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V. Jouault, J.-M. Palau, G. Rimpault, J.-F. Vidal. A New Breakdown Methodology To Estimate Neutronic Model Biases Applied To Apollo3 SFR Core Calculations. M&C 2017 - International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering, Apr 2017, Jeju, South Korea. cea-02434517

HAL Id: cea-02434517

<https://cea.hal.science/cea-02434517>

Submitted on 10 Jan 2020

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A New Breakdown Methodology to Estimate Neutronic Model Biases Applied to APOLLO3[®] SFR Core Calculations

V. Jouault, J.-M. Palau, G. Rimpault, J.-F. Vidal

CEA, DEN, DER/SPRC/LEPh, Cadarache, F-13108 Saint-Paul-lez-Durance, Contact : valentin.jouault@cea.fr

Abstract – This paper presents a new breakdown methodology to estimate independently model biases for each approximations of a given calculation scheme. This new methodology is set to be applied on the new French deterministic neutron transport code APOLLO3[®], and be a part of its advanced V&V process. The first step of the method is the identification of approximations of the different solvers. Then, we measure the impact of each relevant approximation on core characteristics. To do so, we use ad-hoc TRIPOLI-4[®] multi-group calculations, either using APOLLO3[®] cross section, or making it generate its own multi-group cross sections. The methodology is applied on the ASTRID CFV core, and gives satisfactory results. It allows us to evaluate the impact of changes in the calculation scheme, leading to an improved calculation scheme and excellent results for reactivity and reactivity effects, especially in voided configurations.

INTRODUCTION

In order to meet new industrial's expectations in terms of neutronic calculation accuracy and versatility, CEA launched the APOLLO3[®] project [1]. The project main purpose is to develop the deterministic multi-purpose neutronic transport code APOLLO3[®]. This is being done at CEA with the support of EDF and AREVA, with the aim of having a better modeling of physical phenomenon of existing reactor cores (until 3rd generation) but also of future reactor concepts (4th generation). APOLLO3[®] is aiming at replacing the previous 2nd generation of deterministic codes like APOLLO2 [2], CRONOS2 [3] and ECCO/ERANOS [4].

The APOLLO3[®]-SFR package built with APOLLO3[®] solvers defines reference calculation schemes associated with a nuclear data library to calculate all neutronic parameters together with certified biases and uncertainties derived from the VV&UQ process (Verification, Validation and Uncertainty Quantification). This VV&UQ process incorporates numerical verification and validation as well as experimental validation leading to uncertainty quantification. This iterative process has shown its efficiency in the past (for LWR and FBR) but is based on global comparisons (mainly APOLLO2/CRONOS or ECCO/ERANOS vs. TRIPOLI-4[®] pointwise calculations) which do not permit detailed analysis of numerical biases. The purpose of this paper is to present a new V&V methodology, enabling us to estimate numerical biases for each approximation independently. First, it is important to identify the main approximations involved in the APOLLO3[®] reference calculation scheme. Thus, estimation of biases is completed by comparing APOLLO3[®] results with well-chosen reference results (often multigroup Monte-Carlo results). Finally, we will show the results of this methodology applied to the ASTRID CFV core, and how calculation scheme update (improved models) impacts each approximation bias.

I. APOLLO3[®] V&V PROCESS

In order to assess the quality (performance, reliability and flexibility) of the code, a rigorous Verification and Validation (**V&V**) methodology has been established. It is based on a two steps approach.

The first step is **Verification**. It consists in verifying that the numerical resolution of neutronic models and programming of each module is correct. This step should be exhaustive as much as possible and must cover the wide range of functionalities and applications cases. This verification also includes a dedicated "Test Machine" which verifies that tests on old versions remain valid in the new code versions (non regression tests).

The second step is the numerical **Validation**. It quantifies the accuracy of the neutronic models used in APOLLO3[®]. The APOLLO3[®] Validation covers the main functionalities of the code (self-shielding models, flux solvers, homogenization, condensation, depletion, kinetics, perturbation/sensitivity analysis) through a dedicated model based on the PIRT (Phenomena Identification and Ranking Table) methodology [5]. Generally, this validation is based on a comparison of APOLLO3[®] deterministic calculation against TRIPOLI-4[®] [6] continuous-energy Monte-Carlo reference calculation. Both calculations use the same nuclear data library (based on JEFF3.1 evaluation).

