International Conference on Mathematics, Computational Methods & Reactor Physics (M&C 2009)
Saratoga Springs, New York, May 3-7, 2009, on CD-ROM, American Nuclear Society, LaGrange Park, IL (2009)

OVERVIEW AND DISCUSSION OF PHASE I OF THE OECD LWR UAM BENCHMARK ACTIVITY

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ABSTRACT

The ongoing OECD Light Water Reactor (LWR) Uncertainty Analysis in Modeling (UAM) benchmark activity contributes to establishing unified framework to determine the uncertainty in LWR system calculations at all stages of a coupled reactor physics/thermal hydraulics calculation. This benchmark sequence started in 2007, and integrates the expertise in reactor physics, thermal-hydraulics and reactor system modeling as well as uncertainty and sensitivity analysis. Such an effort has been undertaken within the framework of a program of international co-operation that benefits from the coordination of the NEA Nuclear Science Committee (NSC), and from interfacing with the Committee of Safety of Nuclear Installations (CSNI). Reference LWR systems and scenarios for coupled code analysis are defined. Three main LWR types are selected, based on previous benchmark experiences and available data – BWR, PWR and VVER-1000. The full chain of uncertainty propagation from basic data, engineering uncertainties, across different scales (multi-scale), and physics phenomena (multi-physics) is tested on a number of benchmark exercises for which experimental data is available and for which the power plant details have been released. The above-described approach is based on the introduction of nine steps (exercises). These exercises are carried out in three phases, and follow the established routine calculation scheme for LWR design and safety analysis in industry and regulation. This paper provides overview and discussion in detail of the Phase I (Neutronics Phase). In its conclusion part the paper summarizes the priorities of Phase II (Core Phase) and Phase III (System Phase).

Key Words: Uncertainty Analysis in Modeling (UAM), Cross-sections, Covariance Data, Phases, Exercises

1. INTRODUCTION

In the on-going international LWR Uncertainty Analysis in Modeling (UAM) benchmark activity different Uncertainty Analysis (UA) and Sensitivity Analysis (SA) methods for coupled codes will be compared, and their value assessed including the validation of the methodologies for uncertainty propagation. For the first time the uncertainty propagation will be estimated through the whole simulation process on a unified benchmark framework to provide credible coupled code predictions with defensible uncertainty estimations of safety margins at the full core/system level. The benchmark will allow not only to compare and to assess the current UA methods on representative applications but also will stimulate the further development of efficient and powerful UA methods suitable for complex coupled code simulations and will help to formulate

recommendations and guidelines on how to utilize advanced and optimized UA and SA methods in "best estimate" coupled reactor simulations in licensing practices.

To summarize, in addition to LWR best-estimate calculations for design and safety analysis, the different aspects of UAM are to be further developed and validated on scientific grounds in support of its performance. There is a need for efficient and powerful UA and SA methods suitable for such complex coupled multi-physics and multi-scale simulations. The ongoing OECD LWR UAM benchmark sequence addresses this need by integrating the expertise in reactor physics, thermal-hydraulics and reactor system modeling as well as uncertainty and sensitivity analysis, and will contribute to the development and assessment of advanced/optimized uncertainty methods for use in best-estimate reactor simulations. Such an effort has been undertaken within the framework of a program of international co-operation that benefits from the coordination of the Nuclear Energy Agency (NEA) Nuclear Science Committee (NSC) and all participants and by interfacing with the Committee of Safety of Nuclear Installations (CSNI) activities.

2. DESCRIPTION OF OECD LWR UAM BENCHMARK

The objective of the work is to define, conduct, and summarize an OECD benchmark for uncertainty analysis in best-estimate coupled code calculations for design, operation, and safety analysis of LWRs. Reference systems and scenarios for coupled code analysis are defined to study the uncertainty effects for all stages of the system calculations. Measured data from plant operation are available for the chosen scenarios.

