreasing refinement in the energy variable. To save computation time, selfshielded cross sections and fine-group transport calculations are

done for a few one-dimensional representative types of cells. To this end, cells in the assembly with a similar neutronic environment are grouped into types. Each cell type represents one or more physical cells in the assembly and, therefore, the materials for a cell type are obtained by volume averaging of the daughter physical cells. For the burnup calculation, isotopic concentrations are defined for each cell in the assembly and, within each cell, over depletion regions that we usually take to be one-dimensional rings.

3.1 Flux reconstruction

We use the following notation for the energy-integrated, space-averaged fluxes obtained from a transport calculation:

- $\phi_i^g =$ flux in ring i from the fine-group transport calculation for a cell of a given type.
- $\phi_I^G =$ flux in cell I from the intermediary coarse-group 2D cell-homogenized assembly transport calculation.
- $\phi_r^{\mathcal{G}} =$ flux in region r from the large-macrogroup 2D heterogeneous assembly calculation.

The depletion flux $(\phi_i^g)_{BU}$ is reconstructed by combining the fine-group fluxes ϕ_i^g, which are the most detailed energy representation of the pin cells spectra, with the heterogeneous-assembly large-macrogroup flux $\phi_i^{\mathcal{G}}$. The correction is done to account for the specific position of each daughter cell in the assembly. We have explored several possibilities but the best results were obtained from

$$(\phi_i^g)_{BU} = \phi_i^{\mathcal{G}} \times (f_i^g)_w$$

with the fine-group shape factors

$$(f_i^g)_w = \frac{(\phi_i^g)_w}{\sum_{g\in\mathcal{G}}(\phi_i^g)_w}. \tag{5}$$

This formula is based on the idea of reaction-rate conservation, where the fine-group shape factors $(f_i^g)_w$ of Eq. (5) are used to collapse the cross sections for the 2D heterogeneous-cell assembly flux: $\Sigma_i^{\mathcal{G}} = \sum_{g\in\mathcal{G}} \Sigma_i^g (f_i^g)_w$. Then, the reconstructed flux $(\phi_i^g)_{BU}$ not only preserves the fine-spatial distribution of the pivot flux $\phi_i^{\mathcal{G}}$ but it also conserves the coarse-group reaction rates

$$\sum_{g\in\mathcal{G}} \Sigma_i^g (\phi_i^g)_{BU} = \Sigma_i^{\mathcal{G}} \phi_i^{\mathcal{G}}.$$

In order to account for environment effects, the intermediary macrogroup 2D cell-homogenized calculation is used to improve the spatial resolution of the fine-group flux. Instead of using the flux $(\phi_i^g)_w = \phi_i^g$ in Eq. (5) we use the reconstructed flux

$$(\phi_i^g)_w = \phi_I^G \times f_i^g, \tag{6}$$

where

$$f_i^g = \frac{\phi_i^g}{\sum_{g\in G} \phi_i^g}.$$

The cross sections for the intermediary calculation are obtained by collapsing of the fine-group fluxes, $\Sigma_i^G = \sum_{g\in G} \Sigma_i^g f_i^g$.

3.2 Leakage corrections

Leakage corrections have to be introduced to account for the macroscopic variation of the flux in the critical core. In flux reconstruction procedures leakage can be introduced at one or more stages of the calculation. We have found that the best results are obtained by introducing a leakage correction in the fine reconstructed flux used to collapse the cross sections and also in the final burnup flux. We use the flux (6) to homogenize the assembly and compute the infinite medium spectrum ϕ^g_∞ and the associated critical leakage cross section $D^g B^2$. Next, the flux $(\phi^g_i)_w$ is used to compute the spatial shape factors

$$\widehat{f}^g_i = \frac{(\phi^g_i)_w}{\sum_i (\phi^g_i)_w V_i},$$

where the sum is over all regions in the assembly and V_i is the volume of region i, which are then used to normalize $(\phi^g_i)_w$ as follows

$$(\phi^g_i)_w \rightarrow \phi^g_\infty V \times \widehat{f}^g_i,$$

where $V = \sum_i V_i$.

