Treatment of Implicit Effects with XSUSA

Friederike Bostelmann[1,2], Andreas Pautz[2], Winfried Zwermann[1]

[1] *Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) gGmbH, Boltzmannstraße 14, 85748 Garching, Germany*
[2] *École polytechnique fédérale de Lausanne, 1015 Lausanne, Switzerland*
friederike.bostelmann@grs.de, andreas.pautz@epfl.ch, winfried.zwermann@grs.de

Abstract - *For nuclear data uncertainty and sensitivity analysis of neutron transport calculations, the random sampling based XSUSA (Cross Section Uncertainty and Sensitivity Analysis) method has been developed over the years. For the application of the randomly sampled perturbation factors on the corresponding cross sections, the variations of problem-dependent cross sections have so far been assumed to be identical to those of the corresponding problem-independent cross sections; the so-called implicit effects have not been taken into account. In this work, a first-order perturbation theory-based approach for the consideration of implicit effects with XSUSA is presented. The perturbation factors for problem-independent cross sections are adjusted with information given in a single one-dimensional perturbation calculation in order to consider the impact of the self-shielding calculation on the cross section perturbations. In direct perturbation calculations, this approach is applied for the determination of sensitivities of the multiplication factor and the Doppler reactivity to H-1 and U-238 elastic scattering, and to the U-238 n,γ reaction in a light water reactor pin cell. The impact of implicit effects can in particular be observed in the resonance peaks of the sensitivity profiles. The adequate consideration of implicit effects with XSUSA is confirmed in comparisons with corresponding TSUNAMI calculations.*

I. INTRODUCTION

For the propagation of nuclear data uncertainties to output uncertainties in neutron transport calculations, the XSUSA (Cross Section Uncertainty and Sensitivity Analysis) method has been developed over the years [1]. With XSUSA, the nuclear cross sections are randomly sampled on the basis of corresponding covariance data and serve as input for multi-group neutron transport codes. The analysis can be performed on any output quantity of the transport code since the output uncertainties are derived by a statistical analysis of the sample calculations.

For multi-group transport calculations, the problem-independent (unshielded) multi-group cross sections contained in the nuclear data library are modified into problem-dependent (shielded) values by means of so-called self-shielding calculations. In the XSUSA method, the variations of the cross sections in the form of perturbation factors have so far been applied to shielded cross sections. This means that the changes of the shielded cross sections caused by changes in the unshielded cross sections, the so-called implicit effects, have not been taken into account; the variations of the shielded cross sections have been assumed to be identical to those of the unshielded cross sections. This approach is followed in order to reduce the total runtime for the calculations. The self-shielding calculation has to be performed only once for the nominal calculation; the self-shielding calculations for the perturbed calculations are omitted.

In many comparisons with models of a broad variety of spectral conditions, it appeared that the negligence of implicit effects only has a small influence on the investigated output

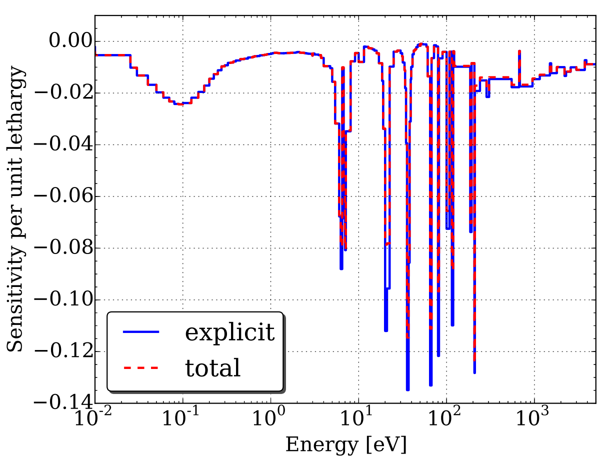

Fig. 1. Sensitivity of k_∞ to U-238 n,γ obtained with TSUNAMI.

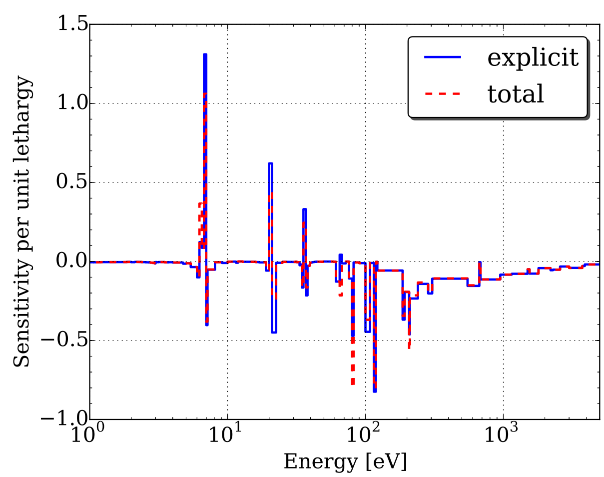

Fig. 2. Sensitivity of ρ to U-238 n,γ obtained with TSUNAMI.

uncertainties [2]. However, it cannot be excluded that there are systems which show larger implicit effects in uncertainty analyses.