The utilized technical approach is to establish a benchmark for uncertainty analysis in best-estimate modeling and coupled multi-physics and multi-scale LWR analysis, using as bases a series of well defined problems with complete sets of input specifications and reference experimental data. The objective is to determine the uncertainty in LWR system calculations at all stages of coupled reactor physics/thermal hydraulics calculation. The full chain of uncertainty propagation from basic data, engineering uncertainties, across different scales (multi-scale), and physics phenomena (multi-physics) is tested on a number of benchmark exercises for which experimental data is available and for which the power plant details have been released.

The principal idea is: a) to subdivide the complex system/scenario into several steps or Exercises, each of which can contribute to the total uncertainty of the final coupled system calculation; b) to identify input, output, and assumptions for each step; c) to calculate the resulting uncertainty in each step; d) to propagate the uncertainties in an integral systems simulation for which high quality plant experimental data exists for the total assessment of the overall computer code uncertainty. The main scope covers uncertainty (and sensitivity) analysis (SA/UA) in best estimate modeling for design and operation of LWRs, including methods that are used for safety evaluations. As part of this effort, the development and assessment of different methods or techniques to account for the uncertainties in the calculations will be investigated and reported to the participants.

The above-described approach is based on the introduction of nine steps (Exercises), which allows for developing a benchmark framework which mixes information from the available

integral facility and NPP experimental data with analytical and numerical benchmarking. Such an approach compares and assesses current and new uncertainty methods on representative applications and simultaneously benefits from different methodologies to arrive at recommendations and guidelines. These nine steps (Exercises) are carried out in three Phases as follows:

Phase I (Neutronics Phase)

a) Exercise 1 (I-1): "Cell Physics" focused on the derivation of the multi-group microscopic cross-section libraries and their uncertainties
b) Exercise 2 (I-2): "Lattice Physics" focused on the derivation of the few-group macroscopic cross-section libraries and their uncertainties
c) Exercise 3 (I-3): "Core Physics" focused on the core steady state stand-alone neutronics calculations and their uncertainties

Phase II (Core Phase)

a) Exercise II-1: Fuel thermal properties relevant for transient performance
b) Exercise II-2: Neutron kinetics stand-alone performance (kinetics data, space-time dependence treatment, etc.)
c) Exercise II-3: Thermal-hydraulic fuel bundle performance

Phase III (System Phase)

a) Exercise III-1: Coupled neutronics/thermal-hydraulics core performance (coupled steady state, coupled depletion, and coupled core transient with boundary conditions)
b) Exercise III-2: Thermal-hydraulics system performance
c) Exercise III-3: Coupled neutronics kinetics thermal-hydraulic core/thermal-hydraulic system performance

Separate Specifications are being prepared for each Phase in order to allow participation in the full Phase or only in a subset of the Exercises. Boundary conditions and necessary input information are provided by the benchmark team. The intention is to follow the calculation scheme for coupled calculations for LWR design and safety analysis established in the nuclear power generation industry and regulation. The specification document that covers Phase I (which includes the first three Exercises) was distributed to the participants [1].

3. DISCUSSION OF PHASE I

Phase I is focused on understanding uncertainties in prediction of key reactor core parameters associated with LWR stand-alone neutronics core simulation. 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:

a) PWR (TMI-1) [2];
b) BWR (Peach Bottom-2) [3];
c) VVER-1000 (Kozloduy-6, Kalinin-3) [4].

For cross-section generation any type of lattice solver can be used. For core calculations the established two-group energy structure for LWR analyses is proposed as the major path of the benchmark activities. However, provisions are made for utilization of other few-group structures

if the participants want to investigate them. The Monte-Carlo method will provide reference solutions for the test problems of each Exercise of Phase I.