It is this scaled flux that is used to define the energy shape factors in Eq. (5) that serve for cross section collapsing and for the reconstruction of the burnup flux. The DB^2 cross section is also collapsed and incorporated in the heterogeneous assembly calculation. Finally, the reconstructed burnup flux is similarly corrected with its infinite medium critical spectrum $(\phi^g_\infty)_{BU}$:

$$(\phi^g_i)_{BU} \rightarrow (\phi^g_\infty)_{BU} V \times \frac{(\phi^g_i)_{BU}}{\sum_i (\phi^g_i)_{BU} V_i}.$$

4. Example calculations

We have analyzed a BWR MOX depletion benchmark for 0%, 40% and 70% void fraction. [3] The geometry of this benchmark, depicted in Fig. 4.1, is that of a 10×10 unrodded assembly with an internal Atrium-like water channel and diagonal symmetry. The assembly contains 77 MOX pins with 5 different enrichments and 14 Gadolinia bearing rods. Because of the diagonal symmetry only 49 pins have to be considered for the burnup calculations.

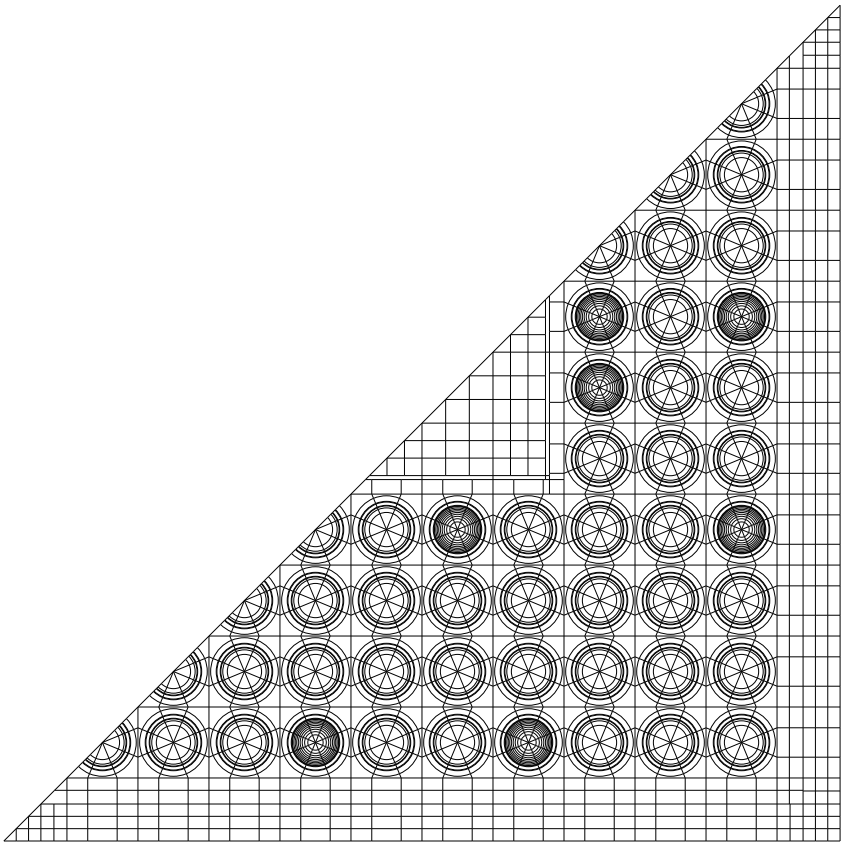
4.1 Flux reconstruction calculation

To account for the different neutronic environments in the assembly, the central zone around the water channel and the peripheral zone, we have defined 10 types of cells (8 MOX and 2 Gadolinia). After each burnup step these 10 cells are constructed by volume averaging of the daughter cells. The fine-group calculation was done with the 172-group (80 thermal) XMAS library with a fast interface-current 'multicell' UP_1 flux solver where cell exchanges account for the different positions of the daughter cells in the assembly. [2] The auxiliary cell-homogenized assembly calculation was done with the IDT short-characteristics module of APOLLO2 with 40 macrogoups (25 thermal) and 16×16 cells, while the 16-macrogroup (13 thermal) detailed heterogeneous-assembly calculation was done with the method of characteristics (MOC) of the TDT module with 3784 regions. [4,5]

Selfshielded cross sections accounting for isotopic mixture and spatial interactions are computed in 1D cylindrical geometry for each cell type. [6] Then, improved selfshielded cross sections for the U238 are obtained from a multicell UP_1 calculation with the 10 cell types. Finally, for the multicell calculations, the water channel box and surrounding water was replaced

by flux averaging of the water-box-water region of an 1D slab (water-box-water-assembly fuel) calculation with an asembly averaged fuel obtained from an 1D cylindrical calculation for a volume-averaged cell. Selshielded cross sections for the water box were obtained from an 1D slab (water-box-water) calculation.

Figure 1: Geometry of the BWR MOX benchmark showing the partition in regions for the MOC calculation.



