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Benchmarking and application of the state-of-the-art uncertainty analysis methods XSUSA and SHARK-X

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ABSTRACT

This study presents collaborative work performed between GRS and PSI on benchmarking and application of the state-of-the-art uncertainty analysis methods XSUSA and SHARK-X. Applied to a PWR pin cell depletion calculation, both methods propagate input uncertainty from nuclear data to output uncertainty. The uncertainty of the multiplication factors, nuclide densities, and fuel temperature coefficients derived by both methods are compared at various burnup steps. Comparisons of these quantities are furthermore performed with the SAMPLER module of SCALE 6.2. The perturbation theory based TSUNAMI module of both SCALE 6.1 and SCALE 6.2 is additionally applied for comparisons of the reactivity coefficient.

1. Introduction

Beside conservative assumptions in nuclear safety analyses for licensing processes, there is an ongoing tendency to use best-estimate codes. This approach is supported by the application of established uncertainty evaluation methods to determine uncertainties of calculated results. In addition to the determination of the accuracy of the numerical method, uncertainty quantification includes propagation of input uncertainty from nuclear data and manufacturing to output uncertainty. The OECD/NEA benchmark for Uncertainty Analysis in Modelling (UAM) Ivanov et al., 2007 was launched almost ten years ago to promote the development of such methods in best-estimate coupled multi-physics and multi-scale simulations of light water reactors. The assessment of uncertainties is important for the determination of appropriate design margins and for understanding how those uncertainties can be reduced.

In recent years, capabilities for uncertainty quantification with respect to nuclear data have been developed at PSI and GRS. Since these methods can already be efficiently applied, uncertainty analyses should always be performed in addition to best-estimate calculations. Consequently, this study is oriented towards the BEPU (best-estimate plus uncertainty) approach by applying best-estimate neutron transport and depletion codes combined with uncertainty quantification of calculated results. GRS and PSI applied their methods on the TMI-1 pin cell depletion exercise which is specified in the context of the UAM benchmark. The multiplication factor uncertainty over burnup is determined along with an evaluation of the main contributors to this uncertainty at specific burnup steps.

Furthermore, at a burnup of 60 MWd/kgHM, uncertainties of nuclide densities are assessed for a selection of nuclides considered important for radiological protection during normal and abnormal operation of a nuclear power plant and for the final disposal of fuel assemblies. During a transient event, the fuel temperature coefficient plays an important role. For this reason, an accurate quantification and its uncertainty is an essential prerequisite for a safe reactor design. An uncertainty quantification and a sensitivity analysis are performed to assess the uncertainty of the fuel temperature reactivity coefficient at the burnup steps 0, 30 and 60 MWd/kgHM.

The uncertainties obtained with the GRS and PSI methods are compared in terms of the mentioned quantities. Additionally, comparisons are performed with the SAMPLER module of SCALE 6.2 (Williams et al., 2013). In terms of the reactivity coefficient, the perturbation theory based TSUNAMI module (Mueller et al., 2009) of both SCALE 6.1 and SCALE 6.2 is applied.

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2. Simulation tools used for UQ/SA analysis

The methodologies used at PSI and GRS to perform uncertainty quantification (UQ) and sensitivity analysis (SA) are detailed below. First the UQ approaches used by both organisations are summarized. Then, the specific methods to perform SA are shown and finally the uncertain inputs considered in this work are presented.

2.1. Uncertainty quantification

The GRS code XSUSA (Cross Section Uncertainty and Sensitivity Analysis) (Zwermann et al., 2009; Bostelmann et al., 2015) and the PSI code SHARK-X (Wieselquist et al., 2013; Ferroukhi et al., 2014; Hursin et al., 2015) are used to determine uncertainties in the results of neutron transport calculations with respect to uncertainties in nuclear data. Both codes rely on the stochastic sampling method: Appropriate probability distributions are assigned to input quantities. These input quantities are then sampled while taking into account correlations between them. For each sample, an independent transport calculation is performed, and the set of sample calculations are statistically analysed in order to obtain output quantities such as the multiplication factor and nuclide densities together with their uncertainties. Both codes allow the assessment of the importance of uncertain input parameters with respect to the total output uncertainty.

In the current version of XSUSA, neutron transport codes in combination with the ENDF/B-VII.0 238-group cross section library and nuclear covariance data of the SCALE 6.1 code package (SCALE, 2011) are applied. The cross sections are perturbed after the self-shielding calculation. The implicit effects (corresponding to the perturbation of the self-shielding factors) are therefore not taken into account.

