STEPS AHEAD IN THE FEW-GROUP CROSS-SECTION LIBRARY GENERATION AT THE PIN LEVEL

N. Petrov
Institute for Nuclear Research and Nuclear Energy, 1784 Sofia, Bulgaria
nlp@inrne.bas.bg

Santiago Sánchez-Cervera and José J. Herrero
Universidad Politécnica de Madrid
C/ José Gutiérrez Abascal, 2 28006 Madrid, Spain
s.sanchezcervera@gmail.com
josejavier.herrero@upm.es

ABSTRACT

There exists an interest in performing pin-by-pin calculations coupled with thermal-hydraulics so as to improve the accuracy of nuclear reactor analysis. In the framework of the EU NURISP project, INRNE and UPM have generated an experimental version of a few-group diffusion cross sections library with discontinuity factors intended for VVER analysis at the pin level with the COBAYA3 code. The transport code APOLLO2 was used to perform the branching calculations.

As a first proof of principle the library was created for fresh fuel and covers almost the full parameter space of steady state and transient conditions. The main objective is to test the calculation schemes and post-processing procedures, including multi-pin branching calculations. Two library options are being studied: one based on linear table interpolation and another one using a functional fitting of the cross sections.

The libraries generated with APOLLO2 have been tested with the pin-by-pin diffusion model in COBAYA3 including discontinuity factors; first comparing 2D results against the APOLLO2 reference solutions and afterwards using the libraries to compute a 3D assembly problem coupled with a simplified thermal-hydraulic model.

1. INTRODUCTION

The tools for safety analysis of reactor core calculations have evolved in the last years to include capabilities of modeling the core at the level of fuel pin and thermal-hydraulic sub-channel. In the framework of the EU NURISP project [1], INRNE and UPM have cooperated to generate and test few-group cross-section libraries to be used in 3D hexagonal pin-by-pin calculations coupled with thermal-hydraulics.

The goal of this work is to present the basic modeling assumptions in APOLLO2 [2] for the library generation, including multi-pin calculations to generate interface discontinuity factors, and to test the performance of parameterized libraries for coupled calculations against the results of a standard library using the table interpolation method.

Section 2 summarizes the techniques used to generate few-group cross-section libraries for the COBAYA3 pin-by-pin diffusion code [3].

2. XS LIBRARY GENERATION

The computation of full core diffusion solutions for LWR is currently performed in a two-step approach. In the first step, a transport code is used to generate homogenized and condensed parameters in few energy groups suitable for diffusion calculations. In the second step, a 3D full core calculation is carried out with a diffusion code. In this process, depletion and branching calculations are performed to create a library containing homogenized parameters at all operational conditions achievable in a nuclear reactor. These conditions are mainly represented by the fuel burn-up and the local operational conditions: fuel Doppler temperature, moderator temperature, moderator density and boron concentration.

In the work presented here the following assumptions were made:

- VVER-1000 UOX assembly with boron burnable absorbers
- 4.4 w/o U5 enrichment of all fuel pins
- Zero burn-up
- Method of Characteristics (MOC) based calculation scheme in APOLLO2
- JEFF3.1.1 based 281-groups library in APOLLO2 and continuous energy cross-sections for the TRIPOLI4 [4] Monte-Carlo reference solutions
- 19-cells clusters used for multi-pin branching calculations
- Use of four local operational conditions by five points each
- Interface currents stored and used to compute the discontinuity factors
- Use of functional fitting vs. table interpolation method

In the considered VVER-1000 fuel assembly there are 331 hexagonal cells. At zero burn-up one can define several types of different fuel cells usually with similar enrichment, surrounding a guide tube, control rod or separable burnable absorber. A set of 19-cell clusters was formed to represent all types in a fuel assembly and to compute cross-sections and interface discontinuity factors for each type of pin as shown in Figure 1.

