Combined use of k-effective and beta-effective measurements for nuclear data validation and improvement

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Abstract. Nuclear cross-sections are being re-evaluated time and again since decades, and in the recent years they are “tuned” to match better in particular the $k_{\text{eff}}$ measurements. However, the $k_{\text{eff}}$ parameter as a very global parameter provides simply too many possible combinations and variations, all more or less in agreement with the differential cross section data measurements and the associated uncertainties. Adding other types of integral measurements, such as shielding and kinetics benchmarks, on the cross-section evaluation menu is expected to provide a complementary and a more complete view on the problem. This paper discusses the advantages of exploiting the effective delayed neutron fraction ($\beta_{\text{eff}}$) measurements for nuclear data (ND) evolution and testing. The cross-section sensitivity and uncertainty analysis revealed some crucial differences in the $k_{\text{eff}}$ and $\beta_{\text{eff}}$ sensitivity profiles which are favorable for ND validation.

1. Introduction

Nuclear data sensitivity and uncertainty (S/U) methodology (either based on the first order perturbation theory or Monte Carlo), combined with the benchmark experiment analysis, play an essential role in assuring the accuracy and reliability of the nuclear reactor computations and provide an insight in the physical phenomena involved in the neutron transport. Critical benchmarks have been traditionally used to validate and improve nuclear data. However, $k_{\text{eff}}$ is only one of the important reactor safety factors requiring accurate nuclear data. Other reactor parameters can likewise provide information relevant for the improvement of nuclear data, such as radiation shielding (reaction rate and spectra) measurements, or kinetic parameters (effective delayed neutron fraction - $\beta_{\text{eff}}$). In this paper the potential of using $\beta_{\text{eff}}$ measurements for improving nuclear data is investigated based on several examples of fast reactors (such as FLATTOP-Pu, Big ten, SNEAK-7a & -7h, etc.) and Accelerator Driven Systems (ADS). The study makes use of $k_{\text{eff}}$ and $\beta_{\text{eff}}$ sensitivity and uncertainty computations performed by means of the SUSD3D code. The sensitivity coefficients of $\beta_{\text{eff}}$ with respect to the basic nuclear data were calculated by deriving the Bretscher’s k-ratio formula as initially proposed in 2010 in the scope of the Uncertainty Analysis in Modeling (UAM) project of the OECD/Nuclear Energy Agency (NEA). Sensitivities of $k_{\text{eff}}$ and $\beta_{\text{eff}}$ with respect to nuclear data are compared in view of exploiting the differences among them for a physically more complete, comprehensive and consistent nuclear data validation and improvement procedure.

An important conclusion of these studies is that due to their high sensitivity and different shapes of sensitivity profiles some $\beta_{\text{eff}}$ experiments can provide a complementary information to critical experiments. These measurements can thus be used to validate other quantities than the delayed nu-bar ($\bar{\nu}_d$) already done in the past. Inelastic and elastic scattering cross sections of $^{238}\text{U}$ are particularly interesting examples where $\beta_{\text{eff}}$ measurements could contribute to improve nuclear data evaluations.

Furthermore, the above S/U method allows to estimate the uncertainty in the calculated $\beta_{\text{eff}}$, which will be particularly important for the future reactor systems that are likely to use wider range of actinide isotopes with lower values of $\beta_{\text{eff}}$ (Pu isotopes, making the reactor control of MOX fueled cores more challenging.

2. Beta-eff sensitivity calculations

2.1. Method

The method for the beta-eff sensitivity and uncertainty calculations is presented in Refs. [1–4]. As demonstrated in these papers (e.g. [3]) the definition of $\beta_{\text{eff}}$ as given in Keepin [5] is equivalent to the sensitivity of $k_{\text{eff}}$ to the delayed neutron yield as defined in the 1\textsuperscript{st} order perturbation theory. $\beta_{\text{eff}}$ and all its components by actinides can be therefore obtained using the 1\textsuperscript{st} order perturbation codes such as SUSD3D as a sum of the $k_{\text{eff}}$ sensitivities with respect to the delayed neutron yields $(\Bar{\nu}_d)$ for all fissile isotopes $i$:

$$\beta_{\text{eff}} = \sum_i \int S_{\nu_i}(E) dE$$

(1)

where:

$$S_{\nu_i}(E) = \frac{1}{R} \int d\Omega \int d\hat{\Omega} \int dE \cdot \Phi(\hat{r}, \hat{\Omega}, E) \cdot \Phi^+(\hat{r}, \hat{\Omega}, E') \chi_d(E')\sigma_i(E) N_i(\hat{r})$$

$\Phi$ and $\Phi^+$ are the direct and adjoint angular fluxes, $\sigma_i$ is fission cross section of the isotope $i$, $\chi_d$ is delayed neutron

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fission spectrum, \( \bar{\nu}_d \) is delayed neutron yield, and \( N_i'(r) \) is number density of the isotope \( i \) at location \( r \). \( R \) is the normalization parameter which in this case assures that the sum of the \( \bar{\nu}_f \) sensitivities of all involved fissile isotopes adds up to 1.

