Review and comparison of effective delayed neutron fraction calculation methods with Monte Carlo codes

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Abstract

The calculation of the effective delayed neutron fraction, β_{eff}, with Monte Carlo codes is a complex task due to the requirement of properly considering the adjoint weighting of delayed neutrons. Nevertheless, several techniques have been proposed to circumvent this difficulty and obtain accurate Monte Carlo results for β_{eff} without the need of explicitly determining the adjoint flux. In this paper, we make a review of some of these techniques; namely we have analyzed two variants of what we call the k-eigenvalue technique and other techniques based on different interpretations of the physical meaning of the adjoint weighting. To test the validity of all these techniques we have implemented them with the MCNPX code and we have benchmarked them against a range of critical and subcritical systems for which either experimental or deterministic values of β_{eff} are available. Furthermore, several nuclear data libraries have been used in order to assess the impact of the uncertainty in nuclear data in the calculated value of β_{eff}.

Keywords: effective delayed neutron fraction, adjoint flux, Monte Carlo, MCNPX

1. Introduction

The effective delayed neutron fraction β_{eff} is a crucial parameter in reactor safety since it corresponds to the maximum reactivity that can be inserted in a critical system without becoming prompt-critical. This parameter is also fundamental to describe the kinetic and dynamic response of both critical and subcritical nuclear systems to internal or external perturbations.

Calculation methodologies for β_{eff} must take into account that it is an adjoint-weighted parameter. Since the calculation of adjoint fluxes with Monte Carlo codes is cumbersome, β_{eff} is usually calculated with deterministic codes. Nevertheless, its calculation with Monte Carlo codes is also desirable since they allow dealing with more complex geometries, different materials and continuous energy cross sections. The need of accurate calculation tools for β_{eff} is specially relevant in the case of ADS that cannot become critical, since the experimental determination of β_{eff} is usually very difficult in a subcritical state.

For this reason, a large number of publications have appeared over the last years considering different techniques for the calculation of β_{eff} with Monte Carlo codes. Trying to group them, we have classified them into two categories. The first one comprises techniques based on k-eigenvalue calculations; the second one comprises techniques based on different interpretations of the adjoint weighting, such as those based on interpreting the adjoint weighting as the next fission probability or the iterated fission probability. In addition, a third category of techniques can be considered to include those based on perturbative methods, such as these derived in Nagaya and Mori (2005, 2011), but we have not considered them in this paper.

In the first of these categories, techniques based on k-eigenvalue calculations, we include techniques based on the definition and calculation of certain parameters by analogy to the effective multiplication constant (k_{eff}), such as those of Bretscher (1997) and Spriggs et al. (2001). Techniques based on the interpretation of the next-fission probability as the adjoint weighting have been analyzed by Nauchi and Kameyana (2005), Meulekamp and Van der Marck (2006) and Nagaya et al. (2010). Techniques based on the interpretation of the iterated fission probability as the adjoint weighting can be seen as an improvement of the previous ones, and they have been proposed by Nauchi and Kameyana (2010), Raskach and Blyskavka (2010), Chiba et al. (2011) and Irwanto et al. (2010). In section 2 we will provide some discussion on the derivation and the physical meaning of all these techniques.

In sections 3 and 4 we will present the results of the application of the above mentioned techniques against a number of critical and subcritical benchmark systems, that we consider to be representative of a wide range of nuclear systems. For this we have used the Monte Carlo code MCNPX[3] (Pelowitz et al. (2006)) with three different nuclear data libraries (ENDF/B-VII.0, JEFF-3.1 and JENDL-3.3). The use of several nuclear data libraries allows us to set a lower limit to the uncertainty on β_{eff} estimators, due to both the accuracy of the different techniques and the uncertainties of the basic nuclear data.

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[3] It must be remarked that the latest versions of the MCNP code can also provide values for adjoint-weighted parameters. The calculation methodology is based on an interpretation of the adjoint flux as iterated fission probability (Kiedrowski (2010); Kiedrowski and Brown (2011)).

2. Calculation methodologies

The usual definition of β_{eff} is:

$$\beta_{eff} = \frac{\left(\Phi_\lambda^\dagger, \hat{F}_d \Phi_\lambda\right)}{\left(\Phi_\lambda^\dagger, \hat{F} \Phi_\lambda\right)} \tag{1}$$

where $\hat{F}$ is the creation operator, that takes into account all neutrons (prompt and delayed) created in the phase space by fission, and $\hat{F}_d$ is the delayed neutron creation operator, that takes into account only delayed neutrons. The brackets indicate integration over the whole phase space. More specifically, the expressions in the numerator and in the denominator of Eq. 1 can be expanded as:

$$\left(\Phi_\lambda^\dagger, \hat{F}_d \Phi_\lambda\right) = \int \Phi_\lambda^\dagger\left(\vec{r}, E, \vec{\Omega}\right) \Sigma_f\left(\vec{r}, E'\right) \nu_d\left(E'\right) \times$$

$$\times \chi_d\left(E', \vec{\Omega}' \to E, \vec{\Omega}\right) \Phi_\lambda\left(\vec{r}, E', \vec{\Omega}'\right) dE' d\vec{\Omega}' dE d\vec{\Omega} d\vec{r} \tag{2}$$

and

$$\left(\Phi_\lambda^\dagger, \hat{F} \Phi_\lambda\right) = \int \Phi_\lambda^\dagger\left(\vec{r}, E, \vec{\Omega}\right) \Sigma_f\left(\vec{r}, E'\right) \nu\left(E'\right) \times$$

$$\times \chi\left(E', \vec{\Omega}' \to E, \vec{\Omega}\right) \Phi_\lambda\left(\vec{r}, E', \vec{\Omega}'\right) dE' d\vec{\Omega}' dE d\vec{\Omega} d\vec{r} \tag{3}$$

$\nu\left(E'\right)$ and $\nu_d\left(E'\right)$ denote, respectively, the average number of total (both prompt and delayed) and delayed neutrons at energy E' produced per fission. $\chi\left(E', \vec{\Omega}' \to E, \vec{\Omega}\right)$ and $\chi_d\left(E', \vec{\Omega}' \to E, \vec{\Omega}\right)$ represent, respectively, the spectrum of energy and angular distribution $\left(E, \vec{\Omega}\right)$ of the total and delayed neutrons produced by an incoming neutron with $\left(E', \vec{\Omega}'\right)$. Σ_f is the macroscopic fission cross section. Finally, Φ_λ and $\Phi_\lambda^\dagger$ are respectively the λ-mode direct and adjoint neutron fluxes, that is, the fundamental mode solutions of the eigenvalue equations[4]:

$$\hat{M}\Phi_\lambda = \frac{1}{k_{eff}} \hat{F}\Phi_\lambda \tag{4}$$

$$\hat{M}^\dagger \Phi_\lambda^\dagger = \frac{1}{k_{eff}} \hat{F}^\dagger \Phi_\lambda^\dagger \tag{5}$$

being $\hat{M}$ the migration and losses operator, that takes into account the net number of neutrons leaving the phase space element by capture, out-scattering or streaming, and $\hat{F}$ is the creation operator, already defined. $\hat{M}^\dagger$ and $\hat{F}^\dagger$ are their corresponding adjoints.