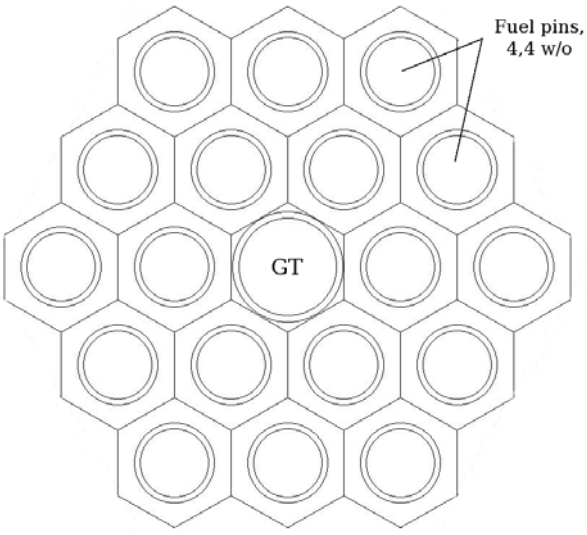

Figure 1 19-cell cluster

The MOC based calculation scheme in APOLLO2 for XS generation in hexagonal geometry [5], [6] was used to generate homogenized and condensed parameters in 2 and 4 energy groups stored in a binary HDF5 format output file. The APOLLO2 solution was verified for certain calculations against Monte Carlo solutions generated with TRIPOLI4.

Specific scripts and a queue client were applied on a multi-processor machine to complete all branching calculations simultaneously. On a machine with 8 cores, each single state point calculation of a 19-cell cluster took about 150 s CPU time and the whole branching calculation took about 4 hours.

Next, the HDF output files were processed to assemble a library in ASCII table format, to be used through linear table interpolation. Since the size of this library rapidly increases with the number of pins to be treated, this work focuses on the functional fitting approach which needs to store only the coefficients of the polynomials fitting the cross sections values.

In order to generate a parameterized library, the tabulated homogenized cross-sections have to be studied with a statistical program such as the R code [7], so that to determine the dependencies of each parameter on the local variables and propose a best fitting polynomial computed by least squares techniques. For these small test cases we have found the polynomials manually avoiding the more practical but costly stepwise regression approach [8] to learn the main dependencies involved for each type of cross-section which will be useful when more automatic procedures will be developed.

The adopted methodology to elaborate the fitting polynomials comprises several steps. First, a graphical representation is done for each cross section against each operational variable. Next, an individual adjustment of the cross section is done to catch the dependency of each local variable separately. After this, multiple adjustments are tackled considering more than one variable at a time; these cases need further attention to determine correctly the crossed effects between variables.

A typical example of a crossed effect appears between the moderator density and the boron concentration, if the water density is modified maintaining the boron concentration, a concentration or dilution of boron is produced implicitly which also affects the homogenized parameters.

Finally all the dependencies are cast together to propose the polynomial that fits best each cross section or discontinuity factor.

When applying the parameterization it has been observed that:

- Most influenced variables are always moderator density and boron concentration for any parameter and energy group. Besides, the behavior with density is always quadratic
- In the fast group, the cross sections are practically independent of the moderator temperature, while in the thermal group there exists a dependency on the moderator temperature but not on fuel temperature
- Scattering cross-sections depend mostly on moderator density linearly, except for up-scattering which depends on moderator temperature.

Two types of interface discontinuity factors definitions have been employed, one is the standard Generalized Equivalence Theory definition [9] which preserves interface flux values from the transport solution, and the other one is a black-box homogenization definition or Selengut type of discontinuity factor [10] which preserves interface partial currents from the reference calculation.

3. CROSS SECTIONS VERIFICATION

The APOLLO2 results were tested against TRIPOLI4 reference solutions at certain parameter's points as listed in Table I. The MOC spatial mesh, tracking parameters were chosen such as to provide converged solutions in a reasonable piece of time.

Table I. State parameters values for testing A2 vs. T4 solutions

Parameters	Moderator density, kg/m3	Moderator temperature, C	Fuel temperature, C	Boron concentration, ppm
Values	750	301	701	500

Three types of clusters formed by a central pin surrounded by fuel pins were considered, with the central position occupied by a guiding tube (GT), a control rod (CR) or a burnable absorber (BA) cell.

