



# Beta-effective sensitivity and uncertainty analysis of MYRRHA reactor for possible use in nuclear data validation and improvement

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## ABSTRACT

New reactor concept studies, such as those of the MYRRHA Accelerator Driven System (ADS), with their extended nuclear data needs relaunched the interest in sensitivity and uncertainty (S/U) studies. S/U analysis play an essential role in assuring the accuracy and reliability of nuclear reactor computations and provide an insight in the physical phenomena involved in the neutron transport. This paper presents the study of the MYRRHA critical core, which is designed to operate at 100 MW thermal power. The previously presented analysis of the MYRRHA effective multiplication factor ( $k_{eff}$ ) was extended to study the sensitivity and uncertainty in kinetic parameters, such as the effective delayed neutron fraction ( $\beta_{eff}$ ). The sensitivity and uncertainty computations were performed by means of the SUSD3D code based on forward and adjoint-flux first-order perturbation theory. The sensitivity coefficients of  $\beta_{eff}$  with respect to the basic nuclear data were calculated by the k-ratio derivation method proposed in 2011. The main components of the uncertainties in  $\beta_{eff}$  were estimated using the JENDL-4.0u covariance data. The energy dependent sensitivity profiles of  $k_{eff}$  and  $\beta_{eff}$  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. The accuracy of the  $k_{eff}$  and  $\beta_{eff}$  measurements and calculations has to be carefully evaluated in order to conclude on the nuclear data status and possible improvements.

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## 1. Introduction

The uncertainty in nuclear data (ND) is one of the most important sources of uncertainty in reactor physics simulations. Although considerable progress has been achieved in the last decades, continuous efforts are still required to fill the gaps in our knowledge, improve the predictive power of the simulations and to meet the target accuracies and reliability needed for nuclear reactor applications. Sensitivity and uncertainty (S/U) analysis allow to identify the most relevant nuclear reaction types and isotopes, and thus to guide future works. Furthermore, the sensitivity coefficients can be used to estimate uncertainties in reactor parameters due to nuclear data uncertainties. Combined with benchmark experiment measurements, they play an essential role in assuring the accuracy and reliability of the nuclear reactor computations. The topic is of high relevance both for the nuclear safety analysis, as well as for the development of future nuclear reactor systems. Several international initiatives have recently expressed interest in nuclear data sensitivity and uncertainty analysis in the areas of fusion (e.g. ITER fusion reactor project in the scope

of Fusion for Energy (F4E) and EURATOM), safety analysis of the present reactors (OECD/Nuclear Energy Agency (NEA) project Uncertainty Analysis in Modelling (UAM) (Ivanov et al., 2013)), and the design and safety analysis of Advanced Fast Reactors and Advanced Fuel Cycle Scenarios (e.g. the ongoing project CHANDA (solving CHallenges in Nuclear Data) (CHANDA, 2013) of the European Commission (EC) and the Working Party on Evaluation Cooperation (WPEC) Subgroup 39) of the Nuclear Energy Agency (NEA) (NEA, 2017; Salvatores et al., 2014). The CHANDA project addresses the challenges in the field of nuclear data for nuclear applications (CHANDA DOW, 2013) with the objective to improve the nuclear data used in simulations, including the corresponding uncertainty files, in order to better understand (and if possible improve) the accuracy of numerical computations and consequently to improve the design and utilization of expensive experimental facilities. In particular, Work Package 10 (WP10) of CHANDA is focused on studying the nuclear data required for the development, safety assessment and licensing of the MYRRHA (Multi-purpose hYbrid Research Reactor for High-tech Applications) experimental reactor (Engelen et al., 2015) and on giving recommendations for data improvements for MYRRHA-relevant elements and isotopes.

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MYRRHA is a flexible experimental reactor being developed at SCK•CEN, aiming to demonstrate the feasibility of the Accelerator-Driven System (ADS) and the lead-cooled fast reactor concepts, with various applications from spent-fuel burning to material irradiation testing for GEN IV systems and fusion reactors. It will be able to work with two possible configurations: sub-critical (coupled to a LINAC proton accelerator) or critical. Since MYRRHA is based on the heavy liquid metal technology, Lead-Bismuth Eutectic, it will be able to significantly contribute to the development of Lead Fast Reactor technology.