Although the impact of implicit effects on integrated values and their uncertainties might be small, an influence could be observed in accompanying sensitivity analyses. Implicit effects are, for example, of particular importance for the n,γ reaction of U-238. In Fig. 1 and 2, exemplary sensitivity profiles for the multiplication factor k_∞ and the Doppler reactivity ρ obtained with TSUNAMI, the first-order perturbation theory based uncertainty analysis tool of the SCALE code package [3], for a light water reactor unit cell are presented. Differences between the explicit sensitivity and the total sensitivity (explicit and implicit) are clearly visible, especially in the resonance peaks.

In this work, an approach for the consideration of implicit effects in uncertainty and sensivity calculations using the random-sampling approach with XSUSA is presented. By means of first-order perturbation theory, the present perturbation factors for the shielded cross sections are adjusted. It shall be emphasized that perturbation theory is only applied to obtain corrections for the varied shielded cross sections arising from implicit effects. The main contributions to the output uncertainties arising from the explicit part are still captured through the random sampling, i.e. without contraints regarding the order of effects.

II. TREATMENT OF IMPLICIT EFFECTS

For the random sampling of cross sections with XSUSA, perturbation factors $p^j_{y,g}$ for the cross sections Σ of each nuclide j with all reactions y in all energy groups g are generated:

$$p^j_{y,g} = 1 + \frac{\Delta\Sigma^j_{y,g}}{\Sigma^j_{y,g}} . \tag{1}$$

For the determination of these perturbation factors, it is referred to previous publications about the GRS random sampling method [1]. The perturbation factors are derived from covariance data belonging to unshielded cross sections. Consequently, a perturbation factor would normally need to be applied to the unshielded macroscopic cross section $\Sigma^j_{y,g}$. Within the XSUSA sampling sequence, however, we want to apply the perturbation on shielded cross sections $\bar{\Sigma}^j_{y,g}$, i.e. a perturbation factor as follows:

$$\bar{p}^j_{y,g} = 1 + \frac{\Delta\bar{\Sigma}^j_{y,g}}{\bar{\Sigma}^j_{y,g}} . \tag{2}$$

In the calculation of this perturbation factor, the impact of the self-shielding on the perturbation shall be considered.

1. Derivation with First-Order Perturbation Theory

In first-order perturbation theory [4], a response R to a perturbation of an input parameter α can be written as

$$\frac{\Delta R}{R} = S_{R,\alpha} \frac{\Delta\alpha}{\alpha} . \tag{3}$$

For sufficiently small α, R depends linearly on α, and the relative sensitivity coefficient of R with respect to α becomes:

$$S_{R,\alpha} = \frac{\alpha}{R}\frac{\mathrm{d}R}{\mathrm{d}\alpha} . \tag{4}$$

Because of the assumption that the response perturbation is linearly related to the perturbation in α, the net response to changes in different input parameters α_i is the sum of the individual perturbations:

$$\frac{\Delta R}{R} = \sum_i \left(S_{R,\alpha_i} \frac{\Delta\alpha_i}{\alpha_i} \right) . \tag{5}$$

Since we are interested in the influence of the unshielded cross sections (individual perturbations) to the shielded cross section (response), we obtain the following relation:

$$\begin{aligned} \frac{\Delta\bar{\Sigma}^j_y}{\bar{\Sigma}^j_y} &= \sum_{i,x} \left(S_{\bar{\Sigma}^j_y,\Sigma^i_x} \frac{\Delta\Sigma^i_x}{\Sigma^i_x} \right) \\ &= \sum_{i,x} \left(\frac{\Sigma^i_x}{\bar{\Sigma}^j_y} \frac{\mathrm{d}\bar{\Sigma}^j_y}{\mathrm{d}\Sigma^i_x} \frac{\Delta\Sigma^i_x}{\Sigma^i} \right) \end{aligned} \tag{6}$$

