Determination of β_{eff} using MCNP-4C2 and application to the CROCUS and PROTEUS reactors

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Abstract

A new Monte Carlo method for the determination of β_{eff} has been recently developed and tested using appropriate models of the experimental reactors CROCUS and PROTEUS. The current paper describes the applied methodology and highlights the resulting improvements compared to the simplest MCNP approach, i.e. the "prompt method" technique. In addition, the flexibility advantages of the developed method are presented. Specifically, the possibility to obtain the effective delayed neutron fraction β_{eff} per delayed neutron group, per fissioning nuclide and per reactor region is illustrated. Finally, the MCNP predictions of β_{eff} are compared to the results of deterministic calculations.

KEYWORDS: β_{eff} determination, MCNP, CROCUS, PROTEUS

1. Introduction

The determination of the delayed neutron fraction β_{eff} using a Monte Carlo code is considered a difficult matter. The accurate prediction of the direct and adjoint neutron fluxes by stochastic methods is rendered problematic by the use of approximate techniques, which can sometimes be inadequate. For example, the easiest way to determine β_{eff} with a Monte Carlo method is based on *k*-eigenvalue predictions with and without accounting for delayed neutrons, some approximations on the flux shape being necessary. This simple technique, called the "prompt method", has the advantage to be usable without specific programming developments. However, the results appear unsatisfactory in many cases [1].

In this context, much effort has been devoted to develop new and more suitable methods for the determination of β_{eff} [2]. More recently, new improvements have been achieved using the Monte Carlo code MCNP-4C2 [3]. One method consists of making several changes directly in the part of the code source files that treats the transport of particles ("Nuclear Research and Consultancy Group (NRG) approach" [1,4]). The current approach is associated with the development of new appropriate subroutines, the theoretical basis being very similar. The NRG method does not slow down the particle transport and has to be considered as the implementation of a new MCNP-4C2 intrinsic feature. The present method is more complex to use (two calculations are needed and the user has to provide different information), but it permits a higher flexibility without having to modify the source code.

The current paper presents the methodology developed and describes its application to standard configurations of the experimental reactors CROCUS and PROTEUS (LWR-PROTEUS I-1A [5]). Comparisons with MCNP-4C2 "prompt method" predictions and with deterministic calculations are also given.

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2. Theoretical approach

2.1 General background

The exact definition of β_{eff} is given by the following equation:

$$\beta_{eff,l} = \frac{\int \varphi^*(\vec{r},E',\Omega') \sum_j \chi^d_{l,j}(E') \nu^d_{l,j}(E) \Sigma_{f,j}(\vec{r},E,\Omega) \varphi(\vec{r},E,\Omega)\, dE\, dE'\, d\vec{r}\, d\Omega}{\int \varphi^*(\vec{r},E',\Omega') \sum_j \chi_j(E') \nu_j(E) \Sigma_{f,j}(\vec{r},E,\Omega) \varphi(\vec{r},E,\Omega)\, dE\, dE'\, d\vec{r}\, d\Omega} \quad (1)$$

where:
l and j indicate the precursor group and the fissile isotope respectively,
$\varphi^*(\vec{r},E',\Omega')$ and $\varphi(\vec{r},E,\Omega)$ are respectively the adjoint and direct flux,
$\chi^d_{l,j}(E')$ is the delayed neutron spectrum,
$\nu^d_{l,j}(E)$ is the average number of delayed neutrons resulting from a fission,
$\chi_j(E')$ is the total neutron spectrum,
$\nu_{l,j}(E)$ is the average number of neutrons (prompt and delay) resulting from a fission and
$\Sigma_{f,j}(\vec{r},E,\Omega)$ is the macroscopic fission cross-section.

For simplification purposes, Equation (1) can also be expressed in a slightly condensed form considering only one precursor group and one fissioning isotope:

$$\beta_{eff} = \frac{\int \varphi^*(\vec{r},E',\Omega') \chi^d(E') \nu^d(E) \Sigma_f(\vec{r},E,\Omega) \varphi(\vec{r},E,\Omega)\, dE\, d\Omega\, dE'\, d\vec{r}\, d\Omega'}{\int \varphi^*(\vec{r},E',\Omega') \chi(E') \nu(E) \Sigma_f(\vec{r},E,\Omega) \varphi(\vec{r},E,\Omega)\, dE\, d\Omega\, dE'\, d\vec{r}\, d\Omega'} = \frac{P^d_{eff}}{P_{eff}} \quad (2)$$

where:
P_{eff}, the denominator, is the so-called spectrum and adjoint weighted neutron production and
P^d_{eff}, the numerator, is the corresponding quantity for delayed neutrons only.