Despite technological improvements in computer science (number of operations per second and storage volume increased), **approximations** are unavoidable in deterministic codes. Yet, those approximations bring more or less important discrepancies on different core characteristics against reference calculations (for example Monte-Carlo). The V&V process is therefore the search of an optimum on these discrepancies between calculation time and accuracy. The current V&V process has shown its efficiency in the past (for LWR and FBR) but is based on global comparisons (mainly deterministic methods against MC pointwise calculations) which do not permit detailed analysis of numerical biases. The innovation in the advanced V&V process presented here comes from the fact

that each approximation existing in a solver is being validating independently, hence removing the possibility of having compensating errors.

I. APOLLO3[®] CALCULATION SCHEME

a. Principle of Calculation Scheme

The use of a scientific calculation code to run a simulation requires, from the user, many choices among the calculation models and options of the code. Those choices should match design specification of different natures (grid, solver type ...), consistently with physics complex phenomena. All those choices establish what we call a **calculation scheme**.

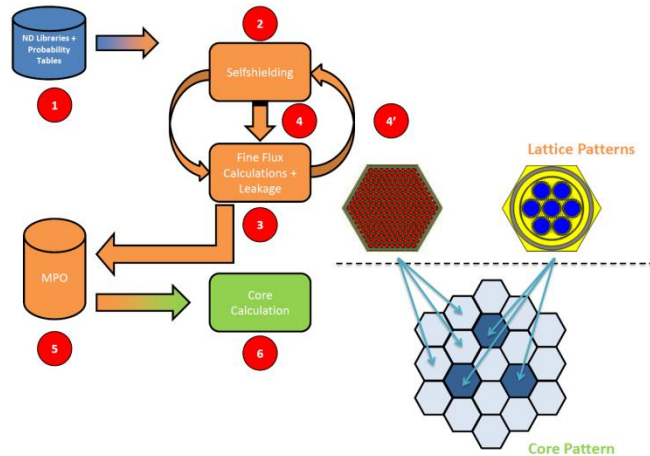


Fig. 1: APOLLO3[®] calculation scheme

The typical calculation scheme for APOLLO3[®] is presented in Fig. 1. It is based on the separation of the cell/lattice calculation (orange) from the core calculation (green).

First, the code sets the nuclear data multi-group libraries, associated with probability tables, following the energy grid choice by the user (1). Then self-shielding calculations (2) are performed to generate self-shielded cross sections of relevant resonant isotopes in different regions. Those cross sections are used in the sub-assembly flux calculation (3), and this process repeats itself (4 and 4') with eventually updating of fission and slowing-down sources (needed for FBR applications). By using ad-hoc leakage and homogenization/condensation models we get self-shielded, condensed and homogenized (5) cross sections which are stored in a Multi-Parametric Output library (MPO). Finally, we use the different MPOs (processed for each kind of sub-assembly) to launch the core calculation with appropriate flux solver (6).

b. SFR Calculation Scheme and its Approximations

Even though APOLLO3[®] is designed to be a multi-purpose code (i.e. treat any kind of reactor), we still need to have different type of calculation schemes depending on which kind of core we are dealing with.

The Table 1 presents the reference APOLLO3[®] calculation scheme (and the corresponding functionalities) for SFR [7].

Approximations are directly linked to the functionalities of the code used to solve the Boltzmann transport Equations. For example, energy discretizations involved in self-shielding (slowing down equations) and flux calculations (Boltzmann equations) are approximations, compared to the continuous-energy TRIPOLI-4[®] calculations. Another example is the order of scattering anisotropy, since it actually comes from a Legendre Polynomials expansion of the scattering cross section. Moreover, the two step calculation (Lattice then Core), combined with the fundamental mode assumption for Lattice calculation leads to another approximation which has to be taken into account.