with sums over i denoting all possible nuclides including j, and x denoting all possible reactions including y. For reasons of simplicity, the group index is omitted. The perturbation factor for the shielded cross sections of Eq. 2 can therefore be described as follows:

$$\begin{aligned} \bar{p}^j_y &= 1 + \sum_{i,x} \left(\frac{\Sigma^i_x}{\bar{\Sigma}^j_y} \frac{\mathrm{d}\bar{\Sigma}^j_y}{\mathrm{d}\Sigma^i_x} \frac{\Delta\Sigma^i_x}{\Sigma^i_x} \right) \\ &\overset{(1)}{=} 1 + \sum_{i,x} \left(\underbrace{\frac{\Sigma^i_x}{\bar{\Sigma}^j_y} \frac{\mathrm{d}\bar{\Sigma}^j_y}{\mathrm{d}\Sigma^i_x}}_{(*)} \left(p^i_x - 1 \right) \right) . \end{aligned} \tag{7}$$

2. Application

As can be seen from Eq. 7, the desired perturbation factors $\bar{p}^j_{y,g}$ can be obtained in a function dependent on the existing perturbation factors for the unshielded cross sections generated with XSUSA, and the sensitivities of the shielded cross sections in terms of the unshielded cross sections. For the latter term that is denoted with $(*)$, the chain rule for derivatives can be applied to obtain an expression with terms that are evaluated by the self-shielding part of the first-order perturbation theory-based TSUNAMI-1D code [5]:

$$\begin{aligned} &\frac{\Sigma^i_{x,g}}{\bar{\Sigma}^j_{y,g}} \frac{\mathrm{d}\bar{\Sigma}^j_{y,g}}{\mathrm{d}\Sigma^i_{x,g}} \\ &= \left(\frac{\Sigma^i_{T,g}}{\bar{\Sigma}^j_{y,g}} \frac{\partial\bar{\Sigma}^j_{y,g}}{\partial\Sigma^i_{T,g}} + \sum_m \left[\frac{C_m}{\bar{\Sigma}^j_{y,g}} \frac{\partial\bar{\Sigma}^j_{y,g}}{\partial C_m} \cdot \frac{\Sigma^i_{T,g}}{C_m} \frac{\partial C_m}{\Sigma^i_{T,g}} \right] \right) \frac{\Sigma^i_{x,g}}{\Sigma^i_{T,g}} \frac{\partial\Sigma^i_{T,g}}{\partial\Sigma^i_{x,g}} \end{aligned} \tag{8}$$

with the unshielded total cross section $\Sigma^i_{T,g}$ and the Dancoff factors C_m for each material zone m. The individual terms are available from TSUNAMI including SAMS, the sensitivity analysis module of SCALE.

With the help of various TSUNAMI and SAMS output files, the unshielded perturbation factors from XSUSA can consequently be modified in order to obtain shielded perturbation factors following Eq. 7. As usual, these perturbation factors can be applied to cross sections in direct perturbation or random sampling calculations.

III. MODEL AND CALCULATION METHOD

The studied model is the TMI-1 PWR unit cell configuration of the OECD/NEA Uncertainty Analysis in Modelling (UAM) benchmark, Exercise I-1b (cf. Fig. 3) [6]. A UO_2 fuel pellet of diameter 9.391 mm is surrounded by a helium filled gap with an outer diameter of 9.582 mm and a Zircaloy-4 cladding with outer diameter 10.928 mm. The fuel has a mass densitiy of 10.283 g/cm^3 and an U-235 enrichment of 4.85 wt.-%, and the cladding mass densitiy is 6.55 g/cm^3. The water moderator density is 748.4 kg/cm^3. The applied temperatures are as follows: 900 K for the fuel, 600 K for the cladding and 562 K for the moderator. For the determination of the Doppler reactivity, the fuel temperature was raised to 1500 K. (When increasing the fuel temperature by 600 K, the linear assumption of the Doppler reactivity was not regarded. This is justified for the present study since the determined reactivity only serves as an exemplary quantity for the comparison of the applied methods.)