4.2 Validation of the reference calculation

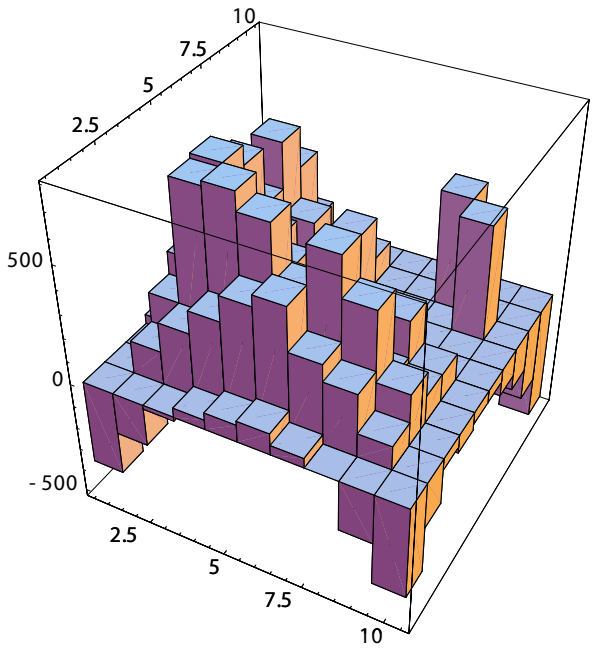
The reference calculation for the depletion run was done with the XMAS library using the TDT solver with the same number of regions and with the same selfshielded cross sections as for the flux reconstruction calculation. We validated this calculation by a comparison with the Monte Carlo TRIPOLI4 code for the startup assembly. [7] The results shown in Table 1 and Fig. 4.2 confirm the accuracy of the reference calculation as well as that of the flux reconstruction scheme. The RMS values in Table 1 are defined as

$$RMS = \sqrt{\frac{\sum_{i=1}^{N}(1-\frac{cal}{ref})^2}{N}}.$$

Table 1: Reference and reconstructed results compared to TRIPOLI4 for the BOL BWR assembly. Pin reaction rates error bounds and RMS in %.

	fission rates		absorption rates		eigenvalue
	(min,max)	RMS	(min,max)	RMS	
reference	(-0.7,1.4)	0.4	(-0.9,1.0)	0.3	-87 pcm
reconstructed	(-1.1,1.7)	0.6	(-1.0,1.6)	0.5	163 pcm

Figure 2: BOL BWR assembly. Reconstructed absorption errors (pcm) with respect to the reference solution.



4.3 Depletion calculations

We have run depletion calculations up to a burnup of 70 GWd/t for the three void fractions of 0, 40 and 70%. Each calculation comprised 3 initial steps with small burnups increments, to account for fast Gadolinia burnup, and 85 steps every 250 MWd/t . Because our depletion calculation uses a corrector-predictor technique, 2 of the 88 steps were recalculated given a total of 90 flux calculations. The results obtained with the reconstruction technique were compared to those from the reference calculation. In a DEC-ALPHA at 1150MHz the running time for an entire depletion calculation was 1h 21m for the reconstruction technique as compared to 12h 30m for the reference calculation. Figure 4.3 shows the errors in reactivity versus burnup for the three void fractions. The error is dominated by the overestimation of Gadolinia burnup. Figure 4.3 depicts the fission rate error bounds for the 40% void case. The figures show that the reactivity error during the burnup calculation does not exceed 90 pcm and the maximum error in pin powers does not exceed 1%. The RMS for the pin power distribution was smaller than 0.5%.

Figure 3: Comparison of reconstructed and reference depletion calculations. Reactivity errors (pcm) versus burnup (MWd/t).

