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APPLICATION OF GLOBAL SENSITIVITY ANALYSIS APPROACH TO EXERCISE I-1 OF THE OECD LWR UAM BENCHMARK

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ABSTRACT

Models of varying complexity are developed to approximate or mimic systems and processes in different aspects of the real world (e.g. physical, environmental, social, or economic). Applying models in such domains inevitably involves uncertainty in both the model representation and in the input data. Uncertainty and sensitivity analysis techniques can be applied to study uncertainty in model predictions arising from imprecisely-known processes and input data. Sensitivity analysis involves determining the contribution of individual inputs to the uncertainty in model predictions.

Global sensitivity analysis deals with uncertainty sources spanning over finite or infinite ranges of uncertainties and with the simultaneous variation of such sources. This in turn enables the identification of high-order interactions among inputs in determining the uncertainty in the output of interest. This paper applies global sensitivity analysis to the modeling of nuclear reactor applications using the Monte Carlo method. In particular, the tests of Exercise 1 (I-1), "Cell Physics", of the OECD Benchmark for Uncertainty Analysis in Best-Estimate Modeling (UAM) for Design, Operation and Safety Analysis of LWRs (OECD LWR UAM Benchmark), are analyzed.

Key Words: MCNP5, Exercise I-1, OECD LWR UAM Benchmark

1. INTRODUCTION

Models of varying complexity are developed to approximate or mimic systems and processes in different aspects of the real world (e.g. physical, environmental, social, or economic). Applying models in such domains inevitably involves uncertainty in both the model representation and in the input data.

Uncertainty and sensitivity analysis techniques can be applied to study uncertainty in model predictions arising from imprecisely-known processes and input data. Sensitivity analysis involves determining the contribution of individual inputs to the uncertainty in model predictions.

Inputs can be poorly known model parameters (kinetic coefficients in chemical models, speed flows of radioactive species in the geo-sphere, etc.), errors in input data, and also more complex entities such as alternative sub-models, flow fields, the use of one mesh size rather than another.

Global sensitivity analysis deals with uncertainty sources spanning over finite or infinite ranges of uncertainties and with the simultaneous variation of such sources. This in turn enables the identification of high-order interactions among inputs in determining the uncertainty in the output of interest.

The OECD Benchmark for Uncertainty Analysis in Modeling (UAM) for Design, Operation and Safety Analysis of LWRs (OECD LWR UAM Benchmark) [1] has been initiated as a result of the increasing demand in recent years from the nuclear community for best estimate predictions supplemented by uncertainty and sensitivity analysis. The main objective of this benchmark activity is to determine the uncertainties in LWR system modeling in all stages of the coupled reactor physics/thermal-hydraulic calculations. The benchmark contains different number of exercises in order to evaluate and propagate the uncertainties from the initial data and engineering uncertainties through different physics phenomena (multi-physics) and modeling scales (multi-scale) and to provide credible coupled code predictions with defensible uncertainty estimations of safety margins at the full core/system level. Following this approach, the complex system is subdivided into nine exercises/steps grouped in three phases. The input, output and assumptions of each exercise/step are identified and the resulting uncertainty of each step is calculated. This paper is focused on application of the global sensitivity analysis approach to Exercise 1 of Phase 1 using the Monte Carlo method.

2. GLOBAL SENSITIVITY ANALYSIS APPROACH

According to [2] Uncertainty Analysis (UA) focuses on quantifying uncertainty in a model output. Sensitivity Analysis (SA) studies how this output uncertainty of a model can be apportioned to different sources of uncertainty in the model input. UA and SA should be run in tandem, usually in an iterative fashion. SA can be classified in two categories – Local Sensitivity Analysis (LSA) and Global Sensitivity Analysis (GSA). The LSA is based on derivatives and is efficient in computer time. However, it has to be implemented in the computer program of the model of interest and it is unwarranted for non-linear models. The derivatives are only informative at the base point where they are computed, and do not provide for an exploration of the rest of the space of the input factors. On the other hand, the GSA approach explores the full space of input factors. The Monte Carlo method can be used in conjunction with the GSA to produce the model outputs by sampling input factors' values from their distributions.