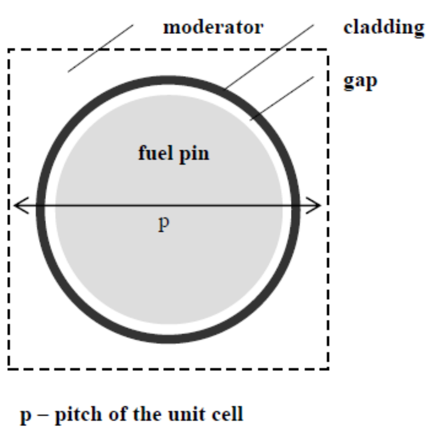

Fig. 3. TMI-1 PWR unit cell [6]

For the present study, XSUSA is applied in direct perturbation mode, i.e. the cross sections of a set of nuclide reactions are group-wise perturbed by a constant value. Direct perturbation calculations were chosen in order to determine sensitivity profiles and to clearly demonstrate the implicit effects. The variations have thereby to be sufficiently large to allow the identification of effects; but at the same time they have to be small enough to avoid higher order effects. These requirements are found to be met with variations of ±5%. The considered cross sections are elastic scattering of U-238 and H-1, and the n,γ reaction of U-238, since it is expected that the influence of these unshielded cross sections to the shielded cross sections is significant.

The calculations are performed with several codes of the SCALE 6.1 code package [3]. The applied transport solver for the individual variation calculations is the two-dimensional deterministic code NEWT, and the adjustment of the perturbation factors as discussed in the previous section is based on a single TSUNAMI-1D calculation. For comparison, corresponding TSUNAMI-2D calculations are performed with and without the consideration of implicit effects. For all calculations, 238-group ENDF/B-VII.0 data is applied.

IV. RESULTS

The sensitivities of the multiplication factor k_∞ and the Doppler reactivity ρ to U-238 elastic scattering, the U-238 n,γ reaction, and to H-1 elastic scattering are compared between XSUSA and TSUNAMI. The calculations without implicit effects (explicit) are thereby compared to corresponding calculations with both explicit and implicit effects (total). In addition to sensitivity profiles, also integrated sensitivities and resulting output uncertainties are determined.

1. Modification of perturbation factors

Since XSUSA is applied in direct perturbation mode with variations of ±5%, the unshielded perturbation factors p_y^i are 0.95 and 1.05 for each energy group, respectively. Due to the application of the presented approach for the consideration of implicit effects, the shielded perturbation factors $\bar{p}_y^j$ of Eq. 7 are obtained. As an example, the sensitivities of the shielded to the unshielded cross sections are displayed in Fig. 4 for the U-238 n,γ and U-238 elastic scattering cross sections. These sensitivities correspond to the term indicated with $(*)$ in Eq. 7 for $x = y$ and $i = j$. The modification is clearly visible in the resonance region of U-238; the perturbation factors are significantly changed in this important energy range.

For the considered system, it is moreover observed that the variations in the considered unshielded cross sections (U-238 n,γ and elastic scattering, and H-1 elastic scattering) mainly influence the shielded U-238 n,γ cross sections; i.e. the major modification of the perturbation factors is caused by the sensitivity of the shielded U-238 n,γ cross section to the other considered unshielded cross sections.

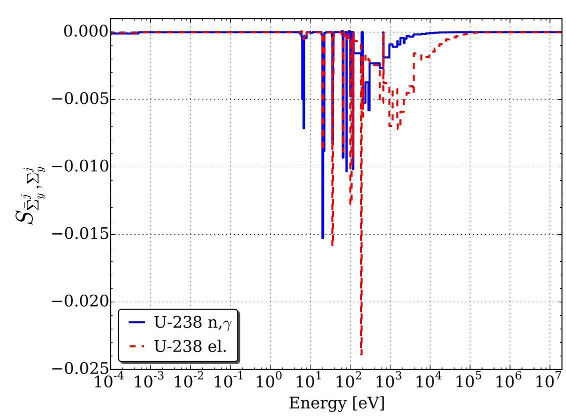

Fig. 4. Sensitivity of the shielded to the unshielded cross section at 900 K.

2. Explicit sensitivity profiles

The explicit sensitivity profiles of TSUNAMI and XSUSA are almost consistent (cf. Fig. 5–6). Only insignificant differences in the resonance peaks can be observed. Since the applied variations are small enough to avoid higher order effects and to allow a direct comparison between the results, it is suggested that the observed slight differences are caused by the underlying method, meaning first-order perturbation theory in contrast to direct perturbation.

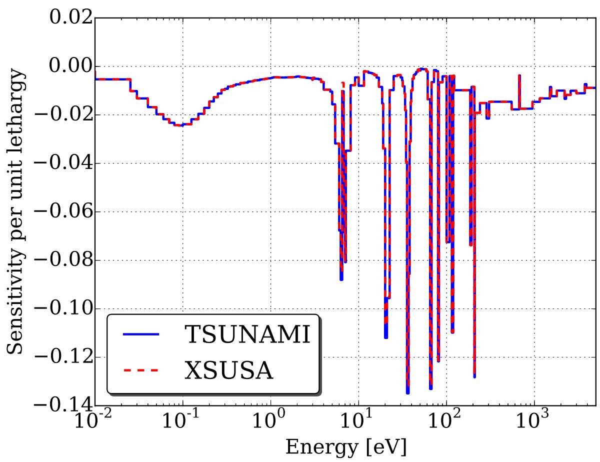

Fig. 5. Explicit sensitivity of k_∞ to U-238 n,γ.