3.1. Exercise I-1: Cell Physics

The Exercise I-1 is focused on derivation of the multi-group microscopic cross-section libraries. Its objective is to address the uncertainties due to the basic nuclear data as well as the impact of processing the nuclear and covariance data, selection of multi-group structure, and self-shielding treatment. The intention for Exercise I-1 is to propagate the uncertainties in evaluated Nuclear Data Libraries - NDL - (microscopic point-wise cross sections) into multi-group microscopic cross-sections used as an input by lattice physics codes. The participants can use any of the major NDLs such as Evaluated Nuclear Data Files (ENDF), Joint European Fission and Fusion files (JEFF), and Japanese Evaluated Nuclear Data Library (JENDL). 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 major NDLs. 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.

Table 1 shows the total number of materials and cross-section reactions with neutron cross-section covariance data in the recent versions of the major evaluated nuclear data files.

Table I. Number of materials and cross-sections with covariances of neutron cross-sections

Data files	Number of materials	Number of cross-sections
ENDF/B-VI.8	44	400
JEFF-3.1	34	350
JENDL-3.3	20	160

The covariance data in the major data files is scarce in terms of materials (including actinides) and types of covariance matrices available. They contain uncertainty information only for few isotopes and reactions and usually for different number and different isotopes in different files. For the isotopes, which are not included, usually their covariances are assumed to be zero, which will result in the underestimation of core parameters uncertainties. In conclusion, the status of available covariance data in the major NDLs is such that it cannot support the objectives of the OECD LWR UAM benchmark. Once the more complete covariance data are ready containing low fidelity covariances that supplement available NDL evaluations for all required materials, it can be used for the purposes of this benchmark within the framework of Exercise I-1. For example, crude but reasonable covariances for all materials are being developed within the framework of ENDF/B-VII.0. When this development is completed and made available it can be used for the purpose of the OECD LWR UAM benchmark.

The current status of the evaluated cross-section NDLs is such that the most comprehensive covariance library is available with SCALE-5.1. For this reason it was decided to utilize the nuclide dependent multi-group covariance data from SCALE-5.1 for the purposes of Exercise I-1. It is based on a 44-group structure. For other group structures, NEA/OECD has provided the tools for handling and transforming the cross-section covariance in a consistent way. Covariance data are relative values and can be used with different NDLs. In order to analyze the results on a common ground, it is recommended to participants to use only these data and tools. The output uncertainties of Exercise I-1 are input uncertainties in Exercise I-2

Following the request from the UAM expert group, the authorization was granted by the SCALE management and US DOE for use of the group cross-section covariance data now distributed with SCALE-5.1 for the purposes of Phase I (Neutronics Phase) of the LWR UAM benchmark activities and in connection with other codes. As a source of their cross-section data the participants can use the NDLs, which are normally used in conjunction with their lattice physics codes. The three major libraries (ENDF, JEFF and JENDL) are possible candidates. For cross-section covariance data the 44-group covariance libraries from SCALE-5.1 are proposed [5]. 44GROUPV6REC is the recommended covariance library based on several sources, including evaluated data files ENDF/B-VI, ENDF/B-V, JENDL, and JEFF. Data missing from all evaluated data files were represented by the "integral approximation", for the resonance and thermal energy ranges only. This approximation was used for approximately 300 materials. The SCALE-5.1 recommended covariance library is currently being updated to include recent high fidelity ENDF/B-VII uncertainty evaluations for the nuclides U-235, U-238, Pu-239, Th-232, and Gd isotopes. Some of the integral approximation data also is being revised to more recent measured values. This is being made available for the UAM effort with SCALE-6.0

In addition to the covariance matrices, a utility program for interpolating or collapsing from a given group structure to another one is provided for participants' use [6]. Participants can choose any multi-group energy structure according to the input requirements of their lattice code to be utilized. The code ANGELO is designed for the interpolation of the multi-group covariance matrices from the original (in this case 44 groups) to a user defined energy structure which is also distributed for the convenience of the users. The algorithm used in the ANGELO code is relatively simple using flat weighting; therefore the interpolations involving the energy group structures which are very different from the original one (especially if the number of groups is reduced considerably) are to be avoided as they may not be accurate. Still, the procedure tends to be conservative. The interpolation procedure was found to give reliable results if the number of groups changed by a factor of up to four. In this range the procedure can therefore be considered as an adequate and easy-to-use alternative to more rigorous methods, like the ERRORR module of NJOY [7].

