Beta effective sensitivity to nuclear data within the APOLLO3® neutronic platform

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ABSTRACT

In this paper, we present a sensitivity analysis of the beta effective to nuclear data for the UM17x17 experiment that has been performed in the EOLE reactor. This work is carried out using the APOLLO3® platform. Regarding the flux calculation, the standard two-step approach (lattice/core) is used. For what concerns the delayed nuclear data, they are processed to be directly used in the core calculation without going through the lattice one. We use the JEFF-3.1.1 nuclear data library for cross-sections and delayed data. The calculation of k-effective and beta effective is validated against a TRIPOLI4® one while the main sensitivities are validated against direct calculation. Finally, uncertainty propagation is performed using the COMAC-V2.0 covariance library.

KEYWORDS: beta effective, perturbation, sensitivity

1. INTRODUCTION

Beta effective is a key parameter that has important implication is the safety domain. To properly compute the beta-effective, we need advanced modeling tools and accurate nuclear data. To this end, we developed within the APOLLO3® platform [1] the possibility to compute the beta effective using delayed nuclear data directly coming from libraries such as JEFF-3.1.1. To test the robustness of such calculations, we implemented also the possibility to compute the sensitivity of the beta effective to nuclear data. In section 2 we recall the formalism and the analytical background to reach this purpose. We also comment on the implementation and the main issues faced during the development. In section 3 we briefly describe a challenging case that we selected to test our implementation. In section 4 we give a few elements about the validation of the implemented methods while in section 5 we present the results of the beta effective sensitivity and uncertainty analysis, giving some physical justification.

2. PERTURBATION THEORY

Perturbation theory in reactor physics, and in particular in transport theory has been introduced by Usachev [2] and Gandini [3] and further studied by Greenspan [4] and Komata [5] among others. The most popular use of perturbation theory is to compute the sensitivity of the k-effective to nuclear data, this is what is usually referred to as standard perturbation theory (SPT). SPT requires to compute the adjoint flux in addition to the forward flux. For more advanced studies one can focus on the sensitivity of linear (i.e. depending only on the flux) or bilinear (i.e. depending on both the forward and adjoint flux) ratios to nuclear data, this is referred to as generalized perturbation theory (GPT). GPT requires to compute importances in addition to the adjoint and direct flux. While extensive description of the method is beyond the purpose of this paper, we present here the equations to solve in order to obtain these importances and how to use them to compute sensitivities.

2.1. Mathematical Description and Formalism

For simplicity, we limit our discussion to the case of the critical calculation, therefore the problem we are going to solve is the following:

$$\left(\mathcal{A} - \frac{\mathcal{F}}{k}\right)\phi = 0 \tag{1}$$

where $\mathcal{F}$ is the fission production operator, $\mathcal{A}$ is the operator containing all the remaining terms (transport, scattering, and removal), k is the k-effective allowing a constant sign solution and ϕ is the flux. The equation for adjoint flux can be obtained from eq. (1) replacing operators with the adjoint ones.

Once we define a quantity B we can compute the importances ψ (forward) and $\psi*$ (adjoint) to B as:

$$\left(\mathcal{A} - \frac{\mathcal{F}}{k}\right)\psi = \frac{\partial B}{\partial \phi^*} \qquad \text{and} \qquad \left(\mathcal{A}^* - \frac{\mathcal{F}^*}{k}\right)\psi^* = \frac{\partial B}{\partial \phi} \tag{2}$$

where the superscript $*$ is used for the adjoint operator and fluxes and k is the k-effective obtained from the critical problem. It is worth noticing that the following relations must be satisfied

$$\left\langle \frac{\partial B}{\partial \phi}, \phi \right\rangle = 0 \qquad \text{and} \qquad \left\langle \frac{\partial B}{\partial \phi^*}, \phi^* \right\rangle = 0 \tag{3}$$

where $\langle , \rangle$ is the scalar product between the two functions that implies the integration over the whole phase space. Notice also that the solution is not unique, we can indeed add any term proportional to the forward and the adjoint flux respectively.

If we impose that

$$\langle \psi^*, \mathcal{F}\phi \rangle = 0 \qquad \text{and} \qquad \langle \phi^*, \mathcal{F}\psi \rangle = 0 \tag{4}$$

we fix the solution and we can then compute the sensitivity of the quantity under exam as follows [3,4]:

$$\frac{dB}{d\sigma} = \frac{\partial B}{\partial \sigma} - \left\langle \psi^*, \frac{\partial\left(\mathcal{A} - \frac{\mathcal{F}}{k}\right)}{\partial \sigma}\phi \right\rangle - \left\langle \phi^*, \frac{\partial\left(\mathcal{A} - \frac{\mathcal{F}}{k}\right)}{\partial \sigma}\psi \right\rangle \tag{5}$$

In the case B is a linear ratio (e.g. ratio of reaction rates) the first equation in (2) and the second in (4) show that ψ can be taken equal to 0 so that the last term on the right-hand side of eq (5) vanishes, therefore we obtain a simpler system. In the case B is a bilinear ratio as for the beta effective we have to compute both importances leading to a more demanding task. From now on, the quantity of interest of this paper is the beta effective, β, defined as follows:

$$\beta = \frac{\langle \phi^*, \mathcal{F}_d \phi \rangle}{\langle \phi^*, \mathcal{F} \phi \rangle} \tag{6}$$

where the subscript d refers to the delayed fraction.