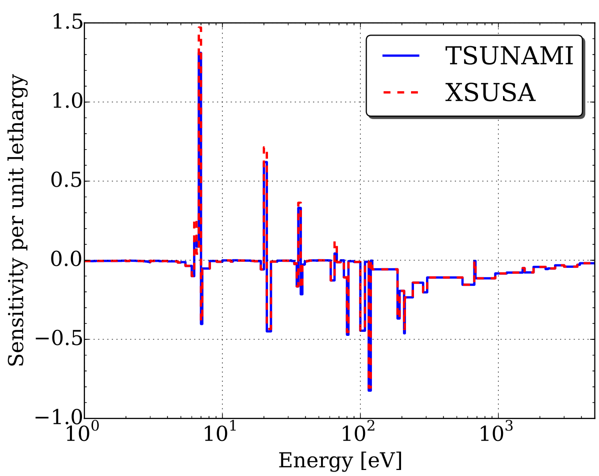

Fig. 6. Explicit sensitivity of ρ to U-238 n,γ.

3. Impact of implicit effects on sensitivity profiles

In both the TSUNAMI and the XSUSA calculations, the impact of implicit effects is clearly visible in the resonance peaks (cf. Fig. 1–2 and Fig. 7–10). For both investigated responses, XSUSA and TSUNAMI show almost consistent results for the total sensitivities, similar to the comparison of the explicit sensitivities (cf. Fig. 11–12). In addition to deviations caused by the different methods, another cause of differences in these cases might be the consideration of only a few major contributors in the implicit treatment with XSUSA. The influence of other unshielded cross sections to shielded cross sections is small and therefore neglected in this study. Furthermore the sensitivity of the shielded cross section to the Dancoff factor (cf. Eq. 8) is considered only for elastic scattering of H-1 since this contribution is negligible for the other reactions. In the full implementation of the method, all sensitivities will be considered independently of their importance.

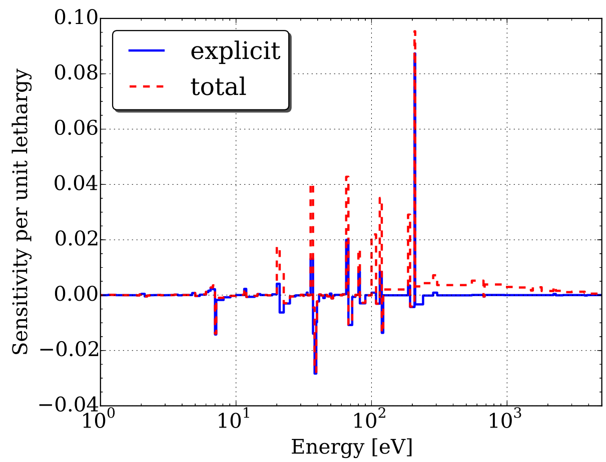

Fig. 7. Sensitivity of k_∞ to U-238 elastic scattering obtained with XSUSA.

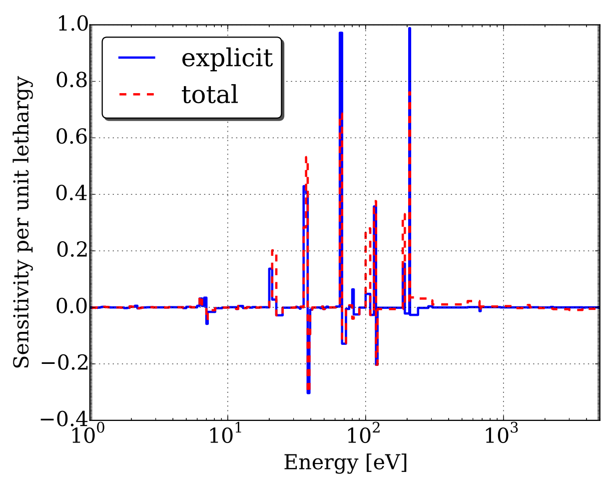

Fig. 8. Sensitivity of ρ to U-238 elastic scattering obtained with XSUSA.

