PHYSOR 2014 – The Role of Reactor Physics Toward a Sustainable Future
The Westin Miyako, Kyoto, Japan, September 28 – October 3, 2014, on CD-ROM (2014)

SENSITIVITY/UNCERTAINTY ANALYSIS FOR BWR CONFIGURATIONS OF EXERCISE I-2 OF UAM BENCHMARK

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ABSTRACT

In order to evaluate the uncertainties in prediction of lattice-averaged parameters, input data of core neutronics codes, Exercise I-2 of the OECD benchmark for uncertainty analysis in modeling (UAM) was proposed.

This work aims to perform a sensitivity/uncertainty analysis of the BWR configurations defined in the benchmark for the purpose of Exercise I-2. Criticality calculations are done for a 7x7 BWR fresh fuel assembly at HFP in four configurations: single unrodded fuel assembly, rodded fuel assembly, assembly/reflector and assembly in a color-set. The SCALE6.1 code package is used to propagate cross section covariance data through lattice physics calculations to both k-effective and two-group assembly-homogenized cross sections uncertainties. Computed sensitivities and uncertainties for all configurations are analyzed and compared. It was found that uncertainties are very similar for the four test-problems, showing that the influence of the assembly environment on uncertainty prediction is very small.

Key Words: **lattice physics uncertainty propagation, sensitivity/uncertainty analysis, few-group homogenized cross section uncertainties**

1. INTRODUCTION

The OECD benchmark for Uncertainty Analysis in Modeling (UAM) for design, operation and safety analysis of LWRs [1] was established in order to quantify the uncertainties at all stages of coupled reactor physics/thermal-hydraulics LWR calculations. It is based on the introduction of 9 steps or Exercises, carried out in 3 phases: neutronics phase, core phase and system phase, following the calculation scheme for LWR design and safety analysis established in the nuclear industry.

Phase I is focused on understanding uncertainties in prediction of core parameters associated with stand-alone core neutronics simulations. In that phase, the main source of uncertainty considered is the cross section uncertainties. It consists of 3 Exercises:

- Exercise I-1 (Cell Physics) propagates the uncertainties starting from evaluated nuclear data libraries to multi-group microscopic cross-section libraries used as input by lattice physics codes.
- Exercise I-2 (Lattice Physics) propagates mainly uncertainties coming from Exercise I-1

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through lattice physics calculations to k-inf and few-group homogenized parameters, used as input data by core neutronics codes.

- Exercise I-3 (Core Physics) propagates uncertainties coming from Exercise I-2 to core stand-alone neutronics parameters.

Three representative designs, corresponding to a PWR, a BWR and a VVER-1000, are defined for the purposes of those Exercises.

In the present work, the uncertainty analysis corresponding to Exercise I-2 for the BWR design is performed using SCALE6.1 code system [2]. The calculation methodology, the models developed for the different BWR configurations proposed in the benchmark and the modeling assumptions are presented. Then, a sensitivity/uncertainty analysis is performed. Computed sensitivities and uncertainties in both k-effective and homogenized two-group cross sections due to cross section covariance data are compared and the influence of the assembly environment is assessed.

2. DESCRIPTION OF BWR TEST PROBLEMS

Cases under study are four different configurations of a BWR fuel assembly representative of the initial loading of Peach Bottom-2 (PB-2) plant: single fuel assembly, rodded fuel assembly, 1-D assembly/reflector and 2-D assembly color set or mini-core. Specifications can be found in [1, Section 3.2].

The fresh fuel assembly is a 7x7 lattice array with 45 UO_2 rods with enrichments ranging from 1.33 w/o to 2.93 w/o and 4 UO_2-Gd_2O_3 rods. The assembly has diagonal symmetry. Criticality calculations are carried out at Hot Full Power (HFP) conditions, as well as uncertainty quantification due to cross section uncertainties.

3. METHODOLOGY

The calculation methodology consisted of employing the TRITON multipurpose sequence of SCALE, version 6.1.2, to perform coupled cross-section processing and transport calculations using the 2-D discrete-ordinates NEWT code, and sensitivity/uncertainty analysis using TSUNAMI-2D.