2.2. Implementation

The GPT was already implemented in APOLLO3® for the linear ratio case [6]. For this work, we have extended the capabilities of the *PerturbationEngine* class [6] to compute direct importances and to deal with delayed nuclear data to compute beta-effective and its sensitivity. As already mentioned to compute direct importances a specific solution has to be selected (4) in order to have the compact formulation for the sensitivities (5). In practice, since we look for the solution by mean of power iteration, the condition (4) has to be imposed at each iteration to avoid instabilities, this is usually referred to as filtering. The previous implementation, that allowed filtering only adjoint importances, has been extended to include the direct ones. Even though the filtering process does not guarantee convergence, in all the cases studied, for this paper or not, we have a proper behavior.

To compute the beta effective, delayed spectrum (χ_d), delayed neutron multiplicity ν_d and precursor families abundances have to be provided to the *PerturbationEngine*. Since the flux and importances calculations are done with ν_{tot} and total fission spectrum, delayed data do not need to be provided to the solver for the operator construction but just to the *PerturbationEngine* to compute sources and integrals. Currently, it is still not possible to feed the core side of APOLLO3® with delayed nuclear data by isotope processed by a lattice calculation, therefore, a simplified approach has been implemented.

Due to the precursor model adopted in JEFF-3.1.1, delayed spectra and decay constants are independent of the fissioning system [7], therefore they can be simply collapsed on the energy mesh we are interested in. The ν_D and abundances present just a weak dependence from the energy of the incoming neutron [7], so this dependence can be either neglected, that is collapsed with a flat flux, or taken into account using a representative flux as done for the preprocessing of the nuclear data at the lattice step. In the present work, we used as a representative flux the one equivalent to the iwt=4 option in the GROUPR module of NJOY with thermal temperature of 0.0253 eV, thermal cutoff of 0.1 eV, $1/E$ dependence for the transition zone, 1.32 MeV as cutoff for the transition zone and a fission temperature of 1.29 MeV.

3. Epicure UM17x17 MODELING

Epicure UM17x17 is an experimental program held in the EOLE facility at CEA Cadarache in the 90s [8]. The Epicure UM17x17 configuration is composed of a central 17x17 MOX-7% assembly surrounded by 3.7% U-235 enriched UO2 assemblies, with a lattice pitch of 1.26 cm. We have selected this system because of its geometry composed of 289 MOX fuel pins and 1351 UOX fuel pins, thus presenting an unusual beta-effective. To model this reactor we proceed with the two-step approach. On the lattice side, we model a 2D section representing cells, cladding, moderator and air without modeling the vessel Figure 1a. We use the JEFF-3.1.1 nuclear data library and

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we perform a 281 energy groups calculation, using the IDT solver from APOLLO3 [9]. Cross-sections are homogenized for the core-level calculation according to the geometry in Figure 1b and condensed from 281 to 26 energy groups.

(a) pin by pin **(b) homogenized**

Figure 1: IDT 2D geometries modeling

On the core side we use the homogenized 2D geometry (Figure 2). Fluxes and importances calculations are done with the MINARET Sn solver from APOLLO3 [10]. MINARET is a discontinuous Galerkin finite element solver. For the calculation, we use 25388 triangular meshes and 26 energy groups and the anisotropy on fluxes and nuclear data are considered up to the first order of the Legendre polynomials. With these options, the calculation for the core step takes about 20 minutes on 32 cores and 4 GB of RAM.