The biases of APOLLO2 vs. TRIPOLI4 solutions are as follows:

- Single pin in infinite media: bias +45 pcm in the multiplication factor and less than 1.E-8 in pin fission rates
- GT cell in the center of the cluster: bias -15 pcm in the multiplication factor

COBAYA3 pin-by-pin diffusion calculations with APOLLO2 generated XS and Interface DF were validated against the reference solutions as follows:

Using either GET or Selengut interface discontinuity factors:

- Single pin in infinite media: all solutions (2 and 4 groups) give deviations less than 1 pcm in multiplication factor and less than 1.E-8 in pin-by-pin fission rates
- GT cell in the center of the cluster: all solutions (2 and 4 groups) give bias less than 1 pcm and less than 0.3% for 2g, or 0.2% for 4g in pin fission rates
- BA cell in the center of the cluster: all solutions (2 and 4 groups) give bias less than 3 pcm and less than -0.4% for 2g, or -0.3% for 4g in pin fission rates
- CR cell in the center of the cluster: all solutions (2 and 4 groups) give bias less than 6 pcm and less than -0.6% for 2-4g in pin fission rates

Not using IDFs leads to hundreds of pcm difference and more than -0.7% deviations in fission reaction rates map.

4. FUEL ASSEMBLY CALCULATIONS

In order to verify the usability of the XS in a full fuel assembly - a simplified one was considered where the water gap was eliminated (Figure 2). For this case: 4 materials were included in the cross sections library used inside the COBAYA3 2D model: a fuel pin from

an infinite lattice calculation, a guide tube and 3 fuel pin types from the cluster calculations surrounding the guiding tube. Cell interface discontinuity factors were included in the library for the two materials using both definitions and considering their dependence on the local variables, which is not important for the infinite lattice fuel pin, but really noticeable for the guiding tube and surrounding pins.

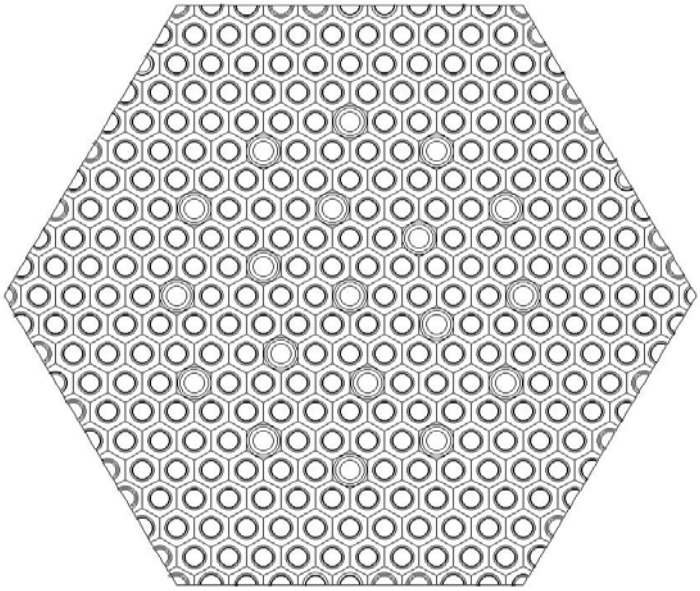

Figure 2 Fuel assembly geometry without water gap

A reference solution of the 2D problem was computed with APOLLO2 and compared with the values obtained by COBAYA3 including IDFs. The deviations are shown in Table II.

Table II. COBAYA3 vs. APOLLO2 deviations in k-eff and pin fission rates for different number of collapsed energy groups

Case	Deviations $\Delta k = k - k_{ref}$ (pcm)	Max deviations in fission RR (%)
C3, 2g, with IDFs	-71	-1.2
C3, 4g, with IDFs	-31	-0.8
C3, 8g, with IDFs	17	-0.6
C3, 8g, no IDFs	44	-1.2

In order to test the parameterized library based on functional fitting, a 3D N/TH fuel assembly calculation was made using the simplified TH module in COBAYA3. The same geometry was extended to 3D with a homogeneous axial composition including axial reflectors at both ends of the FA for which the values of the guide tube cross sections have been used as a first approximation, and all the fuel pins were considered equal for this problem.

