Influence of Nuclear Data Uncertainties on Reactor Core Calculations

To investigate the influence of nuclear data uncertainties on reactor core calculations systematically, the sampling based uncertainty and sensitivity software package SUSA developed at GRS was extended for the use with nuclear covariance data. Varied nuclear data are generated randomly corresponding to the uncertainty information from the covariance matrices. After performing a large number of calculations with these data, the results are statistically evaluated; this can be done not only for integral, but also for local output quantities like the assembly power distribution. The method is applied to multi-group Monte Carlo calculations stationary states of the PWR MOX/UO$_2$ core transient benchmark, and to corresponding nodal diffusion calculations. Unexpectedly large uncertainties result for the radial power distribution. The uncertainties in the nodal results agree very well with those in the Monte Carlo reference results; thus, it is possible to apply the random sampling method to determine the influence of nuclear data uncertainties on transient core calculations.
Einfluss der Unsicherheiten in den Nuklearen Daten auf Reaktorkernberechnungen

1 Introduction

Nuclear data are the basis of all neutron transport calculations. Thus, the quality of the nuclear data used is essential for obtaining reliable results from the nuclear calculation chain. The major evaluated nuclear data are continuously improved. During the last years, the European library was updated from JEF-2.2 to JEFF-3.1 [1] and further to JEFF-3.1.1, the American library from ENDF/B-VI to ENDF/B-VII.0 [2], and the Japanese library from JENDL-3.2 to JENDL-3.3/AC-2008 [3] and further to JENDL-4.0, with the main aim to take into account the newest evaluations of differential experiments as well as findings from nuclear theory. Nevertheless, the precision of nuclear data is limited by the uncertainties of the underlying measurements and the theoretical parameters. The relative uncertainties are sometimes provided in the nuclear covariance data files along with the basic data libraries. There is an increasing effort to improve the amount and the quality of the covariance files accompanying the major data libraries. For now, a rather complete set of covariance data is provided in multi-group format with the SCALE-6 code system [4].

So far, uncertainty and sensitivity investigations with nuclear covariance data, as performed, e.g., with the TSUNAMI code package [5], are based on first order perturbation theory, and primarily consider the multiplication factors and other integral quantities, like reactivity differences, of critical assemblies. In such calculations, the nuclear data uncertainties are taken into account in the spectral and transport calculations for the arrangement under consideration. They so far cannot be applied to reactor core calculations which are based on few-group cross sections obtained from fuel assembly calculations, and where one is interested in local quantities like the power distribution in the core, and finally the time dependence of the system in transient conditions. To systematically investigate the influence of nuclear data uncertainties on the results of calculations for large reactors, a random sampling approach, as for instance the "Total Monte Carlo" method [6], is appropriate. In this paper the sampling based XSUSA ("Cross Section Uncertainty and Sensitivity Analysis") sequence is used, which has been recently developed at GRS as an extension of the SUSA package for the use with nuclear covariance data. With XSUSA uncertainties can be propagated through the complete calculation chain, and resulting uncertainties in any output quantity of the reactor code can be evaluated.

The XSUSA method is described in Section 2. In Section 3, results from Monte Carlo reference calculations for stationary hot zero power states of the core are given. In Section 4, after a description of generating two-group cross sections, nodal diffusion calculations with the QUABOX/CUBBOX code [7] are presented, and the resulting uncertainties are compared with the Monte Carlo results. Conclusions of the investigations are given in Section 5.

2 The XSUSA Method

Within the sampling based GRS method implemented in the code package SUSA ("Software for Uncertainty and Sensitivity Analysis") [8], many calculations for the problem under consideration are performed with varied input data. The variations of the input data are generated randomly from the given probability distributions of the parameters including possible correlations between them. After performing all the calculations (typically 100 or more), the output quantities of interest are statistically analyzed, and their uncertainty ranges and sensitivities to the input parameters are determined.

So far, the GRS method has been mainly applied to problems with a limited number of parameters and only few correlations between them. However, in the case of its application to
the nuclear data uncertainties, various reactions of various nuclides have to be considered. Using the nuclear covariance data from the SCALE-6 code package [4], 44 uncertain parameters for each nuclide and reaction corresponding to the 44 energy group structure are analyzed, resulting in a huge overall number of uncertain parameters. Moreover, a large amount of correlations between the energy group data of each nuclide/reaction combination have to be taken into account, and also cross correlations between data of different reactions and nuclides. Therefore, so far only the uncertain data of a limited number of nuclides and reactions are considered, based on an a priori judgement of their respective importance. The nuclear data covariance matrices only contain the relative variances and covariances of the nuclear data, i.e. the second moments of the distributions; the types of the distributions are not known and for the moment assumed to be Gaussian.