Table 1: APOLLO3[®] SFR Calculation Scheme

Calculation Step	Functionality	Value
Lattice Calculation (2D)	Scattering Anisotropy (1)	P1
	Fission Spectrum incident energy macrogroup (1)	4
	Energy Grid (1)	1968 Groups
	Self-shielding (2)	Sub-group method
	Flux Solver (3)	TDT-MOC (Method of Characteristics)
	Leakage Treatment (3)	B Heterogeneous
Core Calculation (3D)	Energy Grid (5)	33 Groups
	Flux Solver (5)	MINARET (S_N)

2. METHODOLOGY FOR THE ESTIMATION OF BIASES

The methodology consists in identifying approximations in the reference calculation scheme, and thanks to a relevant comparison, estimating the bias induced by each approximation. Since a complete reactor core calculation in APOLLO3[®] requires a two steps calculation, we can apply the methodology on both of those steps.

The estimation of biases in Lattice calculations won't be developed in this work, but an application of the methodology can be found in the article [8].

a. Core calculation Approximations

For core calculations, we chose to focus on three approximations: the flux solver spatial and angular discretizations, the impact of Lattice biases on core calculation and the fundamental mode assumption.

The flux solver used for SFR core calculations is **MINARET** [9], a S_N solver (i.e. the angular variable is treated with the Discrete Ordinates method). **MINARET** solves the time-independent first-order form of the Boltzmann equation using the DGFEM method (Discontinuous Galerkin Finite Element Method) to treat the space variable. The spatial mesh is triangular and unstructured – but conform – in 2D and semi-unstructured in 3D (cylindrical).

We also consider the impact of **lattice biases calculations** on core calculation. Indeed, since there are also approximations in the Lattice calculation, they can have a significant impact on core calculation results, via self-shielded condensed and homogenized cross sections (spectral effects).

Finally, we measure the impact of the **fundamental mode** assumption, and the **two step approach**. It is based on the decomposition of the neutronic flux in two parts: a microscopic flux which describes rapid variations in a sub-assembly, and a macroscopic flux corresponding to the global core flux. We then solve the Boltzmann equation with the microscopic flux on the sub-assembly, by considering an infinite lattice of identical assemblies. This assumption can be valid when we treat simple homogeneous cores with conventional designs (LWR cartesian lattices for instance), but it is less true when treating complex cores with several different assemblies and spatial heterogeneities.

b. Type of calculation required

In order to breakdown the global bias into separate approximations, we need different types of calculation. Each of those types of calculation will be associated with acronyms, for the rest of the document.

First, there is the classical **APOLLO3[®]** calculation (**AP3**). Each sub-assembly is homogeneous and associated with a MPO. This MPO is the result of a Lattice calculation (homogeneous or heterogeneous), with multigroup cross-section coming from the nuclear data libraries.

On the other side, there is the classical **TRIPOLI-4[®]** Monte Carlo calculation (**T4**). We consider the full core, where assemblies are represented according to their **APOLLO3[®]** Lattice calculation representation (if Lattice calculation representation is heterogeneous, the **TRIPOLI-4[®]** representation will be heterogeneous). The input cross-sections are continuous and come from the nuclear data libraries.

We also used the functionality of multi-group Monte Carlo calculations in **TRIPOLI-4[®]**. The **T4 XS AP3** calculation corresponds to a **TRIPOLI-4[®]** calculation with

the multi-group self-shielded condensed and homogenized cross section stored by **APOLLO3[®]** in MPOs. Sub-assemblies are homogeneous in **TRIPOLI-4[®]**, mirroring the **AP3** calculation.

We also generated multi-group cross sections with **TRIPOLI-4[®]**, thanks to this thesis work [10]. To do so, we reproduced the conditions of a Lattice calculation with **APOLLO3[®]** on **TRIPOLI-4[®]** (infinite lattice of sub-assembly, homogenization), for each core sub-assemblies. We then introduced them into an **APOLLO3[®]** calculation (**AP3 XS T4**) or another **TRIPOLI-4[®]** calculation (**T4 XS T4**). For both of those calculations, sub-assemblies are represented homogeneously.