Monte Carlo (M/C) codes usually calculate beta effective using the Bretscher’s approximation [6], sometimes called also the prompt k-ratio method:

\[
\beta_{\text{eff}} = 1 - \frac{k_p}{k} \tag{2}
\]

where \( k_p \) is the \( k_\text{eff} \) taking into account only prompt neutrons and \( k \) is the total (prompt and delayed neutron)\( k_\text{eff} \). In the M/C codes (such as MCNP and SERPENT) \( \beta_{\text{eff}} \) could be also in principle of course also calculated using perturbation theory as the \( k_\text{eff} \) derivative to \( \bar{\nu}_d \).

Since the sensitivity of \( \beta_{\text{eff}} \) would require the calculation of the second derivative (\( \beta_{\text{eff}} \) being already equal the 1st derivative) another approach was developed in the SUSD3D code [7,8] based on the derivation of the Bretscher’s prompt k-ratio method:

\[
S_p = \frac{\sigma}{\beta_{\text{eff}}} \frac{d\beta_{\text{eff}}}{d\sigma} = \frac{k_p}{k \beta_{\text{eff}}} (S_k - S_{\bar{\nu}p}) \tag{3}
\]

The two terms \( S_k \) and \( S_{\bar{\nu}p} \) correspond to the sensitivities of the \( k \) and \( k_p \), which can be obtained using the standard linear perturbation theory. Note also that \( \beta_{\text{eff}} \) sensitivity can be evaluated as the 2nd derivative of \( k_{\text{eff}} \) using M/C technique.

2.2. Computational examples

The above method was implemented in the SUSD3D code to evaluate the uncertainty in beta-effective due to the basic nuclear data and demonstrated at the UAM-5 Meeting in April 2011 [1]. In the past, the following \( \beta_{\text{eff}} \) benchmarks from ICSBEP [9] and IRPhE [10] were already analyses using SUSD3D (see [3] for details):

- **SNEAK-7A & -7B**: MOX fuel reflected by metallic depleted U.
- **Jezebel**: bare sphere of \( ^{239} \text{Pu} \) metal, 6.385-cm radius
- **Skidoo** (Jezebel-23): bare \( \sim 98.1\% \) \( ^{233} \text{U} \) sphere;
- **Popsy** (Flattop-Pu): \( \sim 20\text{-cm} \) natural U reflected \( ^{239} \text{Pu} \) sphere;
- **Topsy** (Flattop-25): \( \sim 20\text{-cm} \) natural U reflected \( ^{235} \text{U} \) sphere;
- **Flattop-23**: \( \sim 20\text{-cm} \) natural U reflected \( ^{233} \text{U} \) sphere;
- **Big Ten**: 10% enriched U with U-reflector, cylinder \( r=41.91 \text{ cm}, h=96.428 \text{ cm} \);
- **ZPPR-9**: MOX core with sodium cooling, depleted U blanket.

Recently, the Berenice Zona2 benchmark and the MYRRHA (ADS) reactor were studied in the scope of the CHANDA project. ENDF/B-VII.1 [11] cross-sections were used in these studies.

As shown in Table 1 below, consistent \( \beta_{\text{eff}} \) values were obtained using the two methods: as the derivative of \( k_{\text{eff}} \) with respect to delayed neutron yield \( \bar{\nu}_p \) (Eq. (1)) using SUSD3D sensitivity codes (exact Keepin formulation) and using the Bretscher’s (prompt k-ratio) method (Eq. (2)) with the \( k \) and \( k_p \) calculated by the deterministic PARTISN [12] and MCNP5 codes.

![Table 1. Measured and calculated values of \( \beta_{\text{eff}} \).](image)

### Table 1. Measured and calculated values of \( \beta_{\text{eff}} \).

| Benchmark     | Measured (pcm) | Calculated (pcm) |
|---------------|----------------|------------------|
|               | SUS3D Eq. (1)  | Prompt k-ratio, Eq. (2) |
| SUSD3D        | PARTISN        | MCNP |
|---------------|----------------|------|
| SNEAK 7A      | 395±5.1%       | 373±2.7% | 379 | 369 |
| SNEAK 7B      | 429±5.1%       | 419±2.9% | 429 | 415 |
| Jezebel       | 195±5%         | 185±2.5% | 186 | 186 |
| Jezebel-\( ^{233} \text{U} \) | 290±3.5%       | 296±7.1% | 297 |
| Flattop-Pu    | 276±2.5%       | 277±2.6% | 278 | 284 |
| Flattop-\( ^{235} \text{U} \) | 665±2%         | 688±2.7% | 690 |
| 23 Flattop    | 360±2.5%       | 374±5.5% | 375 |
| Big-ten       | 720±1%         | 720±2.5% | 734 |
| ZPPR-9        |                      | 360±3.0% | 362 |
| MYRRHA        |                      | 322±2.2% | 323 |
| Berenice Z2   | 349±1.7%       | 344±2.6% | 351 |