To use the GRS method with nuclear covariance data, the ENDF/B-VII based 238-group library of SCALE-6 is collapsed to the 44-group structure of the covariance data using a flux spectrum typical for the system under consideration. With this collapsed master library, all necessary spectral calculations are performed, using the Bondarenko method implemented in the BONAMI module for the unresolved resonance regions, and performing 1-D transport calculations by the CENTRM module with continuous energy data in the resolved resonance region. The resulting data libraries are modified according to the uncertainty information in the covariance matrices for each nuclide/reaction combination considered, taking into account, if present, the covariances between different energy groups, different reactions, and different nuclides. After doing so, it has to be assured that the cross section set is entirely consistent, i.e. that sum rules are fulfilled and that 2-d cross sections (e.g. scattering matrices) are compatible with their 1-d counterparts. With the modified cross sections created in this way, the core calculations are performed and the results are statistically evaluated.

An effect which is not taken into account so far within the XSUSA method is the influence of the nuclear data uncertainties on the spectral calculations. This is due to the fact that the SCALE-6 covariance matrices contain uncertainty information in multi-group representation also in the resonance region. Therefore, for the time being the spectral calculations are performed with undisturbed data, and the same uncertainties are assumed for the resonance-treated data as for the infinite dilution data.

3 Monte Carlo Reference Core Calculations

The XSUSA method is first applied to full scale 2-D calculations for the hot zero power stationary state of the PWR MOX/UO$_2$ Core Transient Benchmark [9]. The specified core, displayed in Fig. 1, is highly heterogeneous, with UO$_2$ and MOX fuel assemblies with burn-ups up to 37 GWd/t HM; the MOX fuel contains a high fraction of $^{239}$Pu. The code KENO-Va from the SCALE-6 system in multi-group mode is used with 44-group ENDF/B-VII based data. Nuclide densities are taken in accordance with the benchmark specification. For the number of neutron histories, a large value of $10^9$ is chosen to assure that differences in the fission rate distributions obtained with varied data do not originate from insufficiently converged solutions. In total, $N = 480$ XSUSA/KENO calculations are run. These calculations are performed on a cluster with twelve nodes, each equipped with two Intel Xeon E5540 quad-core processors running at 2.53 GHz. Each of the KENO calculations takes approx. 12 hrs of CPU time, amounting to slightly more than two and a half days of wall-clock time for the whole batch of runs using all processors simultaneously. Therefore, sampling based uncertainty analyses come into reach of routine application even for CPU time intensive problems. Validation pin cell calculations by comparing with TSUNAMI results and first core calculations were presented in [10].
The calculated multiplication factors turn out to lie in a reasonable band with a relative standard deviation of 0.5 %, in accordance with typical uncertainties for UO$_2$-dominated thermal LWR systems. In the radial fission rate distribution, however, one observes a much larger influence of the nuclear data variations on the result. This is shown in Fig. 2, where the resulting fission rate distribution and its band widths for a row of fuel assemblies are displayed together with the results of a reference calculation with unvaried nuclear data. The resulting relative standard deviation of approximately 5 % in the core centre is unexpectedly high, and the maximum and minimum values of the fission rates obtained for the central fuel assemblies deviate by +/- 14 % from the reference values. Additional calculations with varying single nuclides and reactions separately have shown that the differences in the fission rate distributions are mainly due to the uncertainties in the nuclear data of $^{239}$Pu, specifically nu-bar and, to a less degree, $^{235}$U.

4 Nodal Diffusion Calculations

Today transient core calculations are performed by coupling nodal diffusion codes with a thermo-hydraulics code. In order to determine the influence of nuclear data uncertainties on these transients one has to transfer the covariance to the homogenized few-group cross sections that serve as parameters for the nodal diffusion code. A stepwise approach for the global uncertainty analysis is proposed in the UAM Benchmark specification [11]: first uncertainties and covariances are obtained for single fuel assemblies for every branching point in the cross-section library. After that a global covariance matrix has to be created explicitly. The diagonal elements of this matrix are the variances of the individual cross sections. But also the off-diagonal elements that describe the correlation between the individual cross sections have to be calculated by using the calculation results from different fuel assemblies, temperatures, boron concentrations etc.