In this work, we consider only "effective" the delayed neutron fraction defined in Eq. 1 with the fluxes Φ_λ and $\Phi_\lambda^\dagger$. Several other delayed neutron fractions β can be defined considering fluxes other than Φ_λ or $\Phi_\lambda^\dagger$ but they will not be the "effective"

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[4]Notice that the λ-mode flux, Φ_λ, obtained as solution of Eq. 4 only corresponds to the physical flux for a critical system. As the system departs from criticality, the physical flux also begins to differentiate from Φ_λ. Hence, the concept of effective delayed neutron fraction losses significance for systems far away from critical.

values anymore. See, e.g., Bell and Glasstone (1970), Henry (1975) or Ott and Neuhold (1985) for further discussions on this topic. For instance, considering the adjoint flux to be constant over the whole phase space, we can define a non-adjoint weighted delayed neutron fraction, β_0, that can be expressed as:

$$\beta_0 = \frac{\left(\hat{F}_d \Phi_\lambda\right)}{\left(\hat{F}\Phi_\lambda\right)} \tag{6}$$

The determination of β_0 with Monte Carlo codes poses no major difficulty and can be performed by simply counting the number of total and delayed neutrons produced in fission processes. On the contrary, the determination of adjoint-weighted parameters requires the development of specific methodologies.

2.1. k-eigenvalue methods

Some of these methodologies can be classified as k-eigenvalue methods because they are based in defining and solving eigenvalue equations similar to 4 and 5. A first method is applied by Bretscher (1997) and it has been named the *prompt method* by Meulekamp and Van der Marck (2006) and the *prompt k-ratio method* by Nagaya and Mori (2011). It is obtained by defining the following eigenvalue equations:

$$\hat{M}\Phi_p = \frac{1}{k_p} \hat{F}_p \Phi_p \tag{7}$$

$$\hat{M}^\dagger \Phi_p^\dagger = \frac{1}{k_p} \hat{F}_p^\dagger \Phi_p^\dagger \tag{8}$$

where $\hat{F}_p$ is the prompt neutron creation operator. Assuming that $\Phi_p \simeq \Phi_\lambda$, which in principle seems a good approximation since over 99% of the neutrons produced in fission are prompt neutrons, we can obtain that:

$$\beta_{eff} = \frac{\left(\Phi_\lambda^\dagger, \hat{F}_d \Phi_\lambda\right)}{\left(\Phi_\lambda^\dagger, \hat{F}\Phi_\lambda\right)} = 1 - \frac{\left(\Phi_\lambda^\dagger, \hat{F}_p \Phi_\lambda\right)}{\left(\Phi_\lambda^\dagger, \hat{F}\Phi_\lambda\right)} \simeq$$

$$\simeq 1 - \frac{\left(\Phi_\lambda^\dagger, k_p \hat{M}\Phi_\lambda\right)}{\left(\Phi_\lambda^\dagger, k_{eff} \hat{M}\Phi_\lambda\right)} = 1 - \frac{k_p \left(\Phi_\lambda^\dagger, \hat{M}\Phi_\lambda\right)}{k_{eff}\left(\Phi_\lambda^\dagger, \hat{M}\Phi_\lambda\right)} =$$

$$= 1 - \frac{k_p}{k_{eff}} \tag{9}$$

The eigenvalue k_p can be easily evaluated in MCNPX without requiring any modification of the code, making the most of the ability of this code to "switch off" the delayed neutron transport (this is a standard feature of MCNPX and MCNP since version 4C, and it is performed by overriding the KCODE card with a TOTNU NO card). To perform this calculation it is obviously required that nuclear data libraries contain information about delayed neutron spectra, which is included in the latest versions of the most common ones.

A problem of the prompt method lies, in our opinion, in understanding how it takes into account adjoint weighting. In fact, the calculation of an adjoint-weighted parameter like β_{eff}

should not be possible using expressions that only contain k-eigenvalues, i.e., that are not adjoint-weighted parameters. Notice that both eigenvalues k_{eff} and k_p can be determined (Eqs. 4 and 7) with no need to define any adjoint flux. For instance, Bretscher (1997) considers no adjoint fluxes for deriving the method.

Notice as well that, in principle, any weighting function (e.g. $\Phi_p^\dagger$ as defined by Eq. 8) can be used instead of $\Phi_\lambda^\dagger$ in Eq. 9, leading to the same numerical value for β_{eff}. In particular, we could consider a constant weighting function over the whole phase space and therefore the method must provide values for β_0 instead of β_{eff}. In our opinion, it is not fully understood how the appropriate adjoint weighting is taken into account when applying the prompt method, as defined by Eq. 9, and, in particular, when it is applied with a Monte Carlo code. These issues have not been addressed when the prompt method is discussed by authors like Meulekamp and Van der Marck (2006) or Nagaya and Mori (2011).

In Meulekamp and Van der Marck (2006), it is also remarked that the prompt method is always an approximate method, because of the approximation $\Phi_p \simeq \Phi_\lambda$. For this reason, we have considered the possibility of removing the approximation by defining a new parameter k_p' as:

$$k_p' \equiv \frac{\left(\hat{F}_p \Phi_\lambda\right)}{\left(\hat{M} \Phi_\lambda\right)} \tag{10}$$

Notice that Eq. 10 is not an eigenvalue equation. With this parameter, a new delayed neutron fraction β' can be defined in an analogous manner to Eq. 9:

$$\beta' = 1 - \frac{k_p'}{k_{eff}} \tag{11}$$

Although with this definition of k_p' it is expected that β' will be equivalent to the non-adjoint weighted neutron fraction β_0, as defined by Eq. 6, we have also included the results obtained with this parameter in section 4, to help clarifying how the adjoint weighting influences the prompt method. We will denote the prompt method using k_p' as *prompt method with the total eigenfunction*, as opposite to the previous method, which we will denote as *prompt method with the prompt eigenfunction*.

k_p' can be calculated with MCNP performing a single KCODE cycle switching off the delayed neutron transport and taking as initial fission source distribution a previously calculated one with a flux that includes both prompt and delayed neutrons. An alternative to improve statistics is to perform many of these KCODE switching off delayed neutrons and upgrading the initial fission source in another KCODE cycle run in parallel, this one considering both prompt and delayed neutrons.