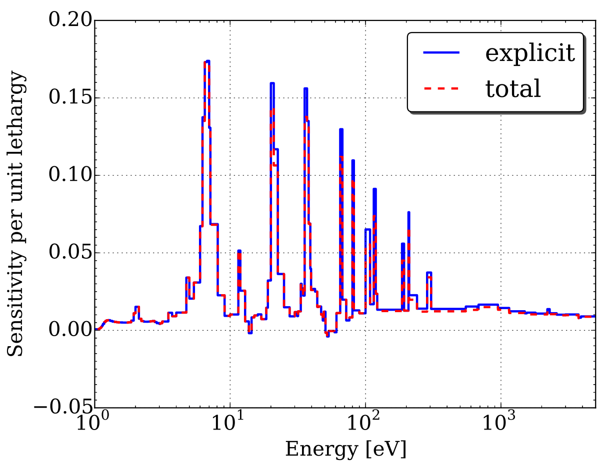

Fig. 9. Sensitivity of k_∞ to H-1 elastic scattering obtained with XSUSA.

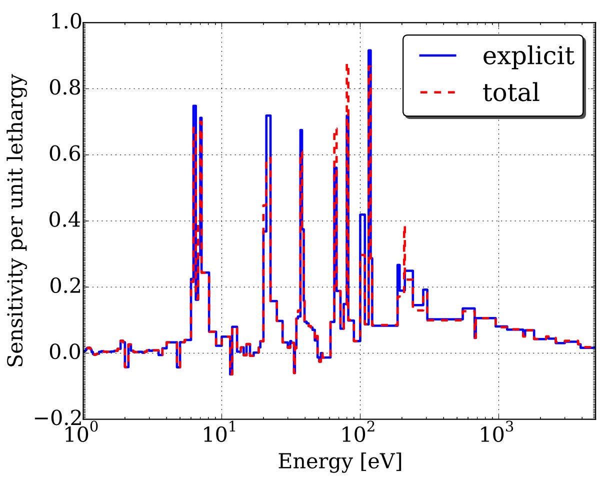

Fig. 10. Sensitivity of ρ to H-1 elastic scattering obtained with XSUSA.

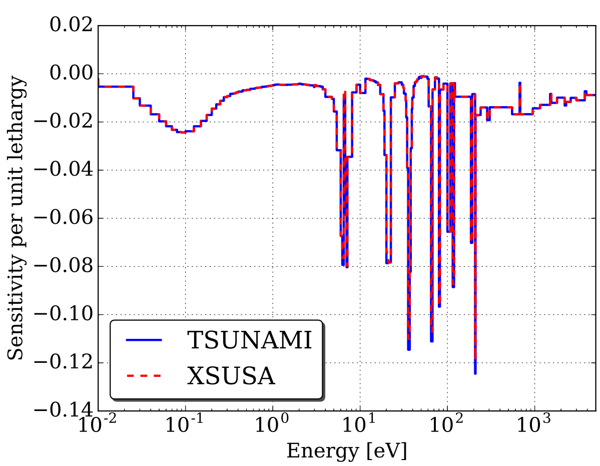

Fig. 11. Total sensitivity of k_∞ to U-238 n,γ.

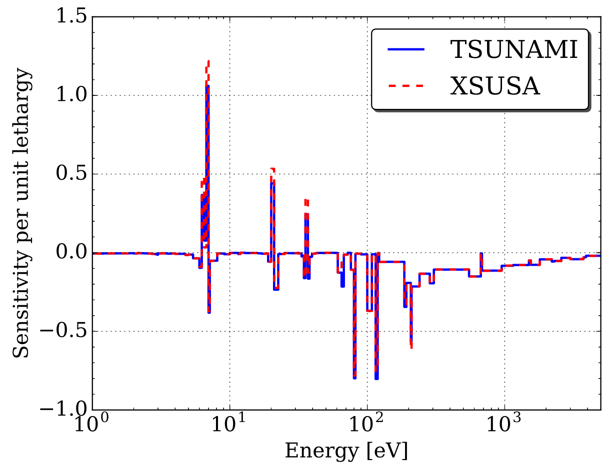

Fig. 12. Total sensitivity of ρ to U-238 n,γ.

4. Impact of implicit effects on integrated sensitivities

In addition to the sensitivity profiles, the integrated sensitivities can be determined to obtain cumulative values for the comparison between XSUSA and TSUNAMI and to estimate a cumulative impact of the implicit effect. The integrated sensitivitis of the multiplication factor and the Doppler reactivity are displayed in Table I.