These two terms have to be compared with P and P_d which represent the neutron production rate by fission and are the basis for the definition of the “fundamental” delayed neutron fraction β_0:

$$\beta_0 = \frac{\int \nu^d(E) \Sigma_f(\vec{r},E,\Omega) \varphi(\vec{r},E,\Omega)\, dE\, d\Omega\, d\vec{r}}{\int \nu(E) \Sigma_f(\vec{r},E,\Omega) \varphi(\vec{r},E,\Omega)\, dE\, d\Omega\, d\vec{r}} = \frac{P^d}{P} \quad (3)$$

In this context, the problem with β_0, which is easily obtained by Monte Carlo calculations, is that this quantity does not permit to assess how effective the delayed neutrons are, making difficult an accurate determination of the reactor kinetic parameters. For this purpose, β_{eff} has to be used, but the determination of this parameter is possible only by the calculation of an adjoint flux (or an adequately approximated adjoint flux) function, as occurs in Equation 2. In addition, it is worth noting that the energy spectra of the emitted neutrons ($\chi(E')$ and $\chi^d(E')$) are also necessary for the assessment of β_{eff}. This is important because the effectiveness of neutrons in inducing fission depends on the initial energy of these neutrons.

Generally speaking, the most challenging difficulty for the determination of β_{eff} by Monte Carlo techniques is to calculate a suitably approximated adjoint function. Effectively, the standard perturbation calculations performed by some deterministic codes can not be reproduced consistently by stochastic methods. However, the adjoint flux can be seen as the significance of a neutron with properties $(\vec{r}, E', \Omega')$ to produce fission [6]. Based on this interpretation, some developments have been made in order to give a definition of β_{eff} related to the so-called theory of effectiveness [4]. In this context, the key point for the determination of β_{eff} by Monte Carlo techniques is to be able to account for the fission multiplication efficiency of the delayed neutrons in function of their energy and their spatial distribution. This quantity is accessible only after some developments, either directly in the source code [4], or with the help of additional subroutines (the currently developed method, see Section 2.3). Apart from these suitable techniques, it is also worth noting that an approximated approach is possible without any changes in the MCNP code. This so-called "prompt method" is described in Section 2.2. We will see that the corresponding results are not satisfactory, justifying the current additional development effort.

2.2 "Prompt method" approach

The "prompt method" approach permits to approximate β_{eff} simply on the basis of two k-eigenvalue-calculations. More precisely, β_{eff} is defined with respect to the following equation ($\int ... dE\, d\Omega\, dE'\, d\vec{r}\, d\Omega = \langle ... \rangle$):

$$\beta_{eff} \cong 1 - \frac{\left\langle \varphi^{*} \chi^{p} \nu^{p} \Sigma_{f} \varphi \right\rangle}{\left\langle \varphi^{*} \chi \nu \Sigma_{f} \varphi \right\rangle} \cong 1 - \frac{k_{p}}{k} \tag{4}$$

where:

χ^{p} is the prompt neutron spectrum,

ν^{p} is the average number of prompt neutrons resulting from a fission,

k_p is the multiplication factor of the system without accounting for the delayed neutrons and
k is simply the multiplication factor of the system (prompt and delayed neutrons considered).

The calculation of k_p and k is straight forward with MCNP, since the *TOTNU* or *TOTNU NO* card are a standard option of a k-eigenvalue calculation. Unfortunately, Equation (4) is only an approximation of β_{eff}. Effectively, Equation (4) is deduced using the following statement:

$$\left\langle \varphi^{*} \chi \nu^{p} \Sigma_{f} \varphi \right\rangle - \left\langle \varphi^{*} (\chi^{d} - \chi) \nu^{d} \Sigma_{f} \varphi \right\rangle = \left\langle \varphi^{*} \chi^{p} \nu^{p} \Sigma_{f} \varphi \right\rangle \tag{5}$$

In addition to this approximation, the practical MCNP calculation of k_p is also not as described in Equation (4), the shapes of φ^{*} and φ being impossible to maintain identical compared to the ones used for calculating k [4]. As presented in Section 4, these approximations make this approach inadequate for an accurate determination of β_{eff} (deviations of typically 10%).