2.2. Methods based on different interpretations of the adjoint flux

A second class of methods for the calculation of β_{eff} is based on the interpretation of the physical meaning of the adjoint weighting. To derive this interpretation, let us consider the case of a subcritical reactor maintained in a steady state by an external neutron source. The neutron transport equation applied for this case takes the form:

$$\hat{F}\Phi - \hat{M}\Phi = -S_{ext} \tag{12}$$

As the adjoint equation, let us consider:

$$\hat{F}^\dagger \Psi^\dagger - \hat{M}^\dagger \Psi^\dagger = -\Sigma_f \tag{13}$$

where we have considered the macroscopic fission cross section as the adjoint source. Then, subtracting Eq. 12 multiplied by $\Psi^\dagger$ and Eq. 13 multiplied by Φ and integrating the resulting expression over the entire range of the variables taking into account the properties of the adjoint operators, we end up with the following expression:

$$\int S_{ext}\left(\vec{r}, \vec{\Omega}, E\right) \Psi^\dagger\left(\vec{r}, \vec{\Omega}, E\right) d\vec{r} d\vec{\Omega} dE =$$
$$= \int \Sigma_f\left(\vec{r}, \vec{\Omega}, E\right) \Phi\left(\vec{r}, \vec{\Omega}, E\right) d\vec{r} d\vec{\Omega} dE \tag{14}$$

The right-hand side of the last equation is just the response of the system to the external source, that is to say, the number of fissions per unit time that takes place in the whole system in the presence of the external source. We can further clarify this if we consider the external source to have the shape of:

$$S_{ext}\left(\vec{r}, \vec{\Omega}, E\right) = \delta\left(\vec{r}_0, \vec{\Omega}_0, E_0\right)$$

Then we find out that[5]:

$$\Psi^\dagger\left(\vec{r}_0, \vec{\Omega}_0, E_0\right) = \int \Sigma_f\left(\vec{r}, \vec{\Omega}, E\right) \Phi\left(\vec{r}, \vec{\Omega}, E\right) d\vec{r} d\vec{\Omega} dE$$

where $\Phi\left(\vec{r}, \vec{\Omega}, E\right)$ is the solution of the equation $\hat{L}\phi\left(\vec{r}, \vec{\Omega}, E\right) = -\delta\left(\vec{r}_0, \vec{\Omega}_0, E_0\right)$. That is to say, the value of the adjoint flux in a point of the phase space is the response of the system to a unit source introduced in this point. Hence, adjoint functions can be interpreted as the *source importance*, meaning the total number of fission reactions caused by the introduction of a source neutron in the point of the phase space $\left(\vec{r}, E', \vec{\Omega}'\right)$.

Alternative ways to derive the interpretation of the adjoint weighting as the neutron importance or the iterated fission probability are presented in Henry (1975) and Hurwitz (1964). Be aware that in the previous derivation, the macroscopic fission cross section has been considered as the adjoint source. Bell and Glasstone (1970), for instance, consider a macroscopic detector cross section instead, and interpret the adjoint flux as the importance of a neutron to the detector response.

To implement the interpretation of the adjoint weighting as neutron source importance to calculate β_{eff} it is necessary to determine the different importances of prompt and delayed neutrons in generating new fissions. For this, first notice that, as it

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[5]Take into account that this is equivalent to the track length estimator of k. Hence, we will use this estimator for all calculations.

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is well known, the total progeny of a given neutron is given by $k + k^2 + k^3 + ...$ in case the multiplication constant k remains constant between fission generations; otherwise it will be given by $k_0 + k_0 k_1 + k_0 k_1 k_2 + ...$ Therefore, it is necessary to determine the multiplication constant of delayed neutrons.

To obtain these values, a modification of the MCNPX code has been implemented to track the delayed neutron creation. In this way, if we start from an already converged fission source distribution, we can now obtain the subset of the fission source corresponding to delayed neutrons. Once this delayed neutron source is known, a value of k_{d0} can be calculated (in MCNPX this is performed with a single KCODE cycle, taking this delayed neutron source as initial fission source distribution). Notice that, with this definition, k_{d0} is not an eigenvalue, as it is calculated from the delayed component of a converged source.

This first KCODE cycle will also provide a second fission source distribution that can be used as the initial fission source distribution for another KCODE cycle, in order to obtain a second multiplicative constant k_{d1} and a third fission source distribution. In turn, this third source distribution can be used to obtain a third multiplicative constant, k_{d2}, and so on. Notice that after several cycles the value of k_{di} will tend to the value of k_{eff}, as the neutron sources used to calculate them tend to reach the initial fission source distribution (considering both prompt and delayed neutrons), and therefore the results obtained with this technique will converge.

Once the values k_{d0}, k_{d1}, etc, have been determined, the value of β_{eff} can be calculated as:

$$\beta_{I.F.P.} = \frac{\text{Equilibrium number of delayed neutrons}}{\text{Equilibrium number of all neutrons}} \times$$

$$\times \frac{\text{Average multiplication of delayed neutrons}}{\text{Average multiplication of all neutrons}} =$$

$$= \beta_0 \lim_{n \to \infty} \frac{k_{d0} + k_{d0}k_{d1} + k_{d0}k_{d1}k_{d2} + ... + \prod_{i=0}^{n-1} k_{di}}{k_{eff} + k_{eff}^2 + k_{eff}^3 + ... + k_{eff}^n} \quad (15)$$

We will denote this technique to calculate β_{eff} as *integrated fission probability* (I.F.P). We introduce this new definition to differentiate it from the concept of *iterated fission probability* introduced in Hurwitz (1964). In Hurwitz's derivation, which is done for a critical system, the iterated fission probability is defined as the number of fissions produced in the n-th generation after a neutron is introduced in the system, and therefore it is usually interpreted as $k_{d0}k_{d1}k_{d2}...k_{dn}$. Nevertheless, although this interpretation is appropriate for a critical system, it seems to us less appropriate for a subcritical system, because it tends to 0 after a large number of generations. Therefore, in this case we consider that a better estimate of the neutron importance is the total (or integrated) number of fissions produced by a given neutron, i.e. $k_{d0} + k_{d0}k_{d1} + k_{d0}k_{d1}k_{d2} + ...$, which tends to converge to a finite value. Thus, this is the interpretation we have adopted in this paper. It must be remarked that this same interpretation has already been applied by Feghhi et al. (2007, 2008) to calculate neutron importance functions and importance-weighted

neutron generation times[6].