However, in voided configurations, this cross section generation doesn't work. Indeed, the homogenization is based on the flux-volume technique, and the volume calculation is performed with a **collision estimator**. Now, in voided regions, there are few collisions, hence flux and volume estimation is impossible, and so are the generated cross sections. Current developments aim at getting around (using a fictitious isotope instead of the vacuum to estimate neutron flux) or fixing the problem (using a track estimator instead of a collision one in transport and collision algorithms).

c. Estimation of separate biases

The combination of the presented types of calculation will enable us to estimate the bias for each approximation in **APOLLO3[®]** core calculation.

To evaluate the impact of the flux solver, a comparison of calculations with identical self-shielded cross sections is required. Thus, two comparisons are possible and have to give similar results: **AP3** vs. **T4 XS AP3** calculations since they have the MPOs' cross sections in common; and **AP3 XS T4** vs. **T4 XS T4** calculations since they have common **TRIPOLI-4[®]** multi-group cross sections. However, the calculations need to be performed with a P0 order of anisotropy, because the treatments of transfer cross sections for order higher than 0 is different between **APOLLO3[®]** and **TRIPOLI-4[®]**. An anisotropy correction bias¹ needs to be taken into account.

On the other hand, to evaluate the impact of sub-assemblies approximations, a comparison with identical flux solvers is required, since the effect only affects MPOs. Two comparisons are also possible and have to give similar results: **AP3** vs. **AP3 XS T4** since they have the **MINARET** solver in common; **T4 XS AP3** vs. **T4 XS T4** calculations since they use the same Monte Carlo method.

Finally, to evaluate the impact of the two step calculation, we have to compare a one step calculation and a two step calculation with the same cross sections and the

¹ This correction corresponds to the difference between the **MINARET** bias (comparison at P0 order) and a similar comparison except that the anisotropy order is P1.

same solvers. Since it is not possible on APOLLO3[®], the only option is *T4 XS T4* vs. *T4*.

The output parameters we will be interested in measuring biases are the reactivity ($\Delta\rho$), the void effect ($\Delta\rho_{void}$) and the control rod worth ($\Delta\rho_{rod}$).

The **Table 2** sums up the methodology for reactivity effects.

Table 2: Approximations, comparisons and notations

Global Bias	AP3 vs. T4	$\Delta\rho$
Flux Solver	AP3 P0 vs. T4 XS AP3 P0	$(\Delta\rho_{MINARET})^{AP3}$
	AP3 XS T4 P0 vs. T4 XS T4 P0	$(\Delta\rho_{MINARET})^{T4}$
Anisotropy Correction	<i>Cf. footnote 1</i>	$(\Delta\rho_{aniso})^{AP3}$ or $(\Delta\rho_{aniso})^{T4}$
Lattice approximations	AP3 vs. AP3 XS T4	$(\Delta\rho_{lattice})^{AP3}$
	T4 XS AP3 vs. T4 XS T4	$(\Delta\rho_{lattice})^{T4}$
Fundamental mode	T4 XS T4 vs. T4	$\Delta\rho_{FM}$

Biases need to respond to the following obligations to be considered valid.

$$\begin{cases} \Delta\rho_{MINARET} = (\Delta\rho_{MINARET})^{AP3} = (\Delta\rho_{MINARET})^{T4} \\ \Delta\rho_{lattice} = (\Delta\rho_{lattice})^{AP3} = (\Delta\rho_{lattice})^{T4} \\ \Delta\rho = \Delta\rho_{MINARET} + \Delta\rho_{lattice} + \Delta\rho_{FM} + \Delta\rho_{aniso} \end{cases} \quad (1)$$

3. RESULTS

In this part, we will show the results of bias decomposition for the Low Void effect core (CFV), in Nominal, Rod inserted and Voided configurations. We will also demonstrate how this method can lead to an improvement of the calculation scheme, especially while taking into account the neutron leakage.

Table 3: Verification of the bias decomposition for CFV core in Nominal configuration. The left part corresponds to the biases labeled AP3, the right part to the biases labeled T4.