3. DESCRIPTION OF EXERCISE I-1

Phase I is focused on understanding uncertainties in prediction of key reactor core parameters associated with LWR stand-alone neutronics core simulations. Such uncertainties occur due to input data uncertainties, modeling errors, and numerical approximations. Input data for core neutronics calculations primarily include the lattice averaged few group cross-sections. Three main LWR types are selected, based on previous benchmark experiences and available data: PWR, BWR and VVER. The work presented in the current paper focuses on Exercise 1 of Phase

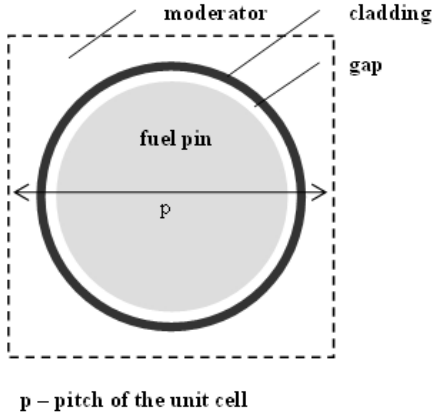
I (I-1), "Cell Physics", which propagates the uncertainties in evaluated nuclear libraries data files, with microscopic point-wise cross-sections, into multi-group microscopic cross-sections in the way used as inputs by the lattice physics codes.

The uncertainty files (nuclear data uncertainties) in the evaluated nuclear data libraries (NDL) are obtained from the analysis of experimental differential data and from nuclear models and are stored as variance and covariance data. The cross-section uncertainty data, within the framework of Exercise I-1, is processed in a multi-group format. The NDL effect is assessed in this paper by running Monte Carlo simulations with these major libraries: ENDF/B-VI.8, ENDF/B-VII.0, JEFF-3.1, and JENDL-3.3.

The final multi-group cross-section libraries and associated uncertainties should be consistent with the requirements of the lattice physics codes, which participants are planning to utilize. Test problems are devised or utilized from the previously defined benchmarks in order to perform a comparative analysis of the multi-group cross-section uncertainty data obtained after processing.

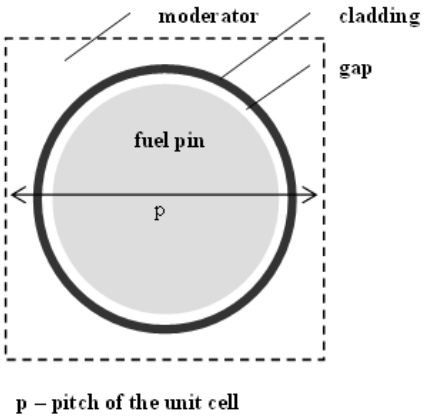
An important feature of the Specification on Phase I [1] is the selected strategy for designing test problems for each exercise. Test problems representatives of the three main LWR types (PWR, BWR, and VVER) are utilized for which the uncertainties are propagated in each Exercise and Phase. These test problems are consistent with the type of calculation done at each step (represented by the corresponding Exercise) within the standard LWR calculation scheme for design and safety analysis.

For Exercise I-1 these problems are the two-dimensional (2D) fuel pin-cell test problems representative of BWR Peach Bottom 2 (PB-2), PWR Three Mile island 1 (TMI-1), and VVER-1000 (Kozloduy-6 and Kalinin-3 plants). The geometry specification of the test problems is illustrated in Fig. 1 for the PB-2 BWR unit cell, in Fig. 2 for the TMI-1 PWR unit cell, and in Fig. 3 for the Kozloduy-6 VVER unit cell.