In practice, we only need to calculate a limited number of values of k_{di}, providing that this number is enough to reach convergence. If we are left with a single cycle we will be considering only the multiplicity of the delayed neutrons but not of their progeny, which is defined as the next fission probability in Meulekamp and Van der Marck (2006):

$$\beta_{N.F.P.} = \beta_0 \frac{k_{d0}}{k_{eff}} \quad (16)$$

In Meulekamp and Van der Marck (2006) it is also discussed the validity of this approximation, arguing that the exact knowledge of the adjoint flux is not critical since the value of β_{eff} is largely determined by the value of β_0 and hence the accuracy in the definition of the adjoint weighting function has little impact. However, the validity of this approach has been questioned by other authors, for instance Irwanto et al. (2010) and Chiba (2009). We discuss the validity of this approximation in section 4

3. Benchmark systems

We have implemented the techniques described in the previous section with a modified version of the Monte Carlo code MCNPX 2.7 and validated them against a set of benchmark experiments for which measured or deterministic data for β_{eff} are available. These benchmarks have been chosen to be representative of wide range of systems. Hence, they include two homogeneous bare fast systems (Godiva and Jezebel), four reflected fast systems (Topsy, Popsy, Big-Ten and CORAL-I), a thermal system (TCA), two configurations of a subcritical system (Yalina-Booster) and three large fast systems (MUSE-4, ESFR and MYRRHA).

MCNP inputs have been taken from the IHECSBE (2008) (the reference number is given), unless indicated otherwise. A brief description of these system follows. The same β_{eff} reference values considered by Meulekamp and Van der Marck (2006) have been used when available; otherwise, the source is referenced.

- Godiva (HEU-MET-FAST-001). A bare, highly enriched (94 w/o) uranium spherical core containing 52.42 kg of uranium. The proposed MCNP model consists of five

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[6]In fact, we consider that for a critical system both interpretations are actually equivalent. In a critical system, the expressions $k_{d0} + k_{d0}k_{d1} + k_{d0}k_{d1}k_{d2} + ...$ in the numerator and $k_{eff} + k_{eff}^2 + k_{eff}^3 + ...$ in the denominator both diverge. Therefore, we can neglect the first m terms (which take a finite value) in both the numerator and the denominator, and take out the common factors, to be left with:

$$\beta_{I.F.P.} = \beta_0 \lim_{n,m \to \infty} \frac{k_{d0}...k_{dm}\left(1 + k_{d(m+1)} + ... + \prod_{i=m+1}^{n-1} k_{di}\right)}{k_{eff}^{m+1}\left(1 + k_{eff} + ... + k_{eff}^{n-m-1}\right)}$$

If after the m-th generation k_{di} has converged to the value of k_{eff}, then the terms between brackets in the numerator and in the denominator must cancel out, and thus we are left with the iterated fission interpretation of the adjoint flux.

ENDF/B-VII.0						
Benchmark	β_{eff} reference	β_0	$\beta_{P.E.}$	$\beta_{T.E.}$	$\beta_{N.F.P.}$	$\beta_{I.F.P.}$
Godiva	659 ± 10	640	651 ± 6	637 ± 3	643.05 ± 0.09	642 ± 1
Jezebel	194 ± 10	204	176 ± 7	210 ± 3	183.35 ± 0.04	178.5 ± 0.3
Topsy	665 ± 13	812	698 ± 6	816 ± 3	620.77 ± 0.13	684 ± 1
Popsy	290 ± 10	536	282 ± 6	546 ± 3	256.73 ± 0.08	273.7 ± 0.5
Big Ten	720 ± 7	904	724 ± 4	906 ± 3	697.72 ± 0.09	712 ± 2
CORAL	663 ± 17	822	679 ± 6	811 ± 8	620.91 ± 0.12	681 ± 1
MUSE-4	331 ± 5	352	313 ± 6	354 ± 3	313.99 ± 0.08	313.6 ± 0.6
TCA	771 ± 17	702	763 ± 8	701 ± 6	763.32 ± 0.21	763 ± 2
Yalina-B (902 f. e.)	761	663	716 ± 8	669 ± 6	724.82 ± 0.24	731 ± 1
Yalina-B (1141 f. e.)	753	662	723 ± 7	665 ± 4	715.69 ± 0.23	719 ± 1

Table 1: β_{eff} and β_0 results (in pcm) with the ENDF/B-VII.0 library. Statistical errors are given when available. $\beta_{P.E.}$: prompt method with the prompt eigenfunction; $\beta_{T.E.}$: prompt method with the total eigenfunction; $\beta_{N.F.P}$: next fission probability; $\beta_{I.F.P}$: integrated fission probability.

JENDL-3.3						
Benchmark	β_{eff} reference	β_0	$\beta_{P.E.}$	$\beta_{T.E.}$	$\beta_{N.F.P.}$	$\beta_{I.F.P.}$
Godiva	659 ± 10	631	640 ± 6	631 ± 3	638.83 ± 0.09	639 ± 1
Jezebel	194 ± 10	203	184 ± 7	200 ± 3	181.11 ± 0.03	176.5 ± 0.3
Topsy	665 ± 13	825	696 ± 6	820 ± 3	614.54 ± 0.14	685 ± 1
Popsy	290 ± 10	563	278 ± 6	545 ± 3	254.50 ± 0.07	276.1 ± 0.4
Big Ten	720 ± 7	926	724 ± 4	918 ± 3	694.15 ± 0.10	710 ± 1
CORAL	663 ± 17	837	695 ± 6	833 ± 7	614.25 ± 0.14	682 ± 1
MUSE-4	331 ± 5	357	318 ± 6	353 ± 3	315.56 ± 0.09	314.6 ± 0.6
TCA	771 ± 17	708	782 ± 8	714 ± 6	777.24 ± 0.20	779 ± 2
Yalina-B (902 f. e.)	761	664	727 ± 8	664 ± 4	731.42 ± 0.27	736 ± 1
Yalina-B (1141 f. e.)	753	662	726 ± 8	660 ± 4	721.93 ± 0.23	725 ± 2

Table 2: β_{eff} and β_0 results (in pcm) with the JENDL-3.3 library.