2.3 Proposed MCNP-4C2 approach

As mentioned, this method is based on the same physical interpretation of β_{eff} as that of the NRG approach [1,4]. However, the effectiveness of the delayed neutrons to produce new fissions in the system (the key point, as stated in Section 2.1) is implemented not directly by modifying the source code files, but rather via the use of two new external subroutines. This possibility stems from certain MCNP-4C2 features (definition of so-called `tallyx` and `source` subroutines). Effectively, the determination of β_{eff} is achieved in the following two calculational steps:

1. The first additional subroutine is used to store (a) the emission location of the delayed neutrons, (b) the energy of the incident neutrons and (c) the corresponding fissionable isotope. These data are collected during an MCNP-4C2 k-eigenvalue transport `kcode` calculation where both prompt and delayed neutrons are taken into account. In addition, this calculation permits to deduce the total fission rate generated in the system.
2. The data generated in Step 1 correspond to the external source for the second calculation. More precisely, this source permits the transport of the delayed neutrons only. Furthermore, the total fission rate induced by the delayed neutron in the next generation is easily accessible using the *NONU* card and by doing a fixed-source MCNP-4C2 transport (`sdef`) calculation. Of course, to make this calculation in an appropriate manner, it is important to associate a specific energy spectrum to these delayed neutrons with respect to the incident neutron energy and to the fissionable isotope. This complementary information, which is needed by MCNP-4C2, can be obtained from standard data files [7,8].

Although this “two-steps method” is not the quickest, it presents several advantages. For instance, the effective delayed neutron fraction can be easily calculated per selected energy group and per fissile isotope. In addition, it is possible to store delayed neutrons per region, thus providing the effectiveness of delayed neutrons per reactor zone. These different options are illustrated in Section 4.

3. MCNP-4C2 modelling

The MCNP-4C2 models studied are those for (a) the standard CROCUS critical configuration [9] and (b) the LWR-PROTEUS Core I-1A configuration [10, 11].

3.1 The CROCUS configuration

The CROCUS facility is a zero-power critical reactor used mainly for educational purposes at the Swiss Federal Institute of Technology (EPFL) in Lausanne. The CROCUS research reactor consists of a two-zone fuel lattice moderated by light water. More precisely, the fuel rods are arranged in square lattices, with a pitch of 1.837cm for the inner uranium oxide zone and 2.917cm for the outer metallic uranium zone. The inner core contains 336 UO_2 fuel rods enriched to 1.806 wt% ^{235}U, while the outer core comprises 176 uranium metal fuel rods with a ^{235}U enrichment of 0.947 wt%. The corresponding MCNP CROCUS model is given in Fig. 1.

3.2 The LWR-PROTEUS I-1A configuration

The PROTEUS facility in its multi-zone form, i.e. as deployed in the LWR-PROTEUS research programme, is characterized by four separate regions (the central test zone, a surrounding buffer zone, an annular D_2O-driver region, and an external graphite driver/reflector region), each of which has a specific role (see Fig. 2, the MCNP whole reactor model). For instance, the central test zone is the region of interest in which the experiments are performed. During the I-1A experiments, the central test zone was configured by 9 advanced BWR assemblies (SVEA-96+). A SVEA-96+ fuel assembly comprises 96 fuel pins arranged in four separate sub-bundles, each containing 24 pins on a square pitch around a central water canal. The ^{235}U enrichment of the UO_2 fuel pins varies between 2.3% and 4.7%, with 12 pins also containing gadolinium as burnable poison with a Gd_2O_3 concentration close to 4% (see Fig. 3).

4. Application of the method and results

First of all, the β_{eff}-values obtained by different methods for the two configurations are given in Tab. 1. In addition, the calculation by MCNP of β_0 is also given in order to highlight the difference between the two parameters. As expected, the lower ^{235}U enrichment of the CROCUS fuel compared to PROTEUS leads to a higher β_{eff}-value (larger proportion of ^{238}U). Otherwise, the results show that a good agreement is obtained between the deterministic β_{eff}-value (based on suitable perturbation calculations) and the "two-steps method" β_{eff}-value for each core, while the results given by the "prompt method" appears different and consequently not satisfactory. Obviously, the "two-steps method" needs further validation, in particular with experimental values, but these first results are very promising and justify the increased use of the technique in the future.

Next, the flexibility of the "two-steps method" is highlighted via the calculation of β_{eff} per delayed neutron energy group, per fissile isotope, and per reactor regions. This has been done for the two different configurations. Thus, Tab. 2 presents each contribution of the delayed neutron energy groups to the β_{eff}-value. For instance, the group number 5 (half-life of 2.37s) is the main contributor for the two configurations. It is also interesting to notice that even if the β_{eff}-values are significantly different for CROCUS and PROTEUS, the distribution of these values (delayed neutrons per precursor group) is very similar.