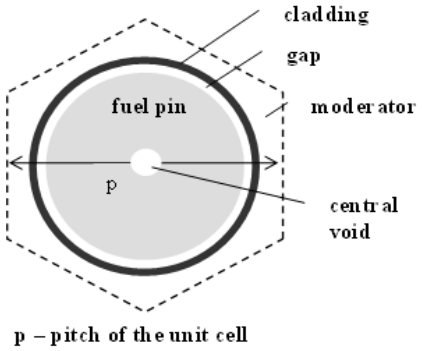
Parameter	*Value*
Unit cell pitch, mm	18.75
Fuel pellet diameter, mm	12.1158
Fuel pellet material	UO_2
Fuel density, g/cm^3	10.42
Fuel enrichment, w/o	2.93
Cladding outside diameter, mm	14.3002
Cladding thickness, mm	0.9398
Cladding material	Zircaloy-2
Gap material	He
Moderator material	H_2O

Figure1. Configuration of PB-2 BWR unit cell



Parameter	*Value*
Unit cell pitch, mm	14.427
Fuel pellet diameter, mm	9.391
Fuel pellet material	UO_2
Fuel density (95% TD), g/cm^3	10.283
Fuel enrichment, w/o	4.85
Cladding outside diameter, mm	10.928
Cladding thickness, mm	0.673
Cladding material	Zircaloy-4
Gap material	He
Moderator material	H_2O

Figure 2. Configuration of TMI-1 PWR unit cell



Parameter	*Value*
Unit cell pitch, mm	12.75
Fuel pellet diameter, mm	7.56
Fuel pellet material	UO_2
Fuel density, g/cm^3	10.4
Fuel enrichment, w/o	3.3
Central void diameter, mm	1.4
Central void material	air
Cladding outside diameter, mm	9.1
Cladding thickness, mm	0.69
Cladding material	Zr +1% Nb
Gap material	He
Moderator material	H_2O

Figure 3. Configuration of Kozloduy-6 VVER unit cell

4. MONTE CARLO MODELING

The continuous energy Monte Carlo method is well suited for providing reference solutions for criticality problems on different spatial scales (cell, super-cell, assembly, and core) with exact representation of complicated real geometry. Core environments that present increased geometry complexity and material heterogeneity are well modeled in MCNP5. The major advantages of the Monte Carlo method over the deterministic methods are, the continuous energy treatment, and the exact three-dimensional geometry modeling. The Monte Carlo method, in particle

transport, can be considered a numerical experiment that represents a high quality reference solution for validation of deterministic codes.

The MCNP5 version (1.40 release) is used in this paper for the studies presented in Section 4 while the MCNP5 version (1.50 release) is utilized for studies summarized in Section 5. In this Section (Section 4) two effects were mainly studied:

- The effect of temperatures - Regular cross-sections (at temperatures for different isotopes available with MCNP5) and New cross-sections (generated at temperatures consistent with the specified HZP conditions)

- The effect of the NDLs on the example of the latest released versions such as ENDF/B-VI.8, ENDF/B-VII.0, JEFF-3.1, and JENDL-3.3.

The MCNP5 geometry and material modeling in two-dimensional representation of the test problems is depicted in Fig. 4.