JEFF-3.1						
Benchmark	β_{eff} reference	β_0	$\beta_{P.E.}$	$\beta_{T.E.}$	$\beta_{N.F.P.}$	$\beta_{I.F.P.}$
Godiva	659 ± 10	633	647 ± 6	630 ± 3	639.01 ± 0.09	637 ± 1
Jezebel	194 ± 10	208	198 ± 6	192 ± 3	188.22 ± 0.04	183.9 ± 0.3
Topsy	665 ± 13	822	702 ± 6	822 ± 2	626.37 ± 0.13	686 ± 1
Popsy	290 ± 10	556	294 ± 6	547 ± 3	267.70 ± 0.07	283.4 ± 0.5
Big Ten	720 ± 7	921	743 ± 4	921 ± 3	714.65 ± 0.09	729 ± 1
CORAL	663 ± 17	833	700 ± 6	830 ± 8	627.44 ± 0.13	683 ± 1
MUSE-4	331 ± 5	366	326 ± 6	361 ± 3	325.24 ± 0.09	324.7 ± 0.6
TCA	771 ± 17	722	790 ± 8	727 ± 6	785.63 ± 0.21	788 ± 2
Yalina-B (902 f. e.)	761	678	739 ± 8	681 ± 4	741.50 ± 0.27	744 ± 1
Yalina-B (1141 f. e.)	753	676	737 ± 7	676 ± 4	732.10 ± 0.26	735 ± 2
ESFR, MOX core, BOL	389.5	491	398 ± 7	465 ± 21	391.62 ± 0.08	388.7 ± 0.7
ESFR, MOX core, 1230 EFPDs	360.3	454	362 ± 6	404 ± 35	360.33 ± 0.07	358.1 ± 0.7
ESFR, (U+Pu+MA)O$_2$ core, BOL	363	477	364 ± 7	475 ± 27	362.22 ± 0.08	357.3 ± 0.8
ESFR, (U+Pu+MA)O$_2$ core, 1230 EFPDs	338.7	436	339 ± 7	393 ± 31	337.59 ± 0.07	335.3 ± 0.9
MYRRHA, critical core, BOC	321	363	331 ± 10	347 ± 13	321.27 ± 0.06	321.3 ± 0.7
MYRRHA, subcritical core, EOC	332	377	331 ± 9	399 ± 12	332.68 ± 0.09	330.5 ± 0.6

Table 3: β_{eff} and β_0 results (in pcm) with the JEFF-3.1 library (JEFF-3.1.1 for the ESFR and Myrrha).

shells with slightly varying composition and an additional sixth shell added to compensate for reflections in the supporting elements and other factors.

- Jezebel (PU-MET-FAST-001). A bare plutonium sphere (4.5 w/o of Pu-240) containing 17.020 kg of a plutonium and gallium alloy (1.02 w/o of gallium).

- Topsy (HEU-MET-FAST-028). A sphere of 93 w/o enriched uranium (17.84 kg) surrounded by a thick (19 inches) U-238 reflector.

- Popsy (PU-MET-FAST-006). A plutonium/gallium sphere (6.06 kg) surrounded by a uranium reflector.

- Big Ten (IEU-MET-FAST-007). The Big Ten core contained uranium with three different enrichments (93%, 10% and natural). It was surrounded by a depleted uranium reflector. Total uranium mass in the reactor was 10 metric tons.

- CORAL-I. A reflected, highly enriched uranium cylinder (containing 26 kg of 90% enriched uranium) surrounded by a reflector of natural uranium (Verdaguer Hernández et al. (1972)). It was in operation at CIEMAT (formerly JEN) between 1968 and 1988. MCNP models for CORAL-I are available (Villamarín et al. (1999)). Experimental β_{eff} data were measured and are presented in De Francisco et al. (1973).

- TCA (LEU-COMP-THERM-006). The TCA (Tank Critical Assembly) consists of a tank containing an array of fuel assemblies of 2.6 w/o UO_2 and water that acts as moderator. The number of fuel rods and the lattice geometry and pitch can be changed. The reactor is made critical by adjusting the water level.

- Yalina-Booster. The Yalina-Booster subcritical facility is located at the JIPNR-Sosny of the National Academy of Sciences of Belarus. The facility consists of a fast and a thermal zones partially decoupled by a thermal neutron absorbing layer between them. The fast zone is formed by HEU (90% and 36% enrichment) in a lead matrix and the thermal zone is formed by LEU (10% enrichment). The whole assembly is surrounded by a graphite reflector. Experimental β_{eff} data are not available, but deterministic calculations with the ERANOS code have been reported by Aliberti et al. (2009) for two different configurations of the system with a different number of fuel rods in the thermal zone (902 and 1141, respectively). The reference value we consider here is the average of several libraries. No estimation of the error is given. MCNP inputs were supplied by JIPNR-Sosny and have been modified to fit these two configurations.

- MUSE-4. The MUSE-4 experiment was carried out at the MASURCA reactor at the CEA-Cadarache facility (France) between 2001 and 2004 and comprised several critical and subcritical configurations. The reference critic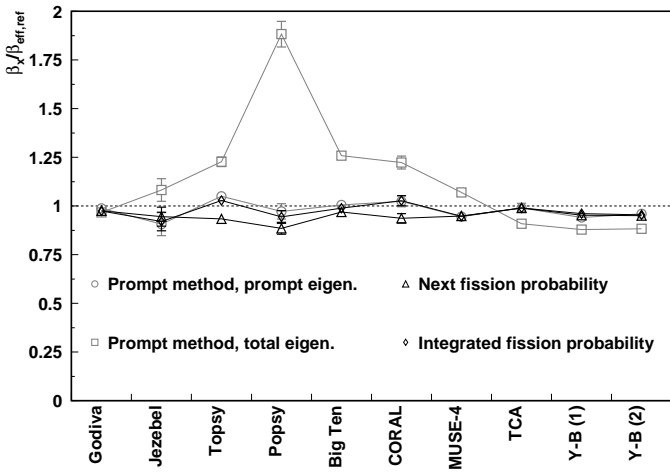al configuration consisted of a core formed by a mixture of MOX fuel and sodium rodlets surrounded by a reflector made up of stainless steel and sodium rodlets. The MCNP input has been made using the specifications given in Soule et al. (2001). β_{eff} data have been taken from Lebrat et al. (2008). It must be remarked that the values of β_{eff} were measured in a later configuration than those of the MCNP input file used, with 1115 fuel elements instead of 1112. These three elements were added to compensate for the decay of some of the Pu-241 in the MOX fuel. Nevertheless the difference in the measured value of β_{eff} is not expected to be significant.

- ESFR (European Sodium Fast Reactor). The 3600 MWth core under consideration is divided in two zones with different Pu content, which is surrounded by a stainless steel reflector. Two different cores are studied. The first core is loaded with $(U,Pu)O_2$ MOX fuel and the second has $(U,Pu,MA)O_2$ fuel. The two zones averaged Pu content is 15 w/o and in the second case the MA content is 4 w/o. In both cases, the results for beginning of life (BOL) and after 1230 equivalent full power days (representative of End of Equilibrium Cycle) are presented. The reference results for β_{eff} were calculated by PSI with the deterministic code ERANOS (Martín-Fuertes et al. (2011)). The MCNP input was developed within the participation of CIEMAT in the CP-ESFR project (Pérez-Martín et al. (2011)).