Global Bias	$\Delta\rho$ (pcm)	+ 140	
MINARET	$\Delta\rho_{MINARET}$ (pcm)	+ 84	+ 83
<i>Anisotropy Correction</i>	$\Delta\rho_{aniso}$ (pcm)	+ 125	+ 119
Lattice Approximations	$\Delta\rho_{lattice}$ (pcm)	- 604	- 594
Fundamental Mode	$\Delta\rho_{FM}$ (pcm)	+ 534	

The combination of the different biases corresponds to the global bias, and each AP3 biases are close to its T4 counterpart, hence the equation (1) is verified.

The global bias is satisfying, but it results from bias compensations. We notice that the MINARET solver has an

In all this part, the uncertainty on the results comes from TRIPOLI-4[®] statistical uncertainties, which is around 6 pcm.

a. The ASTRID core

In the framework of the IVth generation forum, many core designs were developed, in order to enhance safety and keep an equivalent level of performance, compared to reactor cores like Phénix and Superphénix. The SFRv2b core [11] was the result of many optimizations, especially on pins and assemblies. This core has a lower void effect worth, yet still positive.

The CFV concept (low voided effect core) has been selected [12]. The CFV core combines various types of solutions, individually favorable to the sodium void effect reduction compared to the SFRv2b core. The main feature is the appearance of a sodium plenum on top of the fissile zone of the core.

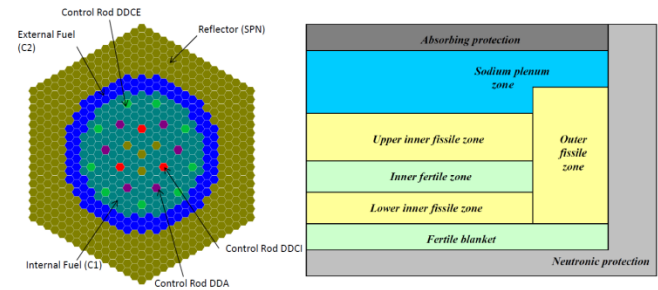


Fig. 2: ASTRID Low Void effect core design

b. Bias decomposition without Leakage

First, we need to check that the equation (1) is respected in the global bias decomposition. To do so, we apply it to the CFV core in Nominal configuration. The results are presented in the **Table 3**.

important impact on the reactivity bias, which comes from the solver options (quadrature order, spatial mesh ...). Moreover, we also observe compensation between Lattice approximations and Fundamental mode biases.

Table 4: Bias decomposition of reactivity and reactivity effects for CFV core in different configuration. No leakage model is considered.

	Nominal	Rod inserted	Voided	Control rod worth	Void effect
Global Bias	+ 140	+ 218	+ 317	+ 78	+ 176
MINARET	+ 84	+ 93	+ 121	+ 9	+ 37
<i>Anisotropy Correction</i>	+ 125	+ 142	+ 166	+ 20	+ 40
Lattice + FM	- 70	- 17	+ 30	+ 49	+ 99
Lattice Approximations	- 604	- 714		- 114	
Fundamental Mode	+ 534	+ 697		+ 163	

Once the method is verified, we apply it to the CFV core on different configuration, to measure the impact of approximations on reactivity and reactivity effects. The **Table 4** summarizes the results.

The global biases are not satisfying, and need to be improved, compared to the targeted accuracy (200 pcm, nuclear data included). As remarked previously, the MINARET solver has a large impact on global biases on reactivity, but a lesser impact on reactivity effect biases. The combined Lattice approximations and Fundamental mode bias has a low impact on global biases, but it hides major compensations. When considered individually, the biases are very important.

The Lattice approximations bias comes from the different biases measured for each sub-assembly in Lattice calculations. A way of decreasing this value would be to improve the lattice calculation scheme.

The Fundamental mode bias mainly describes modeling errors; it translates the difference between lattice calculation representation and core representation. For example, in the current reference calculation scheme, axial fertile blankets are calculated with the cluster representation: the fertile sub-assembly is radially surrounded by fissile sub-assemblies, and axially infinite. However, in the core calculation, axial fertile blanket are placed at the bottom and at the top of the fissile zone. The Fundamental mode bias can be decreased by improving the representation of sub-critical zones.

c. Improving the sub-critical zones' representation

We need to identify zones where a new representation is needed. To do so, we use the new angular flux moments weighting [13] implemented in APOLLO3[®]. This method improves the treatment of exchanges between assemblies of different types, hence it can be used on clusters.