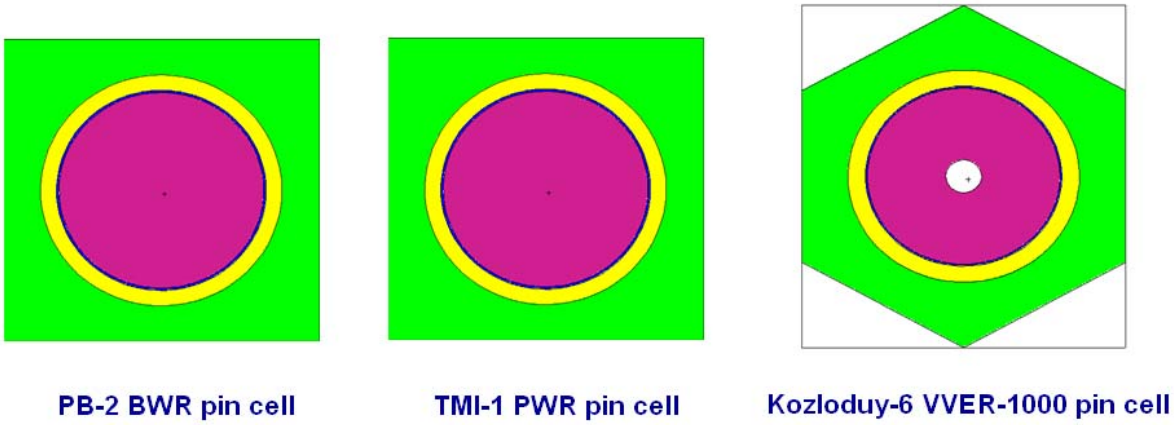


Figure 4. MCNP5 2D models

4.1 Effect of Temperatures

Initially the MCNP5 was used to calculate the above-describe test problems using the so-called Regular cross-sections (at temperatures for different isotopes available with MCNP5). Since the MCNP5 solutions will be sued as reference for deterministic code predictions these calculations were repeated with the so-called New cross-sections (generated at temperatures consistent with the specified HZP conditions). For each of the runs the cross-section libraries were generated using NJOY at 550K with the exception of the hydrogen scattering in light water library, which was at 600K and was included in the MCNP5 distribution (ENDF6.3 library).

The base MCNP5 results New cross-sections illustrating the k_{eff} and the fission source distribution convergence are shown in Fig. 5, Fig. 6 and Fig 7 for each the test problems respectively. Since the results of these tests will be used as reference solutions, it is crucial that the solution provided by the MCNP5 code has converged. It is needed that both, the effective

multiplication factor (k_{eff}) and the fission source distribution, converge in order to start tallying when running criticality calculations. The k_{eff} and the fission source distribution converge differently; k_{eff} converges more rapidly than the source distribution. So the k_{eff} alone cannot be used to asses the solution convergence. The latest MCNP5 release (1.40) incorporates a vital tool to assess fission source distribution convergence[1].

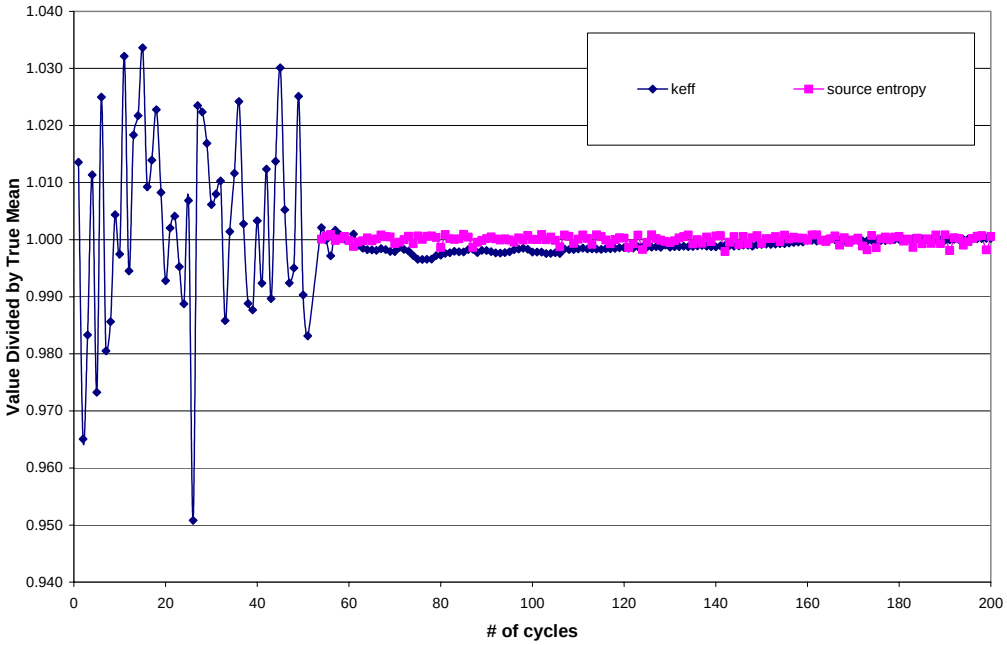


Figure 5. TMI-1 PWR 2D Pin Cell Results with New Cross Sections

[1] This new tool is based on the Shannon Entropy of the fission source distribution [3].