- MYRRHA. This facility is a Lead-Bismuth cooled research reactor planned to be built at SCK-CEN site in Mol (Belgium) (Sarotto et al. (2012)). It is conceived to operate in both critical and subcritical modes, in this case acting as a prototype of accelerator driven system (ADS). Both configurations have been considered in our study: a 100 MW(th) critical core at beginning-of-cycle (fresh fuel Pu content 34% wt.) and a 94 MW subcritical core at end-of-cycle (Pu content 30% wt. in the fresh fuel). Both MCNP reference inputs were developed by SCK-CEN within the CDT FASTEF project. The reference results for β_{eff} were calculated by ENEA using ERANOS code. Fuel depletion calculations for the end-of-cycle core have been performed with the EVOLCODE system (Álvarez-Velarde et al. (2006)).
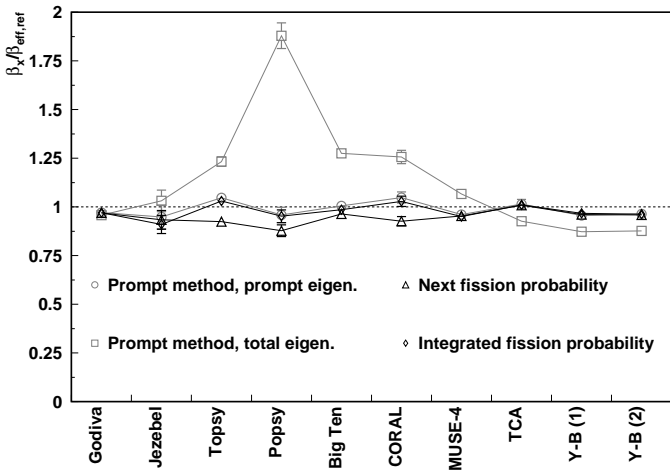
In all the cases except the ESFR and MYRRHA, the β_{eff} results with three different nuclear data libraries (ENDF-VII.0, JEFF-3.1 and JENDL-3.3) processed at room temperature are presented. For the ESFR and MYRRHA, we only present results for the JEFF-3.1.1 library processed at operating temperatures.
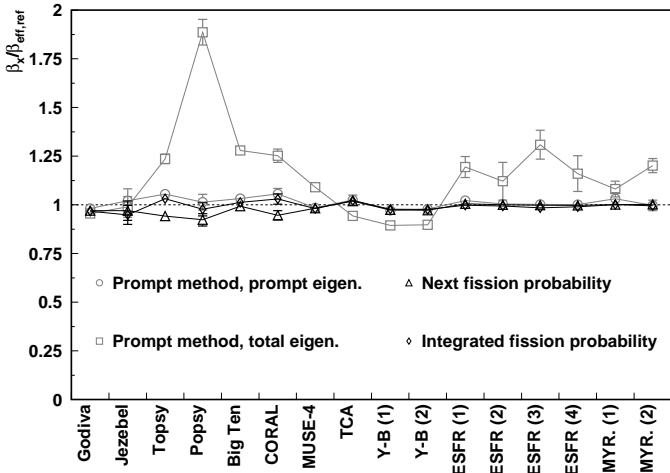
4. Validation results

The results of the validation are presented in Tables 1, 2 and 3. They include results of β_{eff} with the techniques described in section 2 as well as results for β_0. The ratios between the values of β_{eff} calculated with the different techniques and the reference values are presented graphically in Fig. 1.

Figure 1: Graphical depiction of the ratios of the β_{eff} calculated with different techniques to the reference values.

The prompt method (both with the prompt and the total eigenfunction) has been applied considering the simple average of the three k_{eff} estimators provided by MCNPX (collisions, absorptions and track length estimators)[7]. In the case of the I.F.P and N.F.P methods only the track length estimator has been considered.

Results show that the prompt method, with the prompt eigenfunction, fits the reference experimental or deterministic results with good accuracy in all the cases. These results are consistent with the conclusions of previous benchmarks (e.g. Meulekamp and Van der Marck (2006)), in spite of that, as it was commented in section 2, the question of how adjoint weighting is taken into account with this method, is not, to our understanding, fully explained.

On the other hand, the prompt method with the total eigenfunction has been found to provide values of β_0 rather than values of β_{eff}, as expected. Although in homogeneous systems (Godiva, Jezebel) both values are similar, in heterogeneous (reflected) systems (Topsy, Popsy, Big Ten, CORAL), where β_0 and β_{eff} are very different, the prompt method with the total eigenfunction overestimates the value of β_{eff} by a factor of up to two. For thermal systems (TCA and Yalina-B), however, it has been found to underestimate the values by about a 10%.

The integrated fission probability methodology has also been found to provide accurate results for β_{eff} in all cases for the number of KCODE cycles considered (50). If only a single KCODE cycle is performed (next fission probability approximation) the values of β_{eff} obtained can be up to about 10% lower than the reference values for the case of reflected systems (Popsy, Topsy, Big-Ten, CORAL).

In these cases, we have analyzed the number of KCODE cycles required in order to reach convergence in the value of β_{eff}. The results of this analysis are presented in Fig. 2. Notice how the value of β_{eff} increases rapidly with the first cycles, and after about 15 cycles, a relatively constant level is reached. A very accurate determination of k_{eff} is required for this level to remain constant with the number of cycles; otherwise, the bias in k_{eff} will accumulate with the increasing number of cycles and it will result in an increasing systematic deviation in the value of β_{eff} with the number of cycles. Therefore, a larger number of KCODE cycles require a higher precision in the determination of k_{eff} (more statistics).

To better understand the evolution of the β_{eff} results with the number of KCODE cycles, we have obtained the radial distributions of the initial delayed neutron fission source, and the fission sources after a different number of cycles for the cases of the four spherical reactors (Fig. 3). It can be observed how, for the cases of the non-reflected systems (Godiva and Jezebel), the fission source distribution does not experience major changes with the number of cycles. For these systems there was no noticeable difference between the β_{eff} results considering the next fission and the integrated fission probability interpretations of the adjoint weighting. In the reflected systems (Topsy and Popsy),

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[7]It has to be noticed that the β_{eff} estimator must keep the correlation among the two calculations (with and without delayed neutrons), which, in general, is lost using the combined average k_{eff} estimator.

however, there is a considerable difference among the initial delayed neutron fission source, the neutron source obtained from the first KCODE cycle, and subsequent fission sources (from the second one, it is apparent that the fission source has reached a distribution that is stable with the number of cycles). These noticeable differences among fission sources can explain the differences in the β_{eff} results obtained with the N.F.P. and the I.F.P. techniques.