To measure the impact of angular flux moments on core calculation for one sub-assembly, we perform a core calculation in which this sub-assembly's cross section have been collapsed with the moments, and where other sub-assembly's cross sections are collapsed by the flux. We then

compare the measured reactivity with the one obtained with the reference calculation scheme (all sub-assembly's cross section collapsed with the flux). We proceed like this for each sub-assembly.

Table 5: Impact of each sub-critical sub-assembly's representation on reactivity for the CFV core in the Nominal configuration.

Zone	Impact (pcm)
Lower Fertile Blanket	- 201
Inner Fertile	- 60
Sodium Plenum	+ 98
Neutronic protection	- 16
Absorbing Protection	- 38
Control rod	- 18
Control rod follower	+ 32
Radial Reflector	- 1396

The **Table 5** shows that 3 regions aren't well represented: the lower fertile blanket, the sodium plenum and the radial reflector. The lower fertile blanket and the sodium plenum both are within fissile assemblies, below and above fissile regions which means the radial cluster representation is wrong. A way to improve those representations would be to use the MOC-3D [14], to represent exactly the whole fissile assembly, and collapse sub-critical sub-assembly's cross section on the pattern. However, this type of calculation has a high cost of time and memory.

In the radial reflector, the main phenomenon happening is the neutron's slowing-down. Yet, in the lattice calculation, this phenomenon isn't well represented with the cluster modeling. To fix this, in the lattice calculation, the reflector layers have to be explicit, and cross section can be calculated for each reflector layer, to accurately represent the decreasing of the neutron flux. The chosen modeling is presented in **Fig. 3**, and the new results for core calculations are summarized in **Table 6**.

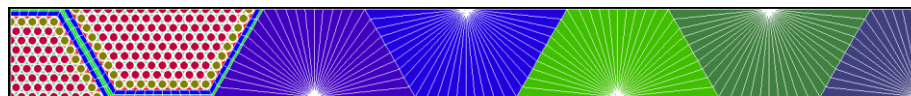


Fig. 3: New radial reflector modeling for lattice calculation. Each reflector sub-assembly is divided into sixty regions. There are reflections on $-X$, $-Y$ and $+Y$ sides of the pattern.

Table 6: New bias decomposition with the new radial reflector modeling for the CFV core.

	Nominal	Rod inserted	Voided	Control rod worth	Void effect
Global Bias	+ 62	+ 118	+ 224	+ 56	+ 162
MINARET	+ 87	+ 89	+ 108	+ 3	+ 21
<i>Anisotropy Correction</i>	+ 122	+ 142	+ 175	+ 20	+ 53
Lattice + FM	- 147	- 113	- 59	+ 34	+ 88
Lattice Approximations	- 637	- 765		- 128	
Fundamental Mode	+ 490	+ 652		+ 161	

Thanks to the new modeling of the radial reflector, the global biases are significantly improved on all reactivity values by ~ -90 pcm compared to the ones of **Table 4**, but only slightly improved for reactivity effects (~ -15 pcm). The new modeling impacts both lattice approximations and Fundamental mode effects (MINARET biases are unchanged), as the bias resulting from the combination of the two increases.

The fundamental mode bias decreases of approximately 45 pcm, because the new representation is more consistent with the core situation than the cluster modeling. At the same time, the lattice approximations bias increases of about 45 pcm, because of the new lattice calculation bias. Indeed, with the former modeling, the bias against TRIPOLI-4[®] was of -6 pcm, but with the new modeling, a new TRIPOLI-4[®] lattice calculation has been performed, and the new bias was of -1191 pcm.

Table 7: Impact of leakage treatment on bias decomposition for the CFV core.