Both codes show a decrease of the integrated sensitivitiy of k to H-1 elastic scattering and U-238 n,γ due to implicit effects by about 5% and 4%, respectively. The sensitivities to U-238 elastic scattering are in contrast strongly increased by factors of about 7 and 10 for TSUNAMI and XSUSA, respectively. The impact of the implicit effects is smaller for the integrated sensitivities of ρ. The sensitivity to U-238 elastic scattering is increased by a factor of about 1.5, and the sensitivities to the other two reactions are decreased by less than 2%.

5. Impact of implicit effects on uncertainty quantification

The variance of output responses can be determined with the so-called sandwich rule:

$$var(R) = S_{R,\alpha} C_{\alpha,\alpha} S^T_{R,\alpha} \tag{9}$$

with $S^T_{R,\alpha}$ being the sensitivity of R to the parameter α, and $C_{\alpha,\alpha}$ being the covariance matrix of the uncertain input parameter α. By using the covariance matrices provided with SCALE 6.1 together with the determined sensitivities, the individual contributions of the investigated nuclide reactions to the uncertainty of the multiplication factor and the Doppler reactivity can be calculated. The results for the reactions under investigation are presented in Table II.

It shall be stressed here that a large sensitivity of a response due to a particular nuclide reaction does not necessarily lead to a large contribution to the total response uncertainty. The integrated absolute sensitivity of k to H-1 elastic scattering is, for example, larger than the integrated sensitivity to U-238 n,γ (cf. Table I). Since the uncertainty of H-1 elastic scattering is about 0.1% in the sensitive energy range compared to more

TABLE I. Integrated sensitivities of k and ρ to the individual nuclide reactions.

	Reaction	TSUNAMI explicit	TSUNAMI total	XSUSA explicit	XSUSA total
k	H-1 el.	-0.2236	-0.2144	-0.2225	-0.2131
	U-238 el.	-0.0023	0.0166	-0.0017	0.0170
	U-238 n,γ	0.1906	0.1806	0.1915	0.1816
ρ	H-1 el.	-0.5086	-0.5090	-0.4861	-0.4808
	U-238 el.	0.0557	0.0898	0.0691	0.0977
	U-238 n,γ	0.7485	0.7401	0.7535	0.7385

TABLE II. Relative uncertainty of k and ρ due to uncertainties of the individual nuclide reactions.

	Reaction	TSUNAMI explicit	TSUNAMI total	XSUSA explicit	XSUSA total
k	H-1 el.	0.0265%	0.0255%	0.0267%	0.0257%
	U-238 el.	0.0115%	0.0250%	0.0091%	0.0264%
	U-238 n,γ	0.2872%	0.2747%	0.2861%	0.2734%
ρ	H-1 el.	0.1292%	0.1276%	0.1301%	0.1281%
	U-238 el.	0.2300%	0.2449%	0.2851%	0.2764%
	U-238 n,γ	0.9236%	0.9178%	0.9113%	0.8965%

than 3% in case of U-238 n,γ, the contribution of H-1 elastic scattering to the total uncertainty of k is still comparatively small.

The impact of the implicit effects on the contribution to the response uncertainty can clearly be observed in Table II. The contribution of H-1 elastic scattering and U-238 n,γ to the uncertainty of k is decreased by about 4% when implicit effects are considered, whereas the contribution of U-238 elastic scattering is more than doubled. XSUSA and TSUNAMI therby show consistent results. For the contribution to the uncertainty of ρ, the impact of implicit effects is slightly different between XSUSA and TSUNAMI. For U-238 elastic scattering, XSUSA shows a decreased contribution to the uncertainty by about 3%, whereas TSUNAMI shows an increased contribution by about 6.5%. Beside the impact of the implicit effects, the individual contributions already show differences between XSUSA and TSUNAMI by about 24% and 13% for the explicit and total calculations, respectively (similar to the differences of the integrated sensitivities). For the other contributions, slightly decreased uncertainties are observed for both XSUSA and TSUNAMI with small differences between the two codes.

V. CONCLUSIONS AND OUTLOOK

A first-order perturbation theory-based approach for the consideration of implicit effects with XSUSA was presented. With the applied procedure, the perturbation factors for unshielded cross sections are adjusted with information given in a single TSUNAMI-1D calculation in order to consider the impact of the self-shielding calculation on the cross section perturbations.