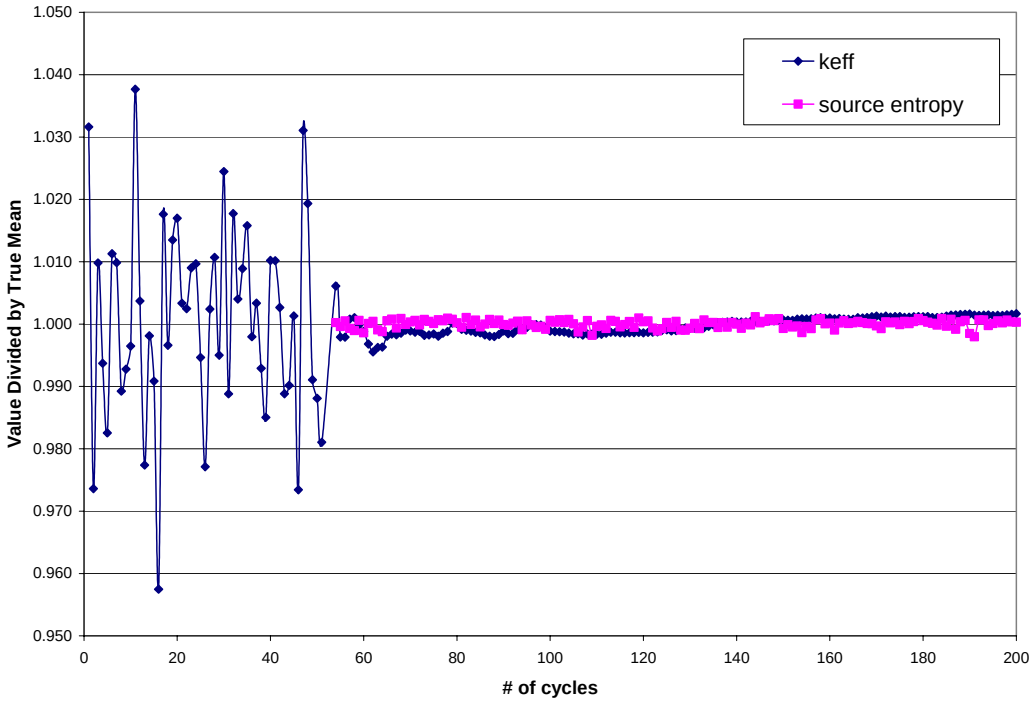


Figure 6. PB-2 BWR 2D Pin Cell Results with New Cross Sections

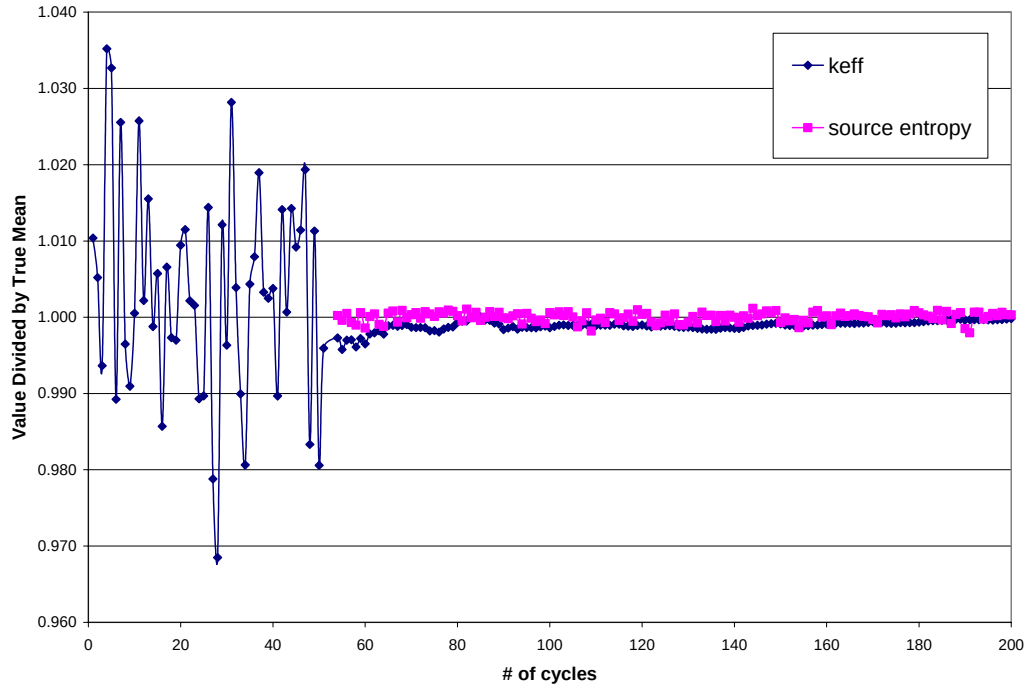


Figure 7. Kozloduy-6 VVER Pin Cell Results with New Cross Sections

4.1 Effect of NDLs

The NJOY code is a nuclear data processing system, which produces point-wise and group-wise cross-sections from the NDLs. It has the capability to generate continuous energy MCNP5 cross-sections. Since the generation process for cross-section libraries is tedious and involves a lot of data manipulation, an automated tool has been developed at the Pennsylvania State University (PSU) to process all the data and manage the processing requirements during the generation process. This automated methodology has been developed as part of the hybrid Monte Carlo-based coupled core calculations. The duration of the cross-section generation procedure has been significantly reduced. This automated tool performs the most time consuming tasks of the cross-sections generation process. The final output of automated tool is a cross-section library together with the directory of cross-section files readily useable by MCNP5.

The automated tool is used to generate temperature dependant cross-section libraries using NDLs. Then, the differences in the effective multiplication factor (k_{eff}) and other parameters, calculated by MCNP5 using the different libraries, are compared.

In these sensitivity studies for each of the pin cell test problems studied, the fuel composition and pin dimensions are the same - only the utilized NDLs are varied. The criticality calculations were performed using the LANL Monte Carlo code, MCNP5 [1], release 1.40. Each of the pin cell test problems was simulated using cross-sections based on ENDF/B-VI.8 [8-9], ENDF/B-VII [8-9], JEFF-3.1 [10], and JENDL-3.3 [11]. Each MCNP5 calculation employed 1500 generations of 5,000 neutrons each. The first 50 