Finally, concerning the uncertainty in the results due to the nuclear data library used, we would like to stress that it is of the same magnitude as the difference between the prompt method (with the prompt eigenfunction) and the integrated fission probability method. With both methods, changing the nuclear data library can drive to changes in the β_{eff} results of up to the order of 10 pcm. Therefore, we cannot conclude whether any library is better suited than the others for β_{eff} calculations for a particular type of systems.

5. Conclusions

We have analyzed and benchmarked the performance of several proposed Monte Carlo techniques for the calculation of the effective delayed neutron fraction, β_{eff}. They are two versions of the so called prompt method, both with the prompt eigenfunction and the total eigenfunction, and the techniques based on the interpretation of the next fission probability (N.F.P.) and the integrated fission probability (I.F.P.) as the adjoint weighting.

Results show that the prompt method with the prompt eigenfunction and the technique based on I.F.P. provide the most accurate values for β_{eff}. The first is the simplest to be applied with MCNPX and does not require any modification of the code. However, it has a weak theoretical justification, as it is necessary to explain how adjoint weighting is approximated with it. The usage of the total eigenfunction instead of the prompt eigenfunction has also been investigated and has been found to provide values for β_0 instead of β_{eff}.

The technique based on I.F.P. provides similar values for β_{eff}. It has been noticed that as the number of KCODE cycles becomes larger, the uncertainties in the determination of k_{eff} and k_{di} cause the uncertainty in the β_{eff} results obtained with this method to increase. The technique based on N.F.P. can be considered the first cycle of the technique based on I.F.P. and has been found to work reasonably well for most of the systems considered but it causes noticeable systematic errors in reflected heterogeneous systems.

Acknowledgments

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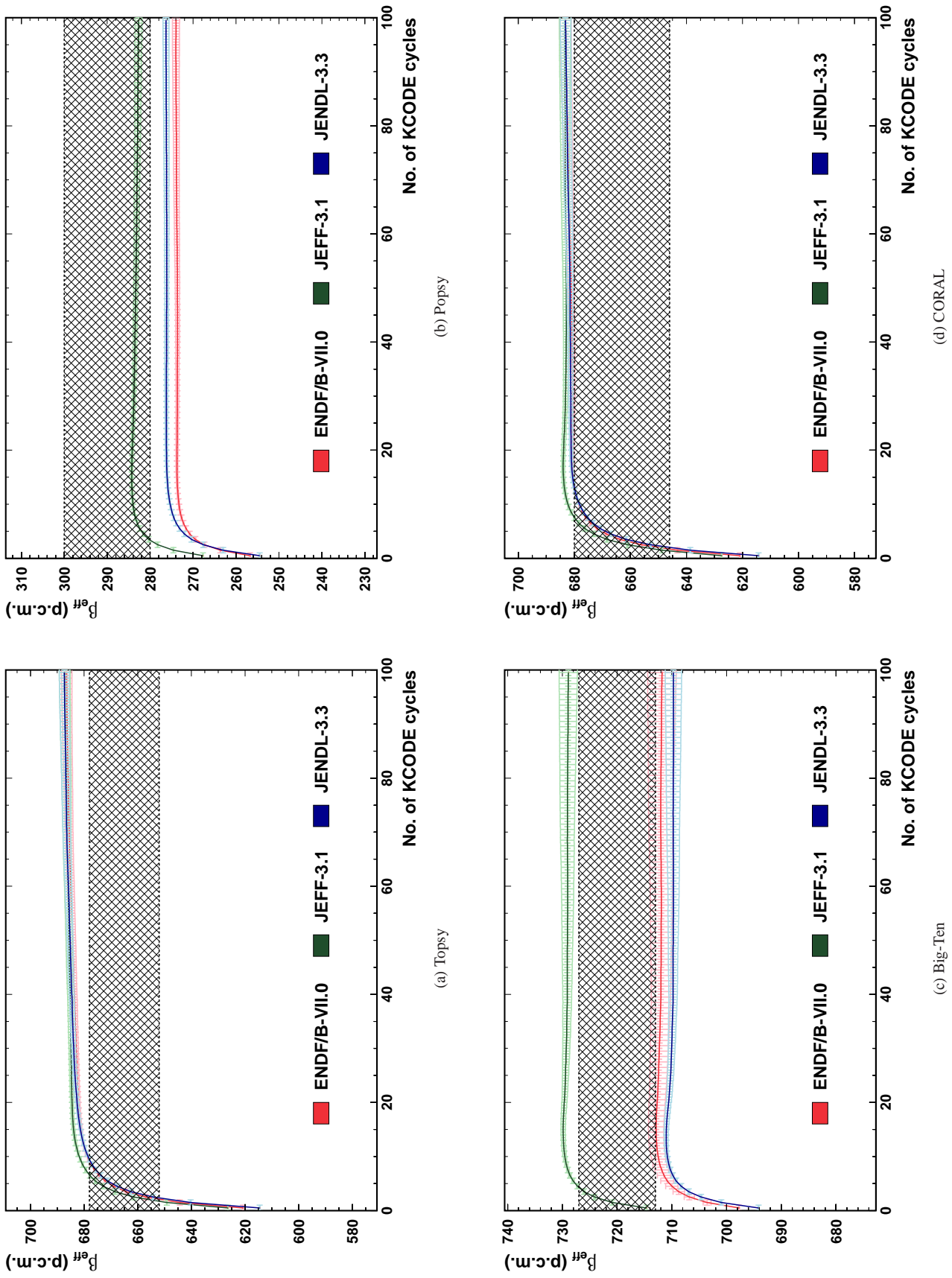Ott, K.O. and Neuhold, R.J. (1985), Introductory Nuclear Reactor Dynamics, American Nuclear Society.