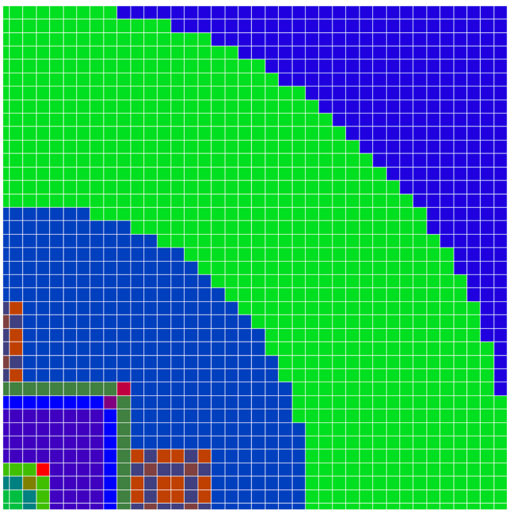

Figure 2: MINARET 2D geometry

4. VALIDATION

The calculations are validated against a TRIPOLI4® one [11], done on the same configuration. IDT obtains a Keff of 1.04678 while TRIPOLI4® has a Keff of 1.048557 ($\pm$ 2.2 pcm); with MINARET we have 1.04712. The beta effective is computed with TRIPOLI4® by means of IFP [12] and the result is (648.6 $\pm$ 0.8) pcm. With MINARET we obtain a beta of 647.1 pcm if we use delayed data preprocessed with a test flux while we get 640.7 pcm if we use a flat flux. Notice that this discrepancy reduces when we increase the number of groups, indeed with 281 energy groups the values with the weighting flux or with a flat one are respectively 648.7 pcm and 648.5 pcm.

The calculation of sensitivities is validated against direct calculations made by changing some input data. In order to do so, we increase by 1% the capture cross-section of the ^{238}U between 34 and 76 meV and between 4 eV and 52 eV and for the ^{235}U between 34 and 76 meV. For the ^{235}U, we perturb also the fission cross-section between 10 and 34 meV and the ν_D between 34 and 76 meV. In all these cases the relative error between the predicted effect on the beta effective and the obtained perturbation is below 1%. To test the robustness of our implementation, we studied also a simplified model of a fast reactor with 6 energy groups. We checked the contribution by energy group and we tested capture, elastic, inelastic scattering and delayed data of ^{238}U, elastic scattering of ^{16}O, fission cross-section and delayed data of ^{235}U and in all the cases we find deviation from the predicted behavior to be within 1%.

5. RESULTS

In the next two sessions, we list the results we obtained for what concerns sensitivities and uncertainty propagation on the beta effective. The results are summarized in two tables and we present only the results for the isotopes contributing to more than 1.0 e-4 to the total uncertainty on the beta effective.

5.1. Sensitivities

For what concern sensitivities, the main conclusion is that direct effects are the dominant contributors as can be seen in Table 1. As we can see all ν_{tot} have a negative impact on the beta (increasing the denominator) while the ν_{D} has a positive impact (being at the numerator). For the present study we take the ν_{tot} and the ν_{D} as being independent one from each other and therefore neglected the (small) effect of an increase of the ν_{D} on the ν_{tot}.

We can notice that the main isotopes contributing to the sensitivity of the beta effective are the ^{235}U with a positive effect through the fission cross-section and the ^{239}Pu with a negative sensitivity on the fission cross-section. This can be explained by the fact that in a mixed UOX-MOX system the beta is a weighted average of the beta of the main fissioning isotopes and since the beta of the ^{235}U is more than three times larger of the one of the ^{239}Pu, we have that increasing the relative fission rate of the U has a positive effect on the beta. Among the indirect effects, we can observe non-negligible effects from the capture of the most present isotopes as ^{1}H, ^{16}O, U and Pu, the elastic scattering of the ^{1}H and ^{16}O and the inelastic scattering of the ^{238}U. However, all these indirect contributions are at most of the order of 10^{-2} %/% and one order of magnitude smaller than the direct ones. Regarding the elastic and inelastic scattering, all the effects are negative. By looking at the energy distribution of sensitivity we can see that the main contribution comes from the energy groups above 1 MeV. Above this energy indeed we have the contribution to the beta effective from the fissions of the ^{238}U that has a beta two times larger than the one of the ^{235}U and that therefore, at these energies, is the main contributor to the beta. This explains why increasing the scattering and therefore increasing the thermalization of the neutrons has a negative impact on the beta. The sensitivities to the spectrum, total and delayed, are not listed in the table (1) since their total value (the one obtained summing over all the energy range) is the same as the total value of the ν [as implied by Eq. (5)] and therefore can be read from there, however it has a different energy distribution that has been used for the uncertainty calculation.

Table 1: Sensitivities (in %/%) of beta effective for the Epicure UM17x17 experiment.