SHARK-X is a set of Perl-based scripts build around the lattice code CASMO-5 (Rhodes et al., 2006) in order to perform uncertainty quantification. The perturbed cross sections are directly introduced in the CASMO-5 code through an in-house routine added to the code. This allows the perturbation of the cross sections after the self-shielding. Thus, the implicit effect (Hursin et al., 2015) is also not taken into account in the PSI methodology. In this work, CASMO-5 uses a 586-group cross section library based on ENDF/B-VII.0 (Rhodes et al., 2009) and nuclear covariance data of the SCALE 6.1 and SCALE 6.2 code packages (Rearden and Jessee, 2016) were applied.

For further comparisons, the TSUNAMI and SAMPLER modules of the SCALE code package in combination with the 44-group ENDF/B-VII.0 Variance Covariance Matrices (VCMs) were used. With TSUNAMI, the multiplication factor uncertainty is obtained by first order perturbation theory. Other responses such as few-group cross sections can be obtained by the application of generalised perturbation theory. SAMPLER is part of SCALE 6.2 (Rearden and Jessee, 2016) and based on a random sampling approach. Perturbation of nuclear data is thereby done before the self-shielding calculation.

2.2. Sensitivity analysis

One of the major issues for the UQ in the stochastic sampling approach is that no sensitivity information is generated as a by-product of the analysis. Such information is however highly desirable to understand the input parameters contributing the most to the overall computed uncertainty.

An approximated method has been developed recently in SHARK-X. The basic idea is to infer the energy independent sensitivity coefficients of the output to the various input parameters from the input samples and the corresponding output samples. The sensitivity coefficients are computed using a least square solver. By folding the sensitivity information with existing input covariance information, it is possible to use the sandwich rule and to determine the fraction of the total variance of the considered response due to each input parameter. The details of the equations can be found in Hursin et al. (2016).

To investigate the major sources of the uncertainty, squared multiple correlation coefficients R^2 were determined for the SAMPLER and XSUSA results. This coefficient reveals the relative amount of the output uncertainty coming from an input quantity. It is determined from correlations of the calculated output quantity with the sampled input quantity, while taking into account correlations between input quantities (Bostelmann et al., 2015). R^2 is calculated for all possible reactions and afterwards ranked according to size in order to obtain the top contributors. As an example, the correlation coefficient R^2 for the output uncertainty of k_∞ coming from a particular cross section σ is calculated as follows:

$$R^2 = (\rho(k_\infty, \sigma_1), \ldots, \rho(k_\infty, \sigma_{44})) \cdot C_\sigma^{-1} \cdot \begin{pmatrix} \rho(k_\infty, \sigma_1) \\ \ldots \\ \rho(k_\infty, \sigma_{44}) \end{pmatrix}$$

$\rho(k_\infty, \sigma_i)$ is the correlation coefficient between k_∞ and the particular input cross section σ_i of energy group $i\epsilon[1,44]$. Those coefficients are calculated easily by means of the 1000 sample calculations of k_∞ and the corresponding sampled cross section. C_a^{-1} is the inverse of the covariance matrix of this particular reaction in 44 groups. R^2 is then providing the amount of the uncertainty of k_∞ that is due to the particular cross section.

2.3. Input uncertainty

The list of uncertain input considered in this work is composed of the cross sections, neutron multiplicity ($\bar{\nu}$) and total fission spectrum (χ). Specifically for depletion calculations, the uncertainties in fission yields and decay constants are also considered. The sources of input uncertainty, i.e. variance and covariance between inputs are detailed below.

2.3.1. Cross sections

Two VCM sources are used in this work. The main source is the SCALE 6.1 VCM library (SCALE, 2011), which contains 401 materials from a variety of sources, including evaluations from ENDF/B-VII.0, ENDF/B-VI.8, JENDL-3.1, plus 300 approximate VCMs such that all relevant nuclides have uncertainty data. The SCALE 6.1 VCM library represents a collaborative effort from Brookhaven National Lab (BNL), Oak Ridge National Lab (ORNL), and Los Alamos National Lab (LANL). It is formatted in a 44-energy group structure.

Recently, ORNL has started testing a new version of SCALE, SCALE 6.2, which contains a 56-group VCM library. This library contains 402 materials from a variety of sources, including evaluations from ENDF/B-VII.1 (187 isotopes), ENDF/B-VII.1 pre-released, ENDF/B-VII.0 and low-fidelity uncertainties from BNL/LANL/ORNL.

2.3.2. Fission yield and decay constants

Perturbation of fission yields and decay constants during depletion calculations is essential to assess the uncertainty of the nuclide composition in spent fuel (Ferroukhi et al., 2014). Fission yields are subjected to constraints such as basic physical laws (e.g. two fission products per fission if the ternary fission is not considered). Classical stochastic sampling of fission yields as applied to cross sections without considering these constraints would therefore not handle fission yields adequately and result in an incorrect estimation of the uncertainty.