LAMBDA is a program to verify some mathematical properties and the physical consistency of the data and the interpolation procedure, in particular the positive definiteness of the multi-group covariance matrices. The trace and the number of positive, negative, and zero eigenvalues are calculated and the matrix is classified on this basis. The correlation matrix is tested to determine if any element exceeds unity. This quality verification is highly recommended before using the

covariance information for data consistency analyses with integral experiments and for data adjustment.

Within the framework of Exercise I-1 the cross-section uncertainty data is processed in a multi-group format. The final multi-group cross-section libraries and associated uncertainties should be consistent with requirements of lattice physics codes, which participants are planning to utilize. In order to perform a comparative analysis of the multi-group cross-section uncertainty data obtained after processing test problems are devised or utilized from the previously defined benchmarks and from the available experimental data.

The first sets of problems are two-dimensional fuel pin-cell test problems representative of BWR PB-2, PWR TMI-1, and VVER-1000 Kozloduy-6. The full geometry and material specifications are provided in [1]. The reflective boundary conditions are utilized at the boundaries of problems. These problems have to be analyzed at Hot Zero Power (HZP) conditions and Hot Full Power (HFP) conditions. The HFP operating conditions cases allow to vary the spectrum in the test problems. First, one group effective uncertainties are to be calculated for subsequent comparisons. The effective uncertainties in this paper are calculated using the 44-group SCALE5.1 uncertainty data associated with the multi-group library used as input in the TRITON lattice physics code. The effective uncertainty (relative error) for neutron cross-sections corresponding to neutron flux spectrum of the pin-cell test problem of interest) is obtained for a given nuclide as shown below:

One-group effective cross-section uncertainty (Δ^2) $= \Sigma \Delta^2_g$
$= \Sigma [\alpha_x \bullet \text{cov}(x, y) \bullet \alpha_y]_g$

where

$\Delta^2 = \Sigma \Delta^2_g$ summation of Δ^2_g from energy group 1 to group G

$\Delta^2_g = \alpha_{x,g} \bullet \text{cov}(x_g, y_g) \bullet \alpha_{y,g}$ each group uncertainty is weighted by x reaction and y reaction

$\alpha_{x,g} = \sigma_{g,x} [\varphi_{g,x} / \varphi_T] / \sigma_x$ weighting factor based on data from x reaction

$\alpha_{y,g} = \sigma_{g,y} [\varphi_{g,y} / \varphi_T] / \sigma_y$ weighting factor based on data from y reaction

cov (x,y) = given covariance matrix

σ_x , σ_y = flux averaged effective cross-sections

x = neutron reaction type

y = neutron reaction type

φ_g = Group flux

φ_T = Total flux

The calculation procedure is illustrated in Fig. 1, where

$\Delta^2_1 = [\alpha_{x,1} \bullet \text{cov}(x_1, y_1) \bullet \alpha_{y,1}] + [\alpha_{x,2} \bullet \text{cov}(x_2, y_1) \bullet \alpha_{y,1}] + \ldots\ldots\ldots\ldots [\alpha_{x,44} \bullet \text{cov}(x_{44}, y_1) \bullet \alpha_{y,1}]$

$\Delta^2_2 = [\alpha_{x,1} \bullet \text{cov}(x_1, y_2) \bullet \alpha_{y,2}] + [\alpha_{x,2} \bullet \text{cov}(x_2, y_2) \bullet \alpha_{y,2}] + \ldots\ldots\ldots\ldots [\alpha_{x,44} \bullet \text{cov}(x_{44}, y_2) \bullet \alpha_{y,2}]$