This may be a reasonable approach for deterministic methods. When applying the XSUSA random sampling method, we chose a different approach for propagating the uncertainties that matches much better with the statistical nature of the method implicitly: a set of $N = 480$ complete few-group cross section libraries is produced by the combination of XSUSA with the spectral code NEWT from SCALE6 [4]. By calculating each parametric point of this library (fuel assembly type, fuel temperature, moderator density, boron concentration etc.) $N$ times with the same set of random numbers, the correlations are preserved naturally and are implicitly contained in the output data. The obtained varied cross-section libraries are then saved. After that all desired transient calculations are performed with every single of these $N = 480$ libraries and evaluated statistically.

To demonstrate the lossless transfer of nuclear uncertainties and correlations from the nuclear data library to a diffusion code, 27 different sets of few-group cross sections and discontinuity factors have been created for the above described PWR reactor with NEWT. The 2D-core steady state calculations were performed with the GRS core simulator QUABOX/CUBBOX (QC) [7]. Calculations with unvaried cross sections showed a good agreement between Monte-Carlo and core simulator: the $k_{eff}$ value for the “all-rods-out” (ARO) state of the 2-D core differed by 247pcm and the differences in the nodal power distribution were not larger than 2.5% (see Fig. 3).

For the calculation of the uncertainties, the same varied 44-energy group cross-section libraries were used as for the KENO calculations described above. Tab. 1 displays mean values and standard deviations for the 2-D hot zero power state of the core compared to the XSUSA/KENO results. When evaluating the uncertainties of integral quantities, the corresponding values were also calculated with TSUNAMI-3D. It can be seen that these
global core values and their uncertainties are in good agreement. It is also possible to calculate a sampling correlation coefficient $R$ which relates the output values of KENO for each run with the respective values obtained by QC. For $k_{\text{eff}}$ this value is $R_{k_{\text{eff}}} = 0.9996$ and thus implies a total dependence of the individual runs, i.e. when the KENO result is an extremely high value, QC will also show an extreme high value.

Statistical values can also be obtained for local core values. The uncertainties of the nodal power distributions are shown in Fig. 4 for both, KENO and QC. The accordance between both methods is very good in every single node. Further values that are important for the transient specified in the benchmark (see Part I-c in [9]) are the uncertainties of the single rod worths which are shown in Tab. 2. Here as well both XSUSA sequences and TSUNAMI-3D yield similar results.

5 Conclusions and Outlook

The influence of nuclear data uncertainties on reactor core calculations were investigated systematically using the sampling based uncertainty and sensitivity software XSUSA. The method was applied to full scale 2-D calculations for the hot zero power state of the core. For the presented UOX/MOX core the uncertainties in the nodal power distribution are 5% in the central fuel assembly. Thus even the most accurate Monte-Carlo codes cannot predict the power distribution in a satisfying degree if the underlying nuclear data has such big uncertainties.

Further investigations on the same core show that it is possible to transfer the nuclear data covariance from the ENDF-library to the two-group library of a diffusion code. Global and local values for uncertainties and mean values are in good agreement between XSUSA/QC, XSUSA/KENO and TSUNAMI-3D. In the future the XSUSA method will be used to create varied nuclear data libraries for transient calculations. The versatility of the method makes it also possible to include not only the nuclear data covariance but also uncertainties of neutron kinetics parameters, fabrication uncertainties and thermo-hydraulic parameters.

In conclusion, it is desirable to routinely accompany reactor calculations by uncertainty and sensitivity analyses in the future, along with aiming for a continuous convergence of different nuclear data evaluations, and a reduction of their uncertainties.

6 Acknowledgements

This work was supported by the German Ministry of Economics and Technology.
7 References


8 The authors of this contribution

Dr. Markus Klein
Lucia Gallner
Bernard Krzykacz-Hausmann
Dr. Andreas Pautz
Dr. Winfried Zwermann

Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) mbH
Boltzmannstraße 14
85748 Garching b. München
GERMANY
Tab. 1 Mean values and standard deviations for the 2D state of the PWR MOX/UO2 Benchmark Core calculated with XSUSA/KEO and XSUSA/NEWT/QC