- All calculations were performed using the SCALE 238-group cross section library from ENDF/B-VII.0 (v7-238). The covariance library was 44GROUPCOV.
- For cross-section processing, the *latticecell* treatment in CENTRM was used for the UO_2 fuel rods. Accurate Dancoff factors were calculated using de MCDancoff module. Rods with the same enrichment and similar Dancoff factors were lumped to reduce the self-shielding processing effort. For Gadolinium-bearing fuel rods, a *multiregion* treatment with five equal-area rings to capture radial depletion of gadolinium was used.
- For the NEWT transport calculations, the order of S_N was set to 10. All fuel mixtures and structural materials used P1 scattering, while all moderator mixtures used P3 scattering. The recommended 4x4 grid mesh was used for the square-pitched units. Convergence criteria for the eigenvalue were set at 1.0E-5. Coarse-mesh finite-difference acceleration (CMFD) option was employed on the global grid, in particular the original method for rectangular-domain

configurations (cmfd=rect). Moreover, the second-level two-group CMFD accelerator was enabled (cmfd2g=yes).

- For S/U calculations, TSUNAMI-2D sequence solved forward and adjoint transport problems using NEWT. Cross-section processing used the modules by default (BONAMIST and CENTRM with ENDF/B-VII.0). Then, the SAMS module was invoked to calculate the sensitivity coefficients in 238 energy groups. Since the covariance matrix in SCALE is given in 44 energy groups, the sensitivity profiles were collapsed inside SAMS and uncertainty quantification carried out using "sandwich formula".

4. SCALE MODELING OF EXERCISE I-2/ BWR

4.1. Unrodded Fuel Assembly (FA) Model

The 2-D single assembly with reflective boundary conditions (standard case used for cross-section generation in LWR analysis) was modeled. Inputs were prepared using the geometry, materials and temperatures at HFP conditions included in the specifications [1] (40% void fraction for the moderator in-channel). For the analysis using SCALE, the whole fuel assembly was modeled, as plotted in Figure 1.a, where different colors identify different materials modeled in the configuration.
Figure 1.b presents the Dancoff factors computed with MCDancoff as well as the SCALE-default value. Wrong Dancoff factors were obtained when the origin of the *global unit* was placed in a corner of the assembly whereas right values were computed placing the origin in the center, as shown in Figure 1.b.

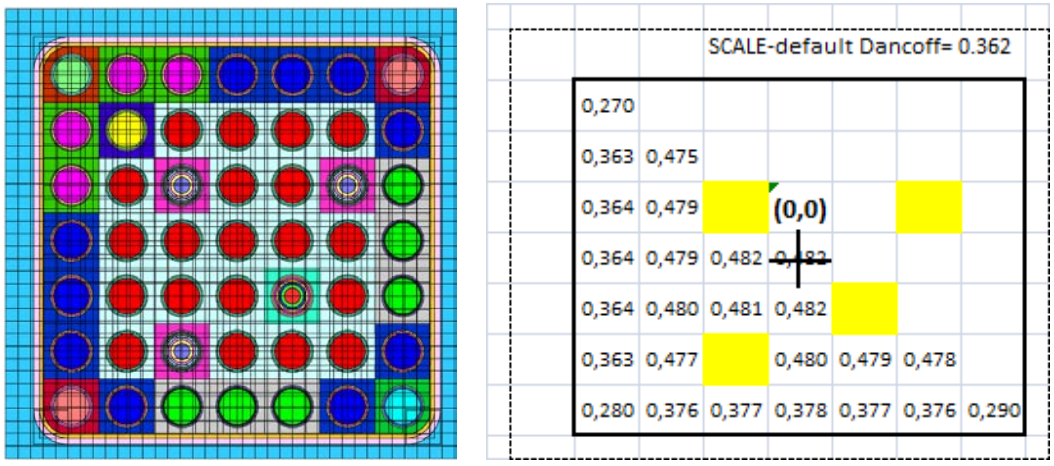

Figure 1. TRITON BWR assembly model and Dancoff factors map

4.2. Rodded Fuel Assembly Model

In order to model the controlled assembly (Figure 2), a cruciform control rod blade was included. Dancoff factors were not re-computed, and the ones calculated for the unrodded assembly were used instead.