In direct perturbation calculations, this approach was applied for the determination of sensitivities of the multiplication factor and the Doppler reactivity to H-1 and U-238 elastic scattering, and to the U-238 n,γ reaction. Comparisons of integrated sensitivities and the individual contributions of the investigated reactions to the multiplication factor and Doppler reactivity uncertainties revealed an impact of implicit effects on the results for H-1 elastic scattering and U-238 n,γ of a few per cent. The impact on U-238 elastic scattering was, however, large such that the contribution to the multiplication factor uncertainty became relevant. The impact of implicit effects could furthermore clearly be observed in the resonance peaks of the sensitivity profiles. Comparisons between XSUSA and TSUNAMI revealed almost consistent results. The observed slight differences might mainly be caused by the underlying methods, meaning first-order perturbation theory in contrast to direct perturbation. It is consequently shown that implicit effects are adequately considered with XSUSA and the presented approach.

It shall be mentioned that it is not intended to regularly use XSUSA in direct perturbation mode. This approach is only followed for the presented study to demonstrate recent advancements of the XSUSA method by calculating sensitivities that can be directly compared to TSUNAMI results, and to apply an approach for which the implicit effects are most clearly visible. Since the random sampling of cross sections is only another way of direct perturbation, the presented method can be applied with random sampling as well.

The advantages of the random sampling approach for uncertainty and sensitivity analysis with XSUSA with the presented method remain fully applicable: The analysis can be performed on any output quantity of the applied neutron transport code; there is no runtime penalty in terms of additional self-shielding calculations for the perturbed calculations such as in the recently released SAMPLER sequence of SCALE 6.2 [7] (only one additional short TSUNAMI-1D calculation is required); the constraint in terms of first-order perturbation theory is only applied for the implicit part of the self-shielding calculation; and in this way, the fast GRS method [8] remains applicable.

It is planned to fully implement this perturbation theory-based approach for the consideration of implicit effects into XSUSA. In this way, implicit effects shall be automatically considered for all nuclides and reactions in direct perturbation and random sampling criticality and depletion calculations.

VI. ACKNOWLEDGMENTS

This work is supported by the German Federal Ministry for Economic Affairs and Energy.

REFERENCES

1. F. BOSTELMANN, W. ZWERMANN, B. KRZYKACZ-HAUSMANN, L. GALLNER, A. AURES, and K. VELKOV, "Sampling-based Nuclear Data Uncertainty Analysis in Criticality and Depletion Calculations," *Proc. ANS MC2015*, Nashville, TN, USA, April 19-23 (2015).
2. F. BOSTELMANN, F.-P. WEISS, A. AURES, K. VELKOV, W. ZWERMANN, B. T. REARDEN, M. A. JESSEE, M. L. WILLIAMS, D. WIARDA, and W. A. WIESELQUIST, "Uncertainty and Sensitivity Analysis in Criticality Calculations with Perturbation Theory and Sampling," *Proc. ANS MC2015*, Nashville, TN, USA, April 19-23 (2015).
3. "SCALE: A Comprehensive Modeling and Simulation Suite for Nuclear Safety Analysis and Design," ORNL/TM-2005/39, Version 6.1, Oak Ridge National Laboratory, Oak Ridge, TN (2011).
4. M. L. WILLIAMS, "Perturbation Theory for Nuclear Reactor Analysis," in Y. RONEN, "Handbook of Nuclear Reactors Calculations, Volume III," CRC Press (1986).
5. B. T. REARDEN, "Perturbation theory eigenvalue sensitivity analysis with Monte Carlo techniques," *Nuclear Science and Engineering*, **146**, 367–382 (2004).
6. K. IVANOV, M. AVRAMOVA, S. KAMEROW, I. KODELI, E. SARTORI, E. IVANOV, and O. CABELLOS, "Benchmark for Uncertainty Analysis in Modelling (UAM) for Design, Operation and Safety Analysis of LWRs, Volume I: Specification and Support Data for the Neutronics Cases (Phase I)," NEA/NSC/DOC(2012)10, Version 2.1 (2016).
7. B. T. REARDEN and M. A. JESSEE, "SCALE Code System," ORNL/TM-2005/39, Version 6.2, Oak Ridge National Laboratory, Oak Ridge, TN, Available from Radiation Safety Information Computational Center as CCC-834 (2016).
8. W. ZWERMANN, B. KRZYKACZ-HAUSMANN, L. GALLNER, M. KLEIN, A. PAUTZ, and K. VELKOV, "Aleatoric and Epistemic Uncertainities in Sampling based Nuclear Data Uncertainty and Sensitivity Analyses," *Proc. PHYSOR2012*, Knoxville, TN, USA, April 15-20 (2012).