The β_{eff}-values per fissile isotope are given in Tab. 3 and compared with the total number of fissions produced by each isotope. This comparison highlights, for each core, the well-known increased emission of delayed neutrons from ^{238}U fissions compared to ^{235}U fissions (for the PROTEUS case, the ^{234}U component is negligible and corresponds to less than 0.01% of the total number of fissions). For instance, for CROCUS, ^{238}U fissions contribute only about 6.5% of the reactor power, but the ^{238}U contribution to the β_{eff}-value is as high 14.6%. Similar is the case for PROTEUS. Of course, this trend is an "expected" result, but the stochastic "two-steps method" makes feasible a quantitative, rather than just a qualitative, assessment. It is also worth mentioning that even if the fission of ^{238}U produces more delayed neutron compared to the fission of ^{235}U, the energy spectrum of the corresponding ^{238}U delayed neutrons is slightly less effective for the two configurations studied. In other words, a delayed neutron produced by ^{238}U fission has a slightly lower probability to cause another fission in the system compared to a delayed neutron born from ^{235}U fission. This type of information is directly accessible from the "two-steps method" outputs.

Finally, the β_{eff}-values per reactor region for CROCUS and PROTEUS (configuration LWR-PROTEUS I-1A) are given in Tab. 4. Following the same technique, the results obtained are compared with the total number of fissions produced by each region. Clearly, the correlation between the β_{eff}-value distribution and the distribution of fissions among the different reactor regions is much stronger than the corresponding one with respect to the fissioning isotopes (Tab. 3). Apart from that, the results of Tab. 4, i.e. the β_{eff} values per region, highlight in a clear manner the strong delayed neutron contribution of the UO_2 zone for CROCUS and of the test zone for PROTEUS.

5. Conclusions

Inspired by a recent theoretical approach of the Nuclear Research and Consultancy Group, Petten, a new subroutine has been developed for the determination of β_{eff} using the MCNP-4C2 code. This subroutine permits to store the distribution of delayed neutrons in the reactor, making accessible the determination of the total fission rate generated only by these delayed neutrons. Then, the β_{eff} is simply defined as the ratio of the total fission rate induced by the delayed neutrons over the total fission rate generated in the system.

This paper proposes a methodology that requires at least two MCNP-4C2 simulations. In addition, the flexibility of the method to provide β_{eff} per energy group, per isotope or per reactor region has also been presented. For the purpose, models of the CROCUS and PROTEUS reactors have been employed.

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Table 1: β_0 and β_{eff} for different cases in [pcm]

Models	β_0 MCNP calculation	β_{eff} "Prompt method"	β_{eff} "Two-steps method"	β_{eff} Deterministic value
CROCUS	750±3	752±5	774±3	781*
PROTEUS (I-1A)	761±3	717±5	729±3	730**

* BOXER with the determination of the adjoint and direct fluxes by a multigroup cylindrical diffusion method
** BOXER/TWODANT(R-Z)/PERT-V combined calculation

Table 2: β_{eff} per energy group for CROCUS and PROTEUS (I-1A)

Group	Half-lives (sec.)	β^i_{eff} CROCUS	β^i_{eff} PROTEUS (I-1A)
1	55.6	23 (3.0%)	21 (2.9%)
2	24.5	112 (14.5%)	106 (14.5%)
3	16.3	66 (8.5%)	60 (8.2%)
4	5.21	146 (18.9%)	137 (18.8%)
5	2.37	251 (32.4%)	237 (32.5%)
6	1.04	82 (10.6%)	78 (10.7%)
7	0.424	68 (8.8%)	65 (8.9%)
8	0.195	26 (3.4%)	25 (3.4%)
Total	-	*774±3 (100%)*	*729±3 (100%)*

Table 3: β_{eff} per fissile isotope (^{235}U and ^{238}U) for CROCUS and PROTEUS (I-1A) compared to number of fissions per isotope

Fissile isotope	β^i_{eff} CROCUS	# fissions	β^i_{eff} PROTEUS (I-1A)	# fissions
^{235}U	661 (85.4%)	93.5%	614 (84.2%)	92.5%
^{238}U	113 (14.6%)	6.5%	115 (15.8%)	7.5%
Total	*774±3 (100%)*	*100%*	*729±5*	*100%*

Table 4: β_{eff} per reactor region for CROCUS and PROTEUS (I-1A) compared to number of fissions per region