3. Comparison of \( k_{\text{eff}} \) and \( \beta_{\text{eff}} \) sensitivity profiles

\( k_{\text{eff}} \) and \( \beta_{\text{eff}} \) parameters being governed by very different physical processes, the corresponding sensitivities are...
Figures 1–6. Examples of the differences between the sensitivity profiles of $\beta_{\text{eff}}$ and $k_{\text{eff}}$ to the main cross sections.
also expected to differ. The values of the delayed neutron fraction depend on the incident neutron energy, and in particular vary from one isotope to the other (from ≈ 210 pcm for $^{239}$Pu, ≈ 650 pcm for $^{238}$U and up to ≈ 1570 pcm for $^{238}$U), meaning that fast fission of $^{238}$U tends to increase, and fission on Pu isotopes (in particular $^{239}$Pu) decreases the $\beta_{\text{eff}}$ value of the system. Consequently, the fission of the isotopes with higher $\beta_{\text{eff}}$ values (such as $^{238}$U) has positive sensitivity, and the fission of low $\beta_{\text{eff}}$ isotopes the negative one. In presence of $^{238}$U in the fuel, the fast fission of $^{238}$U (and all physical processes which tend to maintain neutrons at the energies of $^{238}$U fission) increases $\beta_{\text{eff}}$ (has therefore positive sensitivity), whereas on the contrary the lower energy (and thermal) fission (e.g. of $^{239}$Pu) decreases $\beta_{\text{eff}}$, as well as all reactions leading to neutron thermalisation and have therefore negative sensitivities. This is the opposite of the situation for the $k_{\text{eff}}$ value, where thermal fission is preferred over fast fission. The energy dependence of $\tilde{\nu}_d$ has also an impact on the sensitivity profiles.

The above leads to very different sensitivity profiles of $k_{\text{eff}}$ and $\beta_{\text{eff}}$. Several interesting and possibly ND exploitable examples are shown in Figs. 1–6, such as: a negative $\beta_{\text{eff}}$ sensitivity to some (n,f) reactions (e.g. $^{239}$Pu), strongly negative $\beta_{\text{eff}}$ sensitivity to $^{238}$U(n,n') and positive to $^{238}$U absorption, and, most interestingly, sensitivities to $^{238}$U(n,n) and prompt fission spectra being (PFNS) of opposite sign.

4. Conclusions

Powerful tools for nuclear data sensitivity and uncertainty analysis, both based on deterministic and Monte Carlo methods are available which combined with benchmark experiments, offer an efficient means for evaluation and testing of nuclear data.

The application of sensitivity and uncertainty tools to the effective delayed neutron fraction demonstrated the potential benefits of integrating the kinetics benchmarks into the nuclear data evaluation and validation schemes. The effective delayed neutron fraction is a key reactor safety parameter involved in the control rods worth calculations and transient (reactivity feedbacks effect) studies. It plays an important role in reactivity accident analysis. Precise knowledge of effective delayed neutron fraction ($\beta_{\text{eff}}$) and of the corresponding uncertainty is thus important for reactor safety analysis. It is demonstrated here that, besides its importance for reactor safety, accurate measurements of $\beta_{\text{eff}}$ can provide valuable information on the quality and consistency of basic nuclear data.

The sensitivity coefficients of the effective delayed neutron fraction $\beta_{\text{eff}}$ were obtained by deriving the Breit’s (prompt k-ratio) approximate $\beta_{\text{eff}}$ expression with respect to the basic nuclear data. The method was implemented in the SUS3D sensitivity and uncertainty code and already applied in the past to several fast neutron benchmark experiments from the ICSBEP and IRPhE databases and to the MYRRHA reactor. Uncertainty in $\beta_{\text{eff}}$ is evaluated in terms of the uncertainties of the basic nuclear data and the energy dependence of the neutron fission spectra. JENDL-4 covariance data evaluations cover most of the relevant reactions, except the uncertainties in the delayed neutron fission spectra. According to these covariance data the uncertainty in $\beta_{\text{eff}}$ is mainly due to the uncertainties in delayed (and prompt) neutron yields, inelastic and elastic scattering and fission cross sections, as well as the prompt and delayed fission spectra. For typical MOX cores, the total uncertainty in $\beta_{\text{eff}}$ was found to be around 3%, which is of the order of the experimental uncertainties. More effort should be invested in the corresponding covariance matrix evaluations, and in the realistic estimation of the uncertainties in the measurements.

The sensitivities of $k_{\text{eff}}$ and $\beta_{\text{eff}}$ are shown to present complementary features, suggesting that a combined use of both measurements can be optimal for the validation and improvement of nuclear data. Careful re-evaluation of some measurement uncertainties of the existing, and performing new beta-effective measurements using reactor noise or Cf techniques with, if possible, improved accuracy is recommended.

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