MYRRHA with its specific materials comparing to the conventional nuclear reactors (such as MOX fuel, lead-bismuth coolant) represents several nuclear data challenges. Nuclear data induced uncertainties are of major concern for the accuracy of the simulations and therefore for the reactor safety and design. In this context of new reactor project studies the ND sensitivities and uncertainty tools are particularly valuable in order to understand the physical differences with respect to the present nuclear reactors and to evaluate and extrapolate the present experience and knowledge to future concepts. Reliable estimations of ND uncertainties are essential in order to conclude on the ND needs and guide the experimental activity in support of ND evaluations.

Among the basic fission reactor parameters the kinetic parameters such as the effective delayed neutron fraction ( $\beta_{\text{eff}}$ ) and the neutron generation lifetime ( $\Lambda$ ) play, besides the effective neutron multiplication factor ( $k_{\text{eff}}$ ), a major role in reactor safety and control analysis. The S/U analysis of the MYRRHA neutron multiplication factor  $k_{\text{eff}}$  performed in the framework of the CHANDA project were already presented in Romojaro et al. (2015, 2017). These analyses included the comparison of results obtained using several computer codes (SCALE (ORNL, 2011), MCNP6 (Pelowitz, 2014) and SUSD3D (Kodeli, 2001)), different transport cross sections (ENDF/B-VII.1 (Chadwick et al., 2011), JEFF (Koning, 2007)...) and covariance matrix data (SCALE-6.0 (NEA DB, 2011a), JENDL-4.0u (Iwamoto et al., 2011) and ENDF/B-VII.1).

The present paper extends the previous criticality ( $k_{\text{eff}}$ ) S/U analyses to  $\beta_{\text{eff}}$ .  $\beta_{\text{eff}}$  defines a unit of reactivity known as the dollar and as such, it plays an important role in reactivity accident analysis and is also used for interpretation of reactivity measurements by inverse solution of the kinetic equation. Its accuracy should be therefore well understood and evaluated. The values of  $\beta_{\text{eff}}$  vary from one isotope to the other (i.e. from  $\sim 200$  pcm for  $^{239}\text{Pu}$  to  $\sim 1570$  pcm for  $^{238}\text{U}$ ), therefore the reactor systems containing actinide isotopes in their fuel have to face the problem of lower values of the effective delayed neutron fractions due to the presence of Pu isotopes, making the reactor control of MOX fuelled cores more challenging. A supplementary objective of this work was to contribute to the diversification of the nuclear data validation process, at present to large extent limited to the  $k_{\text{eff}}$  measurements performed in critical benchmark configurations. Kinetic parameters are expected to provide additional and largely complementary information allowing in this way a more complete validation and improvement of nuclear data and radiation transport codes.

## 2. Computation tools and methods - SUSD3D/XSUN-2017

The S/U analysis of the MYRRHA reactor were performed using the SUSD3D (Kodeli, 2001, 2011a) code which is based on the first-order generalised perturbation theory (GPT) (Usachev, 1955; Gandini, 1967). The SUSD3D code derives, from the direct and adjoint fluxes calculated using the deterministic codes, the sensitivity coefficients and the standard deviations of the calculated detector responses or design parameters of interest (such as reaction rates, fluxes,  $k_{\text{eff}}$  and  $\beta_{\text{eff}}$ ) due to the input cross sections and

their uncertainties. The SUSD3D code system was applied in the past 20 years to different problems, from nuclear reactor criticality, radiation shielding of fission, fusion reactors and benchmarks, to medical and industrial applications (e.g. oil well logging).

SUSD3D can take into account the contributions of the uncertainties in the secondary energy and angular distribution (SED/SAD) of the emitted particles. Integral parameter uncertainties due to fission spectra uncertainties can be calculated either using the classical or the constrained sensitivity method (Kodeli et al., 2009). The latest version of the SUSD3D code is available as part of the Windows interface package XSUN-2017 (Kodeli and Slavič, 2017). The XSUN-2017 package includes, besides SUSD3D, also the TRANSX (MacFarlane, 1995) code for the cross section preparation, and the PARTISN neutron/gamma discrete ordinates transport code (Alcouffe et al., 2008), as well as nuclear data and covariance matrix libraries and plotting tools (Soppera, 2016).