generations were excluded from the statistics. As a result, the values of the multiplication factor, k_{eff}, acquired from these calculations are based on 7,250,000 active neutron histories. This amount of histories reduces the Monte Carlo standard deviation for k_{eff} to a maximum of 42 pcm.

The values obtained for k_{eff} for the test problems of the three main LWR types using the NDLs mentioned above are listed in Table I. When comparing the ENDF libraries, ENDF/B-VII.0 produces higher k_{eff} values than ENDF/B-VI.8. The maximum difference of ENDF/B-VI.8 and ENDF/B-VII.0 results for k_{eff} is 312 pcm. JEFF-3.1 produces higher values for k_{eff} than the other libraries for all the cases.

Table I. k_{eff} values for the LWR types for different cross-section libraries

	k_{eff}			
	ENDF/B-VI.8	**ENDF/B-VII**	**JEFF-3.1**	**JENDL-3.3**
BWR	1.35140 +/- .000210	1.35448 +/- 0.00020	1.35651 +/- 0.00020	1.35374 +/- 0.00020
PWR	1.43224 +/- 0.00027	1.43536 +/- 0.00022	1.43659 +/- 0.00021	1.43444 +/- 0.00021
VVER	1.35862 +/- 0.00042	1.36098 +/- 0.00021	1.36299 +/- 0.00022	1.36055 +/- 0.00021

Further studies were performed using MCNP5 tallies to calculate the total fission and absorption cross-sections. The total fission and absorption cross-section values for each of the cross-section libraries are displayed in Table II in units of barns. The maximum absolute difference of ENDF/B-VI.8 and ENDF/B-VII.0 for total fission cross-section values is 0.05 %. One can notice that the largest differences in values for the results presented in Table I and Table II are for the PWR test problem when comparing the different versions of ENDF libraries. The maximum absolute difference of ENDF/B-VI.8 and ENDF/B-VII.0 for total absorption cross-section values

is 0.3 %. Similar to the results presented in Table I, JEFF-3.1 produce higher values for both cross-sections in Table II than the other three libraries.