Table III. k eigenvalue for the 3D FA with coupled NK-TH

	NEMTAB library (table interpolation)	**Parameterized library**	**Difference (pcm)**
No IDF correction 2G	1.30250	1.27416	2834
GET IDF 2G	1.28715	1.26001	2714
Selengut IDF 2G	1.28764	1.26051	2713
No IDF correction 4G	1.30559	1.30509	5
GET IDF 4G	1.28907	1.28925	-43
Selengut IDF 4G	1.28953	1.28969	-16

A very high discrepancy is seen in the results of both library approaches in Table III for the 2-group solution. In this case the solution with the NEMTAB library was taken as reference. This result indicates that the current functional fitting in 2 energy groups fails to give satisfactory accuracy for coupled calculations. This bias persists even when the polynomial expressions have been made as accurate as possible.

As shown in Figure 3, the axial power profiles produced by both libraries in 2 groups also display a large discrepancy, independently of the use or not of IDF. From these two observations, it can be deduced that most part of the bias comes from the poor approximation of cross sections values in 2 groups, rather than from the use of interpolated or parameterized discontinuity factors.

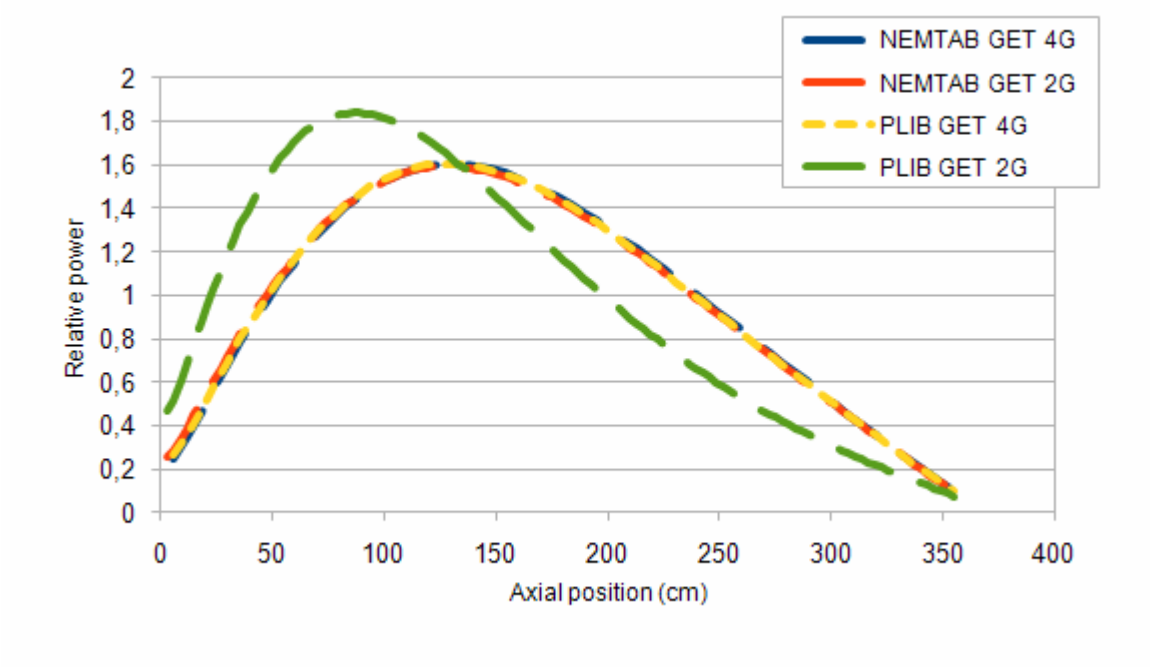

Figure 3 Axial power distribution obtained with different libraries

Deviations of both solutions were already expected as sensitivities of k_{eff} to the cross section values have been studied to know the admissible error on each cross section fitting. In particular, problems have been encountered in 2 energy groups to fit absorption, nu-fission

and down-scattering cross sections in both energy groups for a target accuracy of 10 pcm or less on k_{eff} for the fuel pin, while the guide tube was easily parameterized.