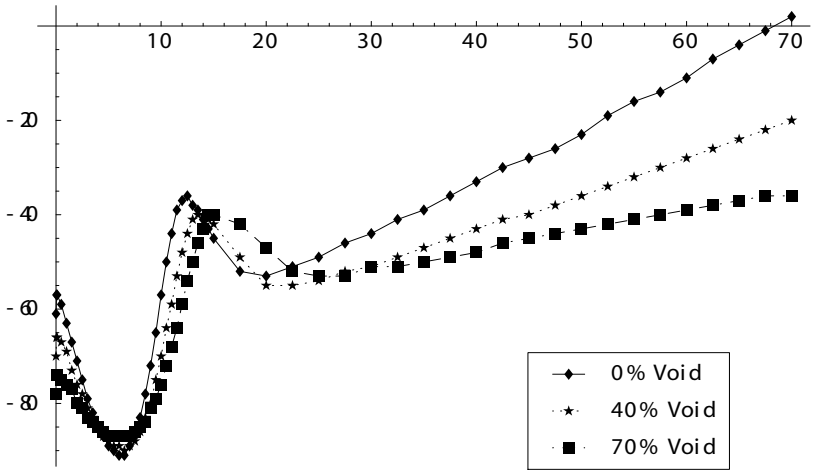
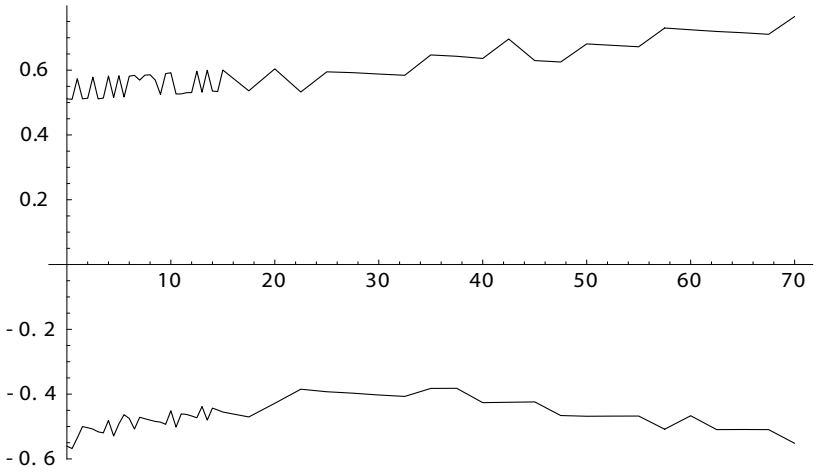


Figure 4: Comparison of reconstructed and reference depletion calculations for 40% void fraction. Fission rate error bounds (%) versus burnup (MWd/t).



5. Conclusions

A technique for flux reconstruction has been incorporated in the APOLLO2 code allowing for fast generation of accurate burnup libraries. The burnup flux is obtained as the product of a pivot flux from a large-macrogroup heterogeneous-assembly MOC calculation times an energy shape factor based on a fine-group flux. The latter is obtained from a fast multicell calculation for a few types of representative cells that are constructed from volume averaging

of their daughter cells. An auxiliary macro-group intermediary cell-homogenized assembly calculation was also introduced to incorporate environment effects in the fine-group flux. One advantage of the reconstruction formula is that it preserves the reaction rates predicted by the large- macrogroup, heterogeneous-assembly MOC calculation.

Our tests have shown that the use of a fast multicell calculation to generate the fine-group cell fluxes, instead of a set of independent 1D cylindrical calculations, significantly improves the accuracy of the results. Spectral leakage corrections are introduced in the fine-group calculation to improve the weighting flux used to collapse cross sections for the detailed MOC calculation and also as a final correction for the reconstructed burnup flux. Our results show the accuracy of the reconstruction scheme that, as compared with a reference fine-group MOC calculation, reduces by a factor of 9.25 the amount of time required for the generation of a burnup library for a 70 GWd/t cycle.

References

1) D. Knott, “Description and validation of the GE lattice physics code LANCER02,” International Topical Meeting MC2005, Avignon, France, Sept. 12 (2005).

2) R. Sanchez *et al.*, “APOLLO II: A user-oriented, portable, modular code for multigroup transport assembly calculations,” *Nucl. Sci. Eng.*, **100**, 352 (1988).

3) A. Yamamoto *et al.*, “Benchmark problem suite for reactor physics study of LWR next generation fuels,” *Nucl. Sci. Technol.*, **39**, 900 (2002).

4) I. Zmijarevic, “Multidimensional discrete ordinates nodal and characteristics methods for the Apollo2 code,” M&C’99 Topical Meeting, Madrid, Spain, Sept. 27 (1999).

5) R. Sanchez and A. Chetaine, “A synthetic acceleration for a two-dimensional characteristic method in unstructured meshes,” *Nucl. Sci. Eng.*, **136**, 122 (2000).

6) M.Coste-Delclaux and S.Mengelle, “New resonant mixture self-shielding treatment in the code APOLLO2”, PHYSOR 2004 Topical Meeting, Chicago, Illinois, April 25 (2004).

7) J.P. Both *et al.*, “A survey of TRIPOLI-4,” Proceedings of the 8th International Conference on Radiation Shielding, Arlington, Texas, April 24 (1994).