Reactor region for CROCUS	β^i_{eff} CROCUS	# fissions	Reactor region for PROTEUS (I-1A)	β^i_{eff} PROTEUS (I-1A)	# fissions
UO_2 zone	516 (66.7%)	61.1%	Test zone	350 (48.0%)	47.9%
U_{met} zone	258 (33.3%)	38.9%	Buffer zone	160 (21.9%)	21.0%
Total	*774±3 (100%)*	*100%*	D2O zone	90 (12.4%)	12.1%
			Graphite zone	129 (17.7%)	19.0%
			Total	*729±3 (100%)*	*100%*

Figure 1: XY-cut of the CROCUS configuration at the core mid-plane

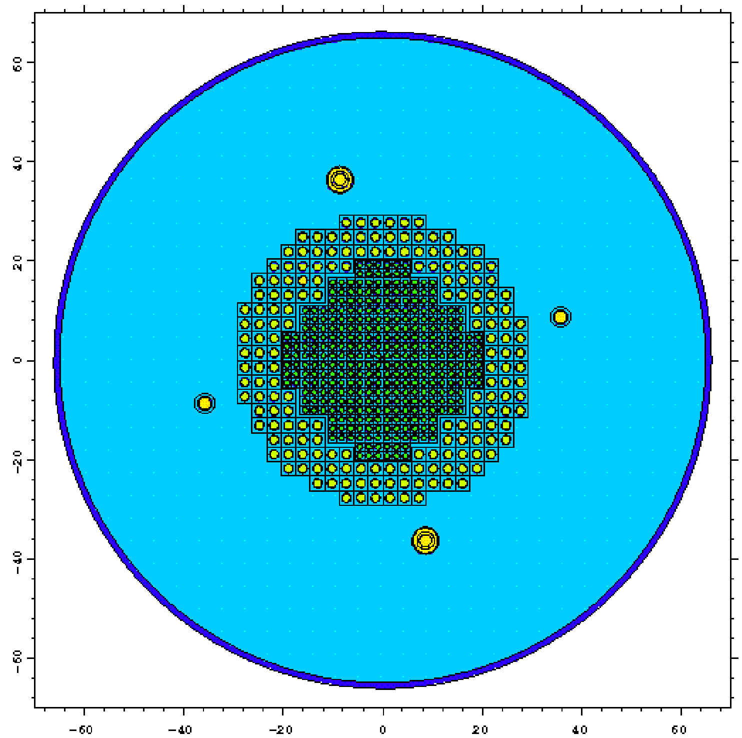

Figure 2: XY-cut of the LWR-PROTEUS I-1A configuration at the core mid-plane

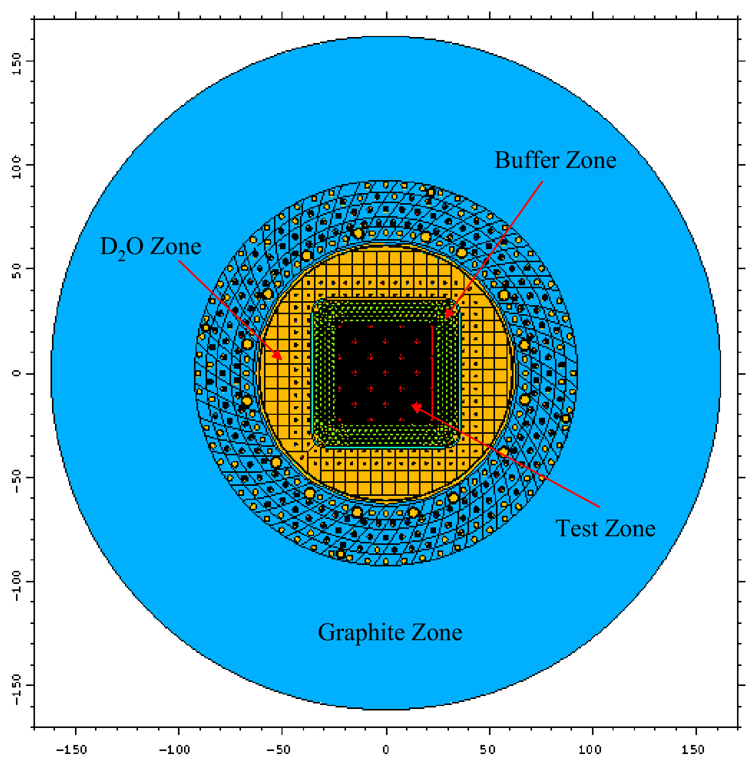

Figure 3: XY-cut of the LWR-PROTEUS I-1A configuration at the core mid-plane (zoom on the test zone)