<table>
<thead>
<tr>
<th></th>
<th>ARO $k_{\text{eff}}$ mean</th>
<th>ARO $k_{\text{eff}}$ $\sigma$</th>
<th>ARI $k_{\text{eff}}$ mean</th>
<th>ARI $k_{\text{eff}}$ $\sigma$</th>
<th>Rod worth mean (pcm)</th>
<th>Rod worth $\sigma$</th>
</tr>
</thead>
<tbody>
<tr>
<td>XSUSA/KEO</td>
<td>1.05913</td>
<td>0.56%</td>
<td>0.98782</td>
<td>0.49%</td>
<td>6802</td>
<td>0.67%</td>
</tr>
<tr>
<td>XSUSA/QC</td>
<td>1.06227</td>
<td>0.55%</td>
<td>0.98939</td>
<td>0.50%</td>
<td>6934</td>
<td>0.78%</td>
</tr>
<tr>
<td>TSUNAMI-3D</td>
<td>1.05670</td>
<td>0.56%</td>
<td>0.98645</td>
<td>0.52%</td>
<td>6764</td>
<td>0.71%</td>
</tr>
</tbody>
</table>
Tab. 2 Relative uncertainties of single rod worths obtained by XSUSA and TSUNAMI-3D

<table>
<thead>
<tr>
<th></th>
<th>A1</th>
<th>A3</th>
<th>A5</th>
<th>A7</th>
<th>C3</th>
<th>E5</th>
</tr>
</thead>
<tbody>
<tr>
<td>XSUSA/KENO</td>
<td>4.35%</td>
<td>N/A</td>
<td>N/A</td>
<td>N/A</td>
<td>N/A</td>
<td>3.02%</td>
</tr>
<tr>
<td>XSUSA/QC</td>
<td>4.24%</td>
<td>1.44%</td>
<td>1.79%</td>
<td>9.66%</td>
<td>2.22%</td>
<td>2.66%</td>
</tr>
<tr>
<td>TSUNAMI-3D</td>
<td>4.69%</td>
<td>1.68%</td>
<td>2.28%</td>
<td>9.66%</td>
<td>2.46%</td>
<td>3.14%</td>
</tr>
</tbody>
</table>
Fig. 1: Core layout of the PWR MOX/UO$_2$ Transient Benchmark Core. UO$_2$ fuel assemblies are drawn in white, MOX fuel assemblies in blue. The row of fuel assemblies for which the power distribution is evaluated is marked in magenta.
Fig. 2: Fission rate distribution for a row of fuel assemblies of the PWR MOX/UO$_2$ core from XSUSA/KENO; mean values from 400 calculations (blue), 1 $\sigma$ band (black), and extreme values (red).
Fig. 3: Power distribution of the PWR MOX/UO₂ Core obtained by KENO Va (top) and relative differences of the QUABOX/CUBBOX solution for the same core (bottom).
<table>
<thead>
<tr>
<th></th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>4.75%</td>
<td>4.55%</td>
<td>3.13%</td>
<td>2.03%</td>
<td>0.71%</td>
<td>2.42%</td>
<td>3.11%</td>
<td>3.53%</td>
</tr>
<tr>
<td>B</td>
<td>4.55%</td>
<td>3.93%</td>
<td>2.76%</td>
<td>1.46%</td>
<td>0.69%</td>
<td>1.95%</td>
<td>3.69%</td>
<td>3.67%</td>
</tr>
<tr>
<td>C</td>
<td>3.13%</td>
<td>2.76%</td>
<td>2.32%</td>
<td>1.85%</td>
<td>0.49%</td>
<td>1.92%</td>
<td>2.77%</td>
<td>3.65%</td>
</tr>
<tr>
<td>D</td>
<td>2.03%</td>
<td>1.46%</td>
<td>1.85%</td>
<td>1.21%</td>
<td>0.94%</td>
<td>1.11%</td>
<td>2.88%</td>
<td>3.17%</td>
</tr>
<tr>
<td>E</td>
<td>0.71%</td>
<td>0.69%</td>
<td>0.49%</td>
<td>0.94%</td>
<td>0.64%</td>
<td>1.10%</td>
<td>1.67%</td>
<td></td>
</tr>
<tr>
<td>F</td>
<td>2.42%</td>
<td>1.95%</td>
<td>1.92%</td>
<td>1.11%</td>
<td>1.10%</td>
<td>1.70%</td>
<td>1.53%</td>
<td></td>
</tr>
<tr>
<td>G</td>
<td>3.11%</td>
<td>3.69%</td>
<td>2.77%</td>
<td>2.88%</td>
<td>1.67%</td>
<td>1.53%</td>
<td></td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>3.53%</td>
<td>3.67%</td>
<td>3.65%</td>
<td>3.17%</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Fig. 4: Uncertainties of the nodal power distribution of the investigated 2-D core. On the left side standard deviations for XSUSA/KENO are shown. The right side shows the respective values for XSUSA/NEWT/QC.