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$\Delta^2_{44} = [\alpha_{x,1} \bullet \text{cov}(x_1, y_{44}) \bullet \alpha_{y,44}] + [\alpha_{x,2} \bullet \text{cov}(x_2, y_{44}) \bullet \alpha_{y,44}] + \ldots\ldots [\alpha_{x,44} \bullet \text{cov}(x_{44}, y_{44}) \bullet \alpha_{y,2}]$

$\Delta^2_{\text{effective}} = + \Delta^2_1 + \Delta^2_2 + \Delta^2_3 + \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots + \Delta^2_{44}$

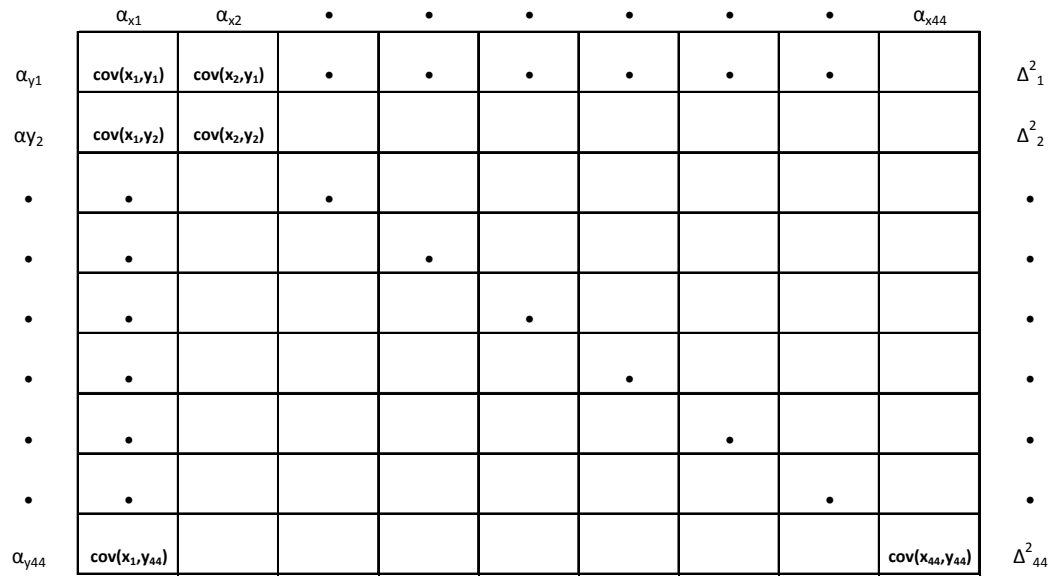

Figure 1. Illustration of calculation procedure for one-group effective cross-section uncertainty for a given nuclide of interest

Figure 2 shows a sample depiction of the effective group uncertainty (Δ^2_g) for the elastic scattering cross-section of Hydrogen.