Isotope	Capture	Elastic	Inelastic	NXN	Fission	ν_{tot}	ν_{D}
^{1}H	-1.46 e-2	-8.51 e-2	-	-	-	-	-
^{16}O	2.30 e-3	-2.40 e-2	-3.38 e-4	-2.35 e-6	-	-	-
^{90}Zr	1.25 e-4	-2.62 e-3	-3.13 e-3	-3.93 e-6	-	-	-
^{91}Zr	-2.07 e-4	-5.23 e-4	-9.65 e-4	-1.80 e-5	-	-	-
^{92}Zr	6.04 e-6	-7.20 e-4	-1.69 e-3	-2.03 e-5	-	-	-
^{94}Zr	4.72 e-5	-7.16 e-4	-1.76 e-3	-3.36 e-5	-	-	-
^{235}U	-3.31 e-2	-1.41 e-4	-5.56 e-4	-3.07 e-5	**1.07 e-1**	**-4.39 e-1**	**7.06 e-1**
^{238}U	-2.94 e-3	-5.78 e-3	-3.29 e-2	-1.73 e-3	6.47 e-2	**-1.30 e-1**	**1.74 e-1**
^{239}Pu	6.46 e-2	-4.76 e-5	-2.21 e-4	-1.09 e-5	**-1.51 e-1**	**-3.58 e-1**	8.24 e-2
^{240}Pu	4.48 e-2	-1.91 e-5	-1.16 e-4	-3.20 e-6	-3.25 e-3	-5.25 e-3	1.02 e-3
^{241}Pu	6.94 e-3	-5.95 e-6	-3.17 e-5	-6.48 e-6	-8.40 e-3	-6.33 e-2	3.48 e-2
^{242}Pu	5.08 e-3	-8.94 e-6	-3.16 e-5	-1.53 e-6	-4.18 e-4	-9.49 e-4	3.61 e-4
^{241}Am	1.09 e-2	-2.18 e-6	-1.72 e-5	-1.75 e-7	-6.81 e-4	-9.60 e-4	8.93 e-5

5.2. Uncertainty

Uncertainty on the beta effective is computed using the so called sandwich formula (7) and using the COMAC-V2.0 covariance library [13]:

$$U = \sqrt{{}^{t}S_{\beta eff} \cdot D \cdot S_{\beta eff}} \tag{7}$$

where $S_{\beta eff}$ is the sensitivity to the beta effective, D is the covariance matrix and ^{t} means transpose.

The results show what already anticipated from the sensitivities: that the indirect contributions are negligible with respect to the direct ones. In particular, the ν_{D} having an higher uncertainty with respect to the ν_{tot}, is the main source of uncertainty (97.5% of the global variance, with a major contribution from ^{235}U: 87% of the global variance).

Table 2: Uncertainty propagation (in %) of beta effective for the Epicure UM17x17 experiment. Negative values stand for imaginary values, negative contribution to the overall variance.

Isotope	Capture	Elastic	Inelastic	NXN	Fission	ν_{tot}	ν_D	χ	TOTAL
^{1}H	0.04	0.14	0.00	0.00	-	-	-	-	0.15
^{16}O	0.05	0.08	0.00	0.00	-	-	-	-	0.10
^{90}Zr	0.00	0.01	0.02	0.00	-	-	-	-	0.02
^{91}Zr	0.00	0.00	0.01	0.00	-	-	-	-	0.01
^{92}Zr	0.00	0.01	0.01	0.00	-	-	-	-	0.01
^{94}Zr	0.00	0.01	0.01	0.00	-	-	-	-	0.01
^{235}U	0.04	0.00	0.00	0.00	0.04	-0.07	**2.23**	0.11	**2.23**
^{238}U	0.01	0.00	0.15	0.04	0.02	0.04	0.57	0.04	0.60
^{239}Pu	0.10	0.00	0.00	0.00	0.13	-0.04	0.50	0.16	0.55
^{240}Pu	0.07	0.00	0.00	0.00	0.02	0.00	0.00	0.00	0.08
^{241}Pu	0.02	0.00	0.00	0.00	0.01	0.03	0.17	0.10	0.20
^{242}Pu	0.06	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.06
^{241}Am	0.03	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.03
TOTAL	0.16	0.16	0.16	0.04	0.14	-0.06	**2.36**	0.22	**2.39**

Among the indirect contributions, elastic scattering of the ^{1}H and inelastic scattering of the ^{238}U are the main contributors. Unfortunately, covariance matrices for the delayed spectrum are not available at this moment and therefore are neglected. This is probably an important source of underestimation since the sensitivities to the delayed spectrum are of the same order of the ones to the ν_D and delayed spectra are poorly known [14]. We can indeed expect that their inclusion in uncertainty calculation can lead to a non-negligible increase of the total uncertainty computed in this work.

6. CONCLUSIONS

In this paper, we demonstrate the possibility to accurately compute the delayed beta and its sensitivity to nuclear data. The latter shows very small dependence from indirect effects but confirms all the expected trends. For what concerns uncertainty, the dominant contribution comes from the ν_D and in particularly from the ν_D of the ^{235}U. However the lack of covariance matrices for the delayed spectrum is a major limitation for a complete assessment of the real uncertainty. Moreover, since the total sensitivity to the delayed spectrum is equal to the one to ν_D and delayed spectra are poorly know, this could be a comparable additional source of uncertainty that would have to be taken into account when covariance matrices for these type of data will be available.

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