Figure 2: β_{eff} results applying the integrated fission probability considering a different number of cycles. The hatched area represents the reference value with its uncertainty.
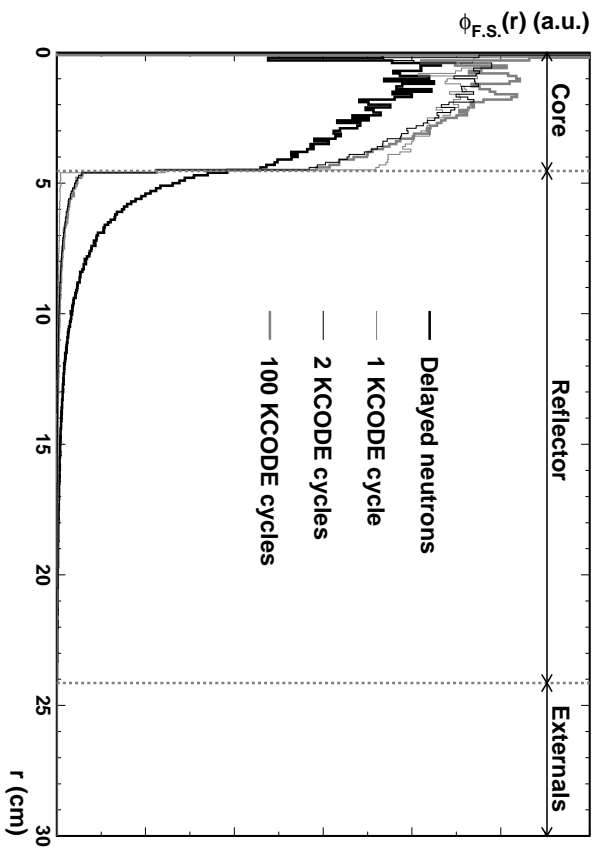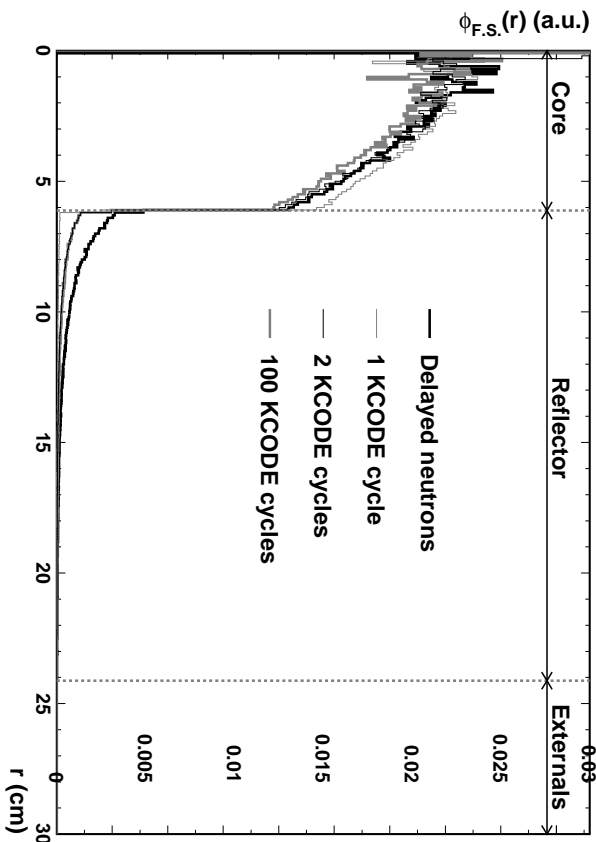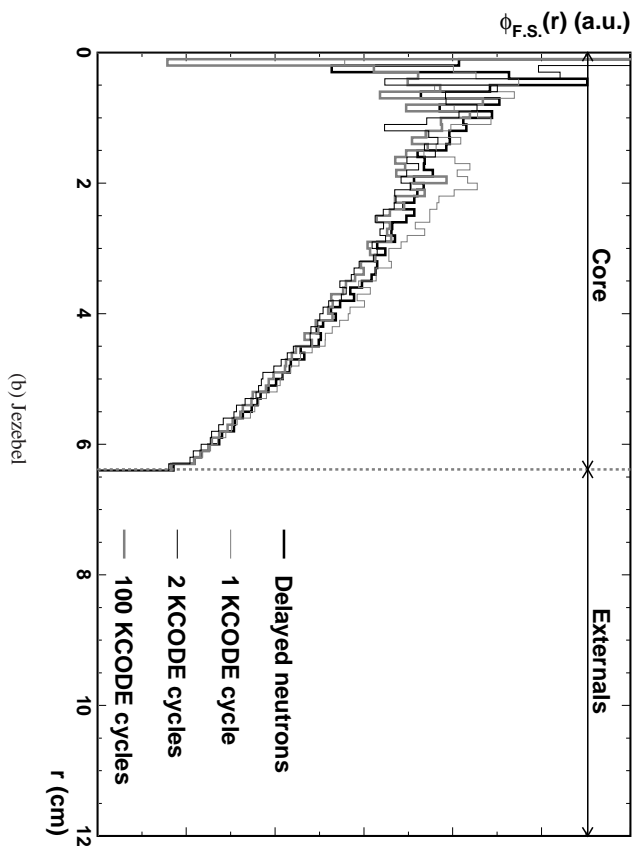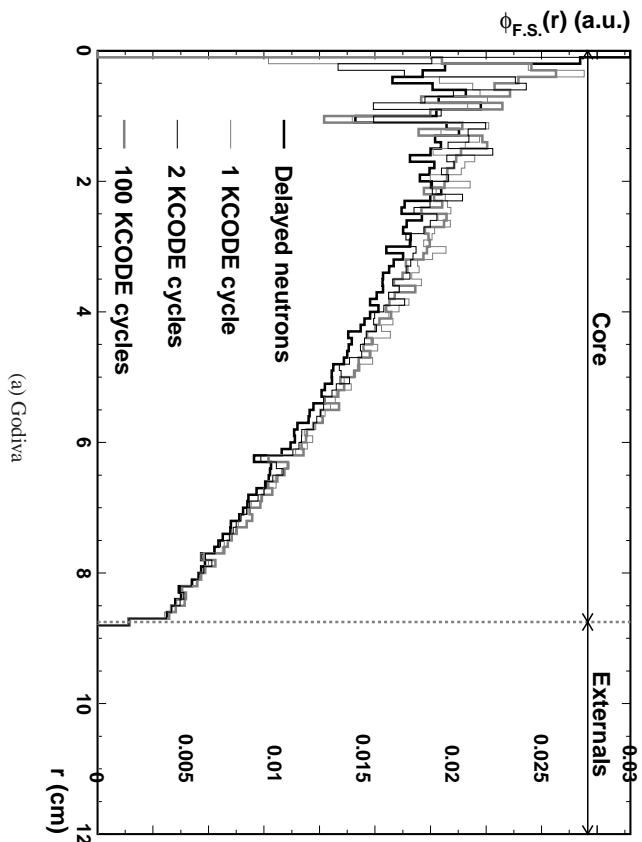
Figure 3: Distribution of delayed and total neutron source for four spherical reactors, normalized to the number of source points.

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