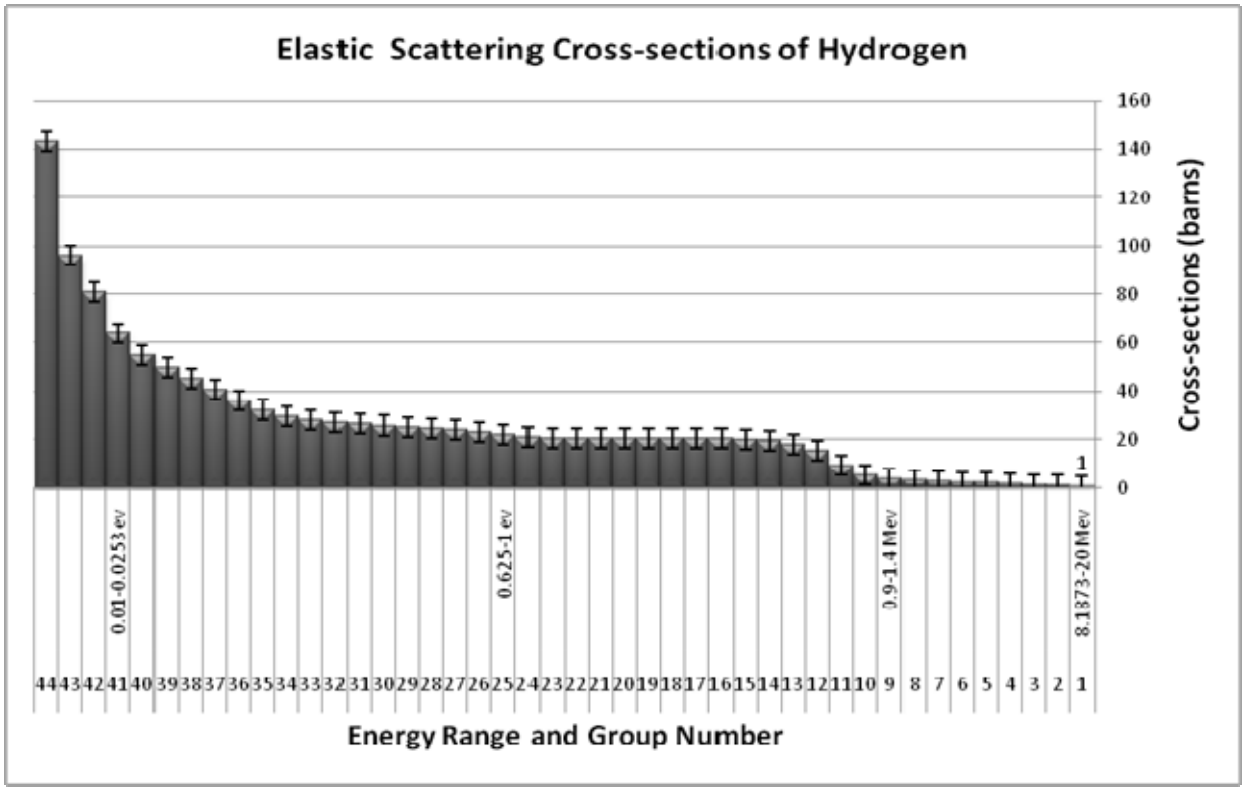

Figure 2. Depiction of the effective group uncertainty for the elastic scattering cross-section of Hydrogen

In order to demonstrate the calculation of the effective one-group uncertainties for the most important reaction cross-sections of three nuclides the benchmark team has utilized the recommended 44GROUPV6REC library from SCALE5.1. The criticality calculations were performed using the SCALE5.1/CSAS1 sequence (which included the 1-D transport solver XSDRNPM) for the three pin-cell test models described above. Using fluxes and cross-section data generated by CSAS1 sequence and XSDRNPM code, the effective one-group uncertainties of the elastic scattering cross-section of Hydrogen (H-1), fission cross-section of U-235 and capture cross-section of U-235 were calculated for each pin-cell model as shown in Table II.

Table II. Effective one-group uncertainties for the most important reactions of three nuclides for the pin-cell test models

Pin-cell model	Nuclide	Reaction x	Reaction y	Effective uncertainty
BWR	H-1	mt-2	mt-2	5.857E-10
	U-235	mt-452	mt-452	9.307E-10
	U-238	mt-18	mt-18	1.249E-07
PWR	H-1	mt-2	mt-2	6.114E-10
	H-235	mt-452	mt-452	8.986E-10
	u-238	mt-18	mt-18	1.490E-07
VVER-1000	H-1	mt-2	mt-2	5.789E-10
	U-235	mt-452	mt-452	9.195E-10
	U-238	mt-18	mt-18	1.459E-07

In the same manner the effective uncertainties can be calculated for the remaining neutron cross-sections of the nuclides present in the pin-cell models. In addition, for each test problem the participants are requested to calculate k_{inf}, and absorption and fission reaction rates for ^{234}U, ^{235}U, and ^{238}U and associated uncertainties due to multi-group cross-sections based on the processed in Exercise I-1 multi-group covariance matrices.