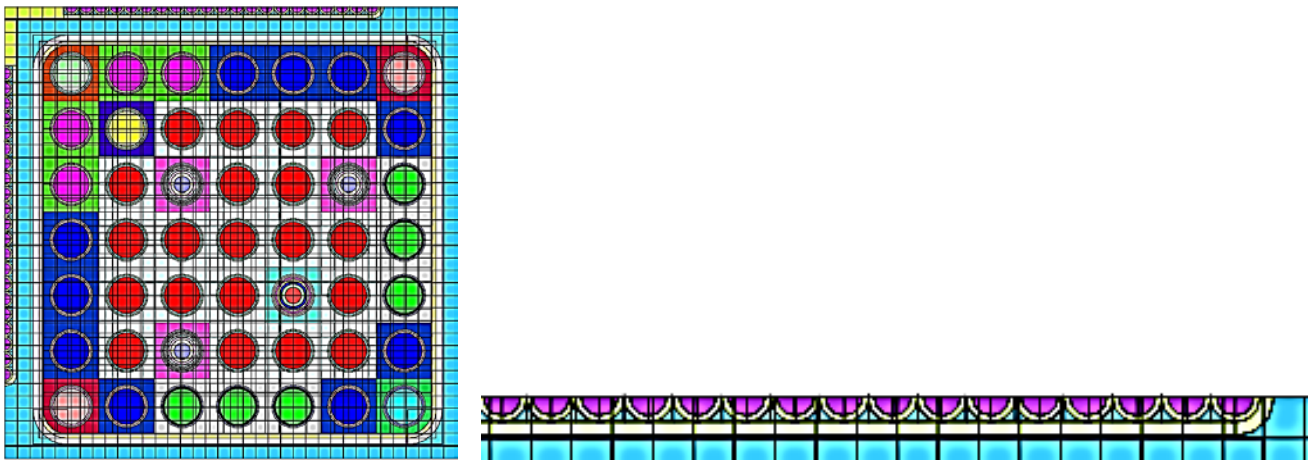

Figure 2. TRITON rodded BWR assembly model and detail of the control rod blade.

4.3. 1-D Assembly/Reflector Model

A 1-D assembly/reflector configuration was modeled, with reflective boundary conditions on the left boundary and vacuum boundary condition on the right boundary. This is the standard model used for reflector cross-section generation in LWR analysis.

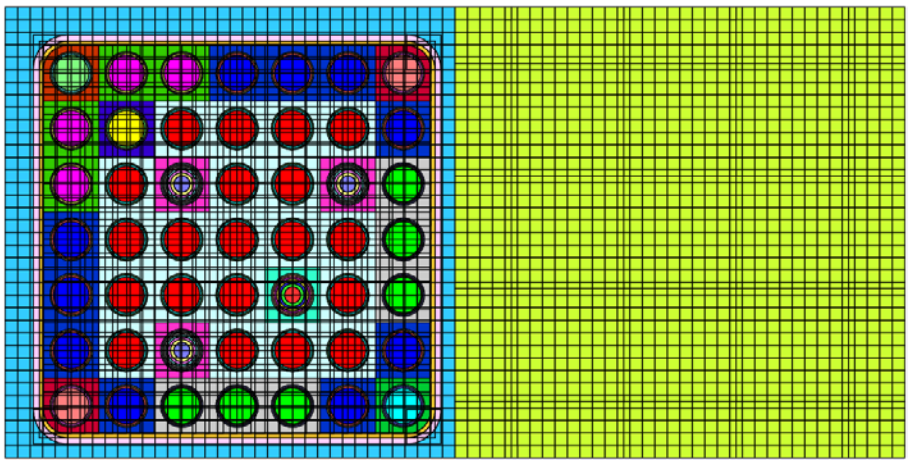

Figure 3. TRITON BWR radial reflector model

4.4. 2-D Color-set (mini-core) Model

A mini-core problem involving unrodded and rodded assemblies was model, with reflective boundary conditions.

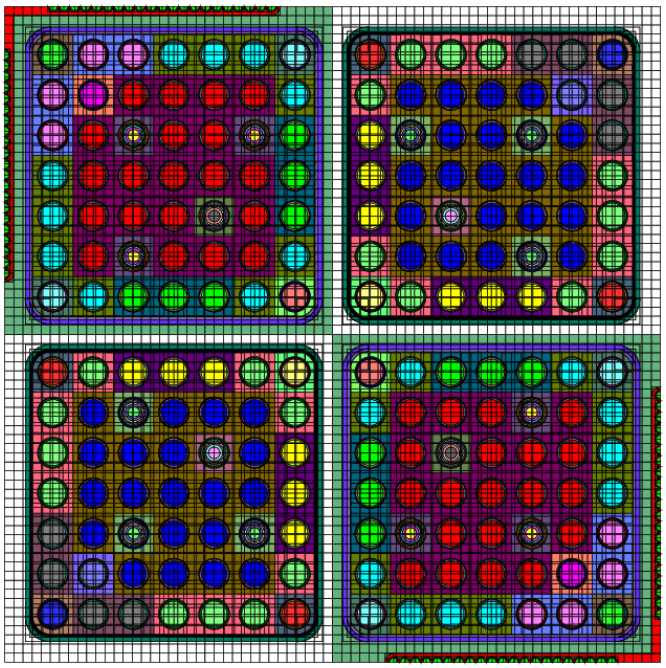

Figure 4. TRITON 2-D BWR color-set model

5. SENSITIVITY/ UNCERTAINTY ANALYSIS