Table II. Total fission and total absorption cross-section data using different libraries

		Total cross-section (b)	
		σ_f	σ_a
BWR	ENDF/B-VI.8	0.035935	0.371765
	ENDF/B-VII	0.036356	0.374339
	JEFF-3.1	0.036433	0.374582
	JENDL-3.3	0.036346	0.375696
PWR	ENDF/B-VI.8	0.041408	0.392008
	ENDF/B-VII	0.041858	0.395007
	JEFF-3.1	0.041921	0.395390
	JENDL-3.3	0.041883	0.396193
VVER	ENDF/B-VI.8	0.039190	0.405403
	ENDF/B-VII	0.039620	0.408371
	JEFF-3.1	0.039715	0.408988
	JENDL-3.3	0.039635	0.410130

In summary, calculations with cross sections derived from ENDF/B-VI.8, ENDF/B-VII, JEFF-3.1 and JENDL-3.3 have been performed for all LWR type test problems. There were significant differences observed between the libraries when calculating the total absorption cross section. This fact indicates that the choice of NDL used to derive cross-section data is important. Further studies to see how results vary with change of enrichment and the effect of the Doppler coefficient are planned as future work.

5. SENSITIVITY ANALYSIS

The evaluation of nuclear data induced uncertainty is possible by the use of nuclear data covariance information. The development of nuclear data covariance files is in progress in the major NDLs. The uncertainty within the nuclear data files is difficult to assess. The uncertainty data, expressed in percentage with respect to the nominal value of a given cross section for a given energy, is available for few isotopes and not all the nuclear data files include uncertainties. For the purposes of the OECD LWR UAM benchmark the availability of covariance data is important for all relevant nuclides (actinides, fission products, absorbers and burnable poisons, structural materials and etc.), present in the reactor core and reflector regions of LWRs, covering the entire energy range of interest (from 0 to 10 MeV), and for all relevant reaction cross-section types.

In order to conduct a preliminary sensitivity test, we have identified, among the available uncertainty data, the reactions that have cross section larger than 100 barns, considering that the uncertainty effect of less probable reactions have no effect on k_{eff}. We have assumed that the cross sections values are normally distributed with a mean value given by the nominal value (generally used in the computations) and a standard deviation that is given by the product of the nominal cross section and the uncertainty value expressed in percentage points.

Ideally, the uncertainties of the cross sections should be modified within the nuclear data file. Unfortunately, the parameters within the ENDF files needed to be reconstructed, which involves taking the resonance and other parameters into consideration. This process is extremely complex for continuous energy calculations and will be studied in the future.

In this preliminary test, only the uncertainties of the thermal cross sections of U-235 and Li-6 were considered. A two-column sample matrix with 320 rows was generated to represent such uncertainties. Each row represents two cross section values that are used to simulate one energy group MCNP5 criticality calculation. This approach was implemented using the one-group transport calculations available in the latest MCNP5 version (release 1.50) named "onegxs". This new feature is first used to construct one-group cross section files for each isotope in a format recognized by MCNP5. This then allows MCNP5 to run in a multi-group mode using the one-group data files. For the remaining isotopes the one-group nominal cross-section values were used (no uncertainties were attached).