The second set of test problems are based on the KRITZ-2 LEU critical experiments [9] and for these problems we have utilized the NEA/OECD SUSD3D tool [10] in order to propagate cross-section uncertainties to calculate quantities of interest in nuclear analysis. Example of the uncertainties in k_{eff} (in pcm) due to cross section uncertainties for the benchmark configuration KRITZ-2.13C based on various covariance data is shown in Fig. 3. The same sensitivity profiles were used in all three cases and only the covariance data were varied.

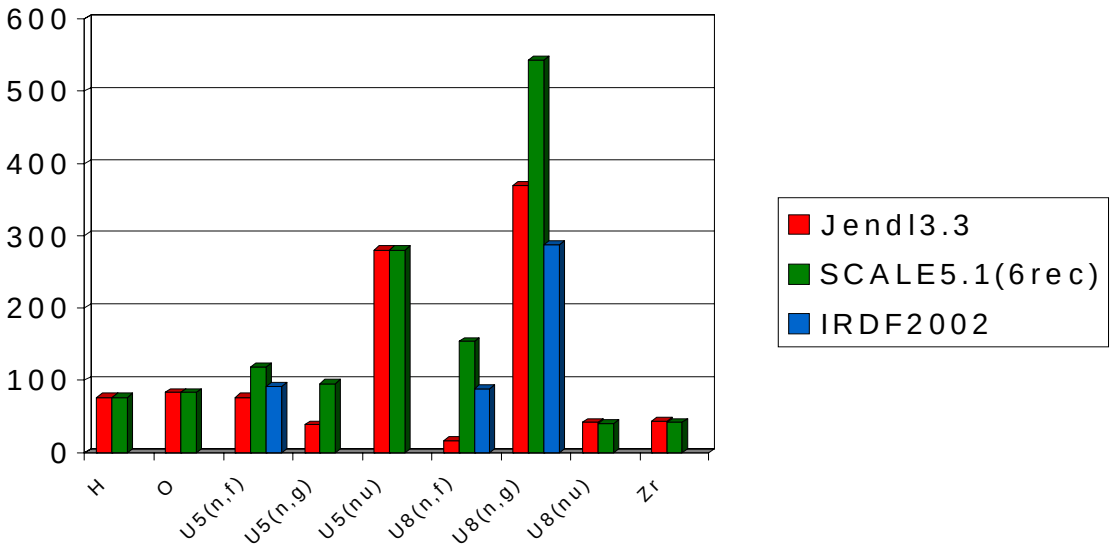

Figure 3. Uncertainties in k_{eff} (in pcm) due to cross section uncertainties

3.2 Exercise I-2: Lattice Physics

In the current established calculation scheme for LWR design and safety analysis, multi-group microscopic cross-section libraries are an input to lattice physics calculations. The multi-group cross-section uncertainties (multi-group cross-section covariance matrix) should be obtained by participants as output uncertainties within the framework of Exercise I-1. In Exercise I-2 the multi-group cross-section uncertainties are input uncertainties and must be propagated through the lattice physics calculations to few-group cross-section uncertainties (few-group covariance matrix). The other input uncertainties in Exercises I-2 are new uncertainties added during the cross-section generation process.