The 2-group fitted values are inside the limits to get bias in k_{eff} in the order of 100 pcm per each unitary change in most cross sections which from our experience means that one can expect biases of 10 times more because of accumulation of errors, which agrees well with the biases observed on the range of 1000 pcm.

On the other hand, the same Table III and Figure 3 show a very good agreement of the solutions obtained with the 4-group libraries for both NEMTAB and parameterized libraries. And the difference between the two solutions is actually inside the uncertainty of the NEMTAB library so that the parameterized library is able to achieve the same level of accuracy on the cross sections values.

5. SUMMARY AND CONCLUSIONS

Few-group libraries for pin-by-pin diffusion calculations have been generated with APOLLO2 in two different formats, tabulated and parameterized, for several types of cells.

Verification of the 2D 19-cell clusters and fuel assembly solutions shows excellent potential and is a good sign to continue the work on V&V of the pin-by-pin XS library. Further work should be done on completing the real fuel assembly case – the one with inter-assembly water gap. And next step is to include burn-up in the library.

The performance of the parameterized library based on functional fitting has been tested on a 3D VVER-1000 assembly problem coupled with simplified thermal-hydraulics.

A systematic bias is observed between the solutions produced by both libraries, which indicates that the parameterized library in 2 groups fails to achieve the required precision in the cross section functional fitting.

Good performance is displayed when using the library in 4 energy groups. The results indicate that the fitting is acceptable and this number of energy groups is suitable to be used in parameterized libraries for pin-by-pin diffusion calculations of VVER reactors.

ACKNOWLEDGEMENTS

This work is partially funded by the NURISP project (Contract n° 232124) in the 7th Euratom Framework Program of the European Union.

REFERENCES

1. C. Chauliac, J.M. Aragonés, D. Bestion, D.G. Cacuci, N. Crouzet, F.-P. Weiss, M.A. Zimmermann, 2011. NURESIM - A European simulation platform for nuclear reactor safety: Multi-scale and multi-physics calculations, sensitivity and uncertainty analysis. *Nuclear Engineering and Design*, **241** (9), 3416 – 3426.
2. I. Zmjarevic, P. Bellier, S. Mengelle, S. Santandrea. APOLLO2 v2.8e Reference manual. CEA Saclay, 2011

3. J.J. Herrero, C. Ahnert and J.M. Aragonés. 3D whole core fine mesh multigroup diffusion calculations by domain decomposition through alternate dissections. Proc. M&C 2007, Monterey, 15-19 April 2007
4. TRIPOLI4 Project Team. TRIPOLI4 User Guide. CEA-R-6169, 2008
5. N. Petrov, G. Todorova, N. Kolev, F. Damian, P. Bellier. Advanced calculation schemes for cross-section library generation with APOLLO2 at the nodal level. EU NURISP SP1 Project Meeting, Varna, 2010
6. N. Petrov, G. Todorova, N. Kolev, F. Damian. Two-level MOC calculation scheme in APOLLO2 for cross-section library generation for LWR hexagonal assemblies. Proc. M&C 2011, Rio de Janeiro, Brazil, May 8-12, 2011
7. R Development Core Team. R: A Language and Environment for Statistical Computing. Vienna, Austria, 2010. ISBN 3-900051-07-0
8. Zimin, V.G., Semenov, A.A., 2005. Building neutron cross-section dependencies for few-group reactor calculations using stepwise regression. *Annals of Nuclear Energy* **32** (1), 119–136.
9. K.S. Smith, Assembly homogenization techniques for light water reactor analysis, *Progress in Nuclear Energy*, **17** (1986) 303
10. R. Sánchez, Assembly homogenization techniques for core calculations, *Progress in Nuclear Energy*, **51** (2009) 14-31