Among others, the SUSD3D code also calculates  $\beta_{\text{eff}}$  and the corresponding sensitivities and uncertainties.  $\beta_{\text{eff}}$  and all its components by actinides are calculated as the  $k_{\text{eff}}$  sensitivities with respect to the delayed neutron yields ( $\bar{v}_{d,i}$ ) for all fissionable isotopes  $i$ . Indeed, as demonstrated in Kodeli (2013) the definition of  $\beta_{\text{eff}}$  as given in Keepin (1965) is equivalent to the sensitivity of  $k_{\text{eff}}$  to the delayed neutron fission yield as defined in the 1<sup>st</sup> order perturbation theory:

$$\beta_{\text{eff}} = \frac{\langle \Phi^+, F_d \Phi \rangle}{\langle \Phi^+, F \Phi \rangle} = \sum_i \frac{v_{d,i}}{k_{\text{eff}}} \frac{\partial k_{\text{eff}}}{\partial v_{d,i}} = \sum_i S_{v_{d,i}} \quad (1)$$

where:  $\Phi$  and  $\Phi^+$  denote the direct and adjoint angular fluxes,  $F$  and  $F_d$  are the total and delayed neutron generator operators. The summation goes over all fissionable isotopes  $i$  present in the model. The brackets  $\langle \rangle$  represent the inner product integrated over all independent variables (space, energy and angle).

Adjoint calculations are much more challenging for the continuous energy Monte Carlo codes, however  $\beta_{\text{eff}}$  can still be calculated from Eq. (1) using Monte Carlo codes with implemented GPT capability, which thus represents an exact alternative to the Bretscher's (prompt k-ratio) approximation (Bretscher, 1997):

$$\beta_{\text{eff}} = 1 - \frac{k_p}{k} \quad (2)$$

From the above it also follows that,  $\beta_{\text{eff}}$  being the 1<sup>st</sup> derivative, the sensitivity of  $\beta_{\text{eff}}$  can be obtained as a 2<sup>nd</sup> derivative of  $k_{\text{eff}}$ . Calculation of second order sensitivities is computationally intensive, but is possible using some Monte Carlo codes such as SERPENT GPT and MCNP6.

In the SUSD3D deterministic code, a different approach was developed in 2011 for the S/U calculations, which is based on the derivation of the Bretscher's (prompt k-ratio) approximation (Kodeli, 2011b, 2013):

$$S_\beta = \frac{\sigma}{\beta_{\text{eff}}} \frac{\partial \beta_{\text{eff}}}{\partial \sigma} = \frac{1 - \beta_{\text{eff}}}{\beta_{\text{eff}}} (S_k - S_{k_p}) \quad (3)$$

where  $k_p$  is the  $k_{\text{eff}}$  taking into account only prompt neutrons and  $k$  is the total (prompt and delayed neutron)  $k_{\text{eff}}$ . The two terms  $S_k$  and  $S_{k_p}$  correspond to the sensitivities of the factors  $k$  and  $k_p$  which are calculated using the standard linear perturbation theory.

Since  $k_p$  does not depend on  $v_{d,i}$ , it is easy to see that the  $\beta_{\text{eff}}$  sensitivity to  $v_{d,i}$ , usually of principal importance, is simply proportional to the  $k_{\text{eff}}$  sensitivity to  $v_{d,i}$  ( $S_{k_{v_{d,i}}}$ ):

$$S_{\beta_{v_{d,i}}} = \frac{v_{d,i}}{\beta_{\text{eff}}} \frac{\partial \beta_{\text{eff}}}{\partial v_{d,i}} = \frac{1 - \beta_{\text{eff}}}{\beta_{\text{eff}}} S_{k_{v_{d,i}}} \quad (4)$$

A similar method was later the same year independently proposed by Chiba et al. (2011).

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