In order to propagate the input uncertainties through lattice physics calculations to determine uncertainties in output lattice-averaged parameters within the framework of Exercise I-2 the utilization of a lattice physics code is necessary. Participants can use/select their own lattice physics codes in conjunction with their own UA and SA tools for the purposes of this exercise. Different stand-alone neutronics single assembly and mini-core test problems have been designed for the purposes of the Exercise I-2 utilizing information from the previous OECD coupled code benchmarks. Continuous Monte Carlo (MCNP5) solutions with sufficient statistics to assure not only k_{inf} (k_{eff}) but also fission source convergence will be used as reference solutions. In addition, the KRITZ-2 [9] LEU mini-core test cases and the VVER physics experiments [11] (for which there is available experimental data) are utilized.

The output uncertainty of Exercise I-2 is propagated in Exercises I-3, II-3, III-1 and III-3. The major effort is focused on obtaining uncertainties in two group homogenized parameters based on the standard two-group structure (with 0.625 eV cut-off) utilized in the LWR industrial calculation scheme. Provision for few group (more than two energy group) homogenized parameters and associated uncertainties with selected by participants few-group structures is made.

3.3 Exercise I-3: Core Physics

In the current established calculation scheme for LWR design and safety analysis the lattice averaged (homogenized) few-group cross-sections are an input to core calculations. The few-group cross-section uncertainties (few-group covariance matrix) should be obtained by participants as output uncertainties within the framework of Exercise I-2. In Exercise I-3 the few-group cross-section uncertainties are input uncertainties and must be propagated to uncertainties in evaluated stand-alone neutronics core parameters. The other input uncertainties in Exercises I-3 are new uncertainties added during the core stand-alone calculations.

Understanding the uncertainties in key output reactor core parameters associated with steady state core simulation is important in regard to introducing appropriate design margins and deciding where efforts should be directed to reduce uncertainties. The propagation of the input uncertainties through core calculations to determine uncertainties in output core parameters within the framework of Exercise I-3 requires utilization of a core simulator code. Participants can use/select their own core simulator codes in conjunction with their own UA and SA tools for the purposes of this exercise.

Three-dimensional (3-D) test problems on two different levels are defined to be used within Exercise I-3: HZP core test cases (for which the continuous energy Monte Carlo method is used for reference calculations), and documented experimental benchmark plant cold critical data and critical lattice data.

In summary this exercise is focused on stand-alone neutronics core calculations and associated prediction uncertainties. It does not analyze uncertainties related to cycle and depletion calculations. No feedback modeling is assumed, thus it will address the propagation of uncertainties associated with few-group cross-section generation but not cross-section modeling i.e. methodologies used for cross-section parameterization as a function of history and instantaneous variables.

3. CONCLUSIONS

The three exercises within Phase I follow the established in the industry and regulation routine calculation scheme for LWR design and safety analysis. The Phase I is focused on understanding uncertainties in the prediction of key reactor core parameters associated with LWR stand-alone neutronics core simulation. The obtained output uncertainties from Phase I of the OECD LWR UAM benchmark will be utilized as input uncertainties in the remaining two phases – Phase II (Core Phase) and Phase III (System Phase).

Phase II will address core neutron kinetics, thermal-hydraulics and fuel performance, without any coupling between the three physics phenomena. Phase III will include system thermal-hydraulics and coupling between fuel, neutronics and thermal-hydraulics for steady-state, depletion and transient analysis.

The benchmark team is preparing Specifications for each Phase in order to allow participation in the full Phase or only in a subset of the Exercises or in a separate Exercise. Boundary conditions

and necessary input information will be provided by the benchmark team. Each organization interested in the UAM benchmark has to identify its own objectives and priorities. In particular for the preparation of Phases 2 and 3, it might be necessary to rank the priorities between the reactor types or the transients to be analyzed.

The presented OECD LWR UAM benchmark activity is challenging and responds to the needs of estimating confidence bounds for results from simulations and analysis in real applications. It will create the favorable environment for the development of UA and SA methods and their use and become a standard. In order to achieve this, the UAM scientific board members recommended that research organizations and institutions reserve the necessary funds to support this activity and that an uncertainty analysis culture is developed in nuclear engineering.

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