The sensitivity analysis methodology applied in this preliminary test, originally due to Sobol [7], has been ameliorated by Saltelli [12]. The method of Sobol is variance-based, meaning that the variance of the model output can be decomposed into terms of increasing dimension, called partial variances, that represent the contribution of each single input (but even pairs, triplets, etc) to the overall uncertainty of the model output. This method allows the simultaneous exploration of the space of the uncertain inputs, which is carried out via Monte Carlo or quasi Monte Carlo sampling. Statistical estimators of partial variances are available to quantify the sensitivities of all the inputs and of groups of inputs through multi-dimensional integrals.

The computational cost, in terms of model simulations, required to estimate the sensitivities of higher-order interactions between inputs can be very high. To preclude this, the concept of total sensitivity index has been introduced by [13], which requires much less computational effort. The total sensitivity index provides an indication of the overall effect of a given input, taking into account all possible interaction of that input with all the others. We refer to the above mentioned literature for the technical details of the methods. In this paper we estimate both first order and total sensitivity indices.

The results show that the uncertainty of the thermal cross section for U-235 is entirely responsible for the uncertainty of k_{eff} (i.e., both the first order and the total sensitivity indices are equal to 1), whereas the uncertainty of the Li-6 cross section does not affect k_{eff} at all (i.e., its first order and total sensitivity indices are equal to 0). This means that the uncertainty of Li-6 cross section can be ignored in subsequent simulations. Additional analyses will be conducted by increasing the number of energy groups to investigate to what extent the uncertainties of the cross sections contribute to the uncertainty of k_{eff}.

5. CONCLUSIONS

Global sensitivity analysis deals with uncertainty sources spanning over finite or infinite ranges of uncertainties and with the simultaneous variation of such sources. This in turn enables the identification of high-order interactions among inputs in determining the uncertainty in the output of interest. This paper applies global sensitivity analysis to the modeling of nuclear

reactor applications using the Monte Carlo method. In particular, the test problems of Exercise 1 (I-1), "Cell Physics", of the OECD LWR UAM Benchmark, are analyzed.

REFERENCES

1. K. Ivanov, M. Avramova, I. Kodeli, E. Sartori, "Benchmark for Uncertainty Analysis in Modeling (UAM) for Design, Operation and Safety Analysis of LWRs. Volume 1 – Specification and Supporting Data for the Neutronics Cases (Phase I) Version 1.0", NEA/NSC/DOC(2007)23.
2. A. Saltelli, et al., "Global Sensitivity Analysis – The Primer", John Wiley & Sons, Ltd, 2008.
3. "MCNP - A General Monte Carlo N-Particle Transport Code, Version 5," Los Alamos National Laboratory (2004).
4. F. Brown, et al., "Convergence Testing for MCNP5 Monte Carlo Eigenvalue Calculations", *Proceedings of Mathematics & Computation and Supercomputing in Nuclear Applications*. Monterey, California, April 2007.
5. F. Brown, N. Barnett, "A Tutorial on Using MCNP for 1-Group Transport Calculations" Los Alamos National Laboratory, 2008.
6. H. Lemmel and P. McLaughlin, "ENDF/B-6 Standards Library 1987", International Atomic Energy Agency, Nuclear Data Services, IAEA-NDS-88, Rev.4 Feb 2002.
7. I. Sobol, "Sensitivity analysis for non linear mathematical models, Math. Modelling and Computational Experiment", 1: 407-414, 1993.
8. A. Vasilev, et al., "On the performance of ENDF/B-VII.0 data for fast neutron fluence calculations". Annals of Nuclear Energy, 35 (2008) 2432–2435.
9. T-2 Nuclear Information service, 2003 T-2 Nuclear Information Service, Los Alamos National Laboratory, 2003. Available from: <http://t2.lanl.gov/data/data.html>
10. NEA, "Joint Evaluated Fission and Fusion and File (JEFF-3.1)," OECD, Paris, France, 2005.
11. NEA/OECD, "Japanese Evaluated Neutron Data Library," OECD, Paris, France, 2002.
12. A. Saltelli, "Making Best Use of Model Evaluations to Compute Sensitivity Indices", Computer Physics Communication, 145: 280-297, 2002.
13. T. Homma, A. Saltelli, "Reliability Engineering and System Safety", 52, 1, 1996.