	Nominal	Rod inserted	Voided	Control rod worth	Void effect
Global Bias	+ 75	+ 87	+ 143	+ 13	+ 69
MINARET	+ 87	+ 89	+ 108	+ 3	+ 21
<i>Anisotropy Correction</i>	+ 126	+ 152	+ 177	+ 25	+ 51
Lattice + FM	- 138	- 154	- 141	- 15	- 3

Neutron leakage has a little impact on reactivity bias in nominal configuration. However, we observe a reactivity improvement in rod inserted and voided configurations above all. In voided configuration, the sodium plenum is voided entirely; hence the neutron leakage is important. That accuracy gain is also reflected in reactivity effects, leading to very satisfying results.

As expected, the MINARET bias is unchanged, since all neutron leakage treatment impact is measured on the fundamental mode bias. We can assume that this bias decreases since the lattice + FM bias decreases. Further

d. Impact of leakage treatment on bias decomposition

In order to improve results, we use the B Heterogeneous model to simulate leakage in fissile sub-assemblies. We will also use angular flux moments collapsing on those sub-assemblies, as a result of [13]. This modification should have an impact on fundamental mode bias, because the spectrum in fissile sub-assemblies will be more consistent with the one in core situation. However, we won't be able to measure this impact because we can't discriminate lattice approximations and fundamental mode biases when using a leakage model, due to the lack of critical buckling research in TRIPOLI-4[®], which means we can't generate TRIPOLI-4[®] cross sections consistent with the one of APOLLO3[®] (no $T4$ XS $T4$ calculation).

investigations need to be lead in order to validate this assumption.

CONCLUSION

In this paper, we presented a new methodology enabling us to estimate biases for each approximations independently. This new methodology is set to be applied on the new French deterministic neutron transport code APOLLO3[®], and be a part of its advanced V&V process.

The first step of the method is the identification of approximations of the different solvers. Within the

APOLLO3[®] reference calculation scheme we chose, we identify the different solvers being used and the way they are operating to reach the most accurate result.

The next step is to measure the impact of the different approximations on core characteristics. Since APOLLO3[®] has a two-step calculation scheme, there are two kinds of approximations: sub-assembly approximations, which have an indirect impact on the final result; and core approximations, which have a direct impact.

To estimate the bias brought by each approximation, we need new types of calculations, since we can't achieve that goal only with classic APOLLO3[®] and TRIPOLI-4[®] calculations. The main feature of this article is to propose a method involving TRIPOLI-4[®] multi-group calculation, either by giving it MPOs' cross sections or making it generate its own multi-group cross sections.

The methodology was applied on the ASTRID CFV core and gave good results. It also permitted us to upgrade the calculation scheme, as a new radial reflector modeling has been developed. This new representation plus the adding of neutron leakage treatment gave us satisfying results for core calculations, with a great improvement of voided configurations calculations.

Further work is still to be done. First, new developments have to be made in TRIPOLI-4[®] in order to improve cross section generation in voided configuration (homogenization in space and collapsing in energy with angular moments of the flux), and also add a critical buckling search to have lattice calculations consistent with APOLLO3[®] B homogeneous and heterogeneous models. Finally, we could apply this methodology on thermal reactors, since APOLLO3[®] is a multi-purpose code and that nothing in the methodology is exclusive to SFR.

ACKNOWLEDGMENTS

APOLLO3[®] and TRIPOLI-4[®] are registered trademark of CEA. We gratefully acknowledge CEA, AREVA and EDF for their long term partnership and their support. The first author would like to thank the APOLLO3[®] development team for their efforts in implementing the models described here.

NOMENCLATURES

MPO = Multi-Parametric Output;
AP3 = Classic APOLLO3[®] calculation;
T4 = Classic TRIPOLI-4[®] calculation;
T4 XS AP3 = Multi-group TRIPOLI-4[®] calculation, with MPOs' cross sections;
AP3 XS T4 = APOLLO3[®] calculation with TRIPOLI-4[®] sub-assembly cross sections;
T4 XS T4 = TRIPOLI-4[®] calculation with TRIPOLI-4[®] multi-group sub-assembly cross sections;
ASTRID = Advanced Sodium Technological Reactor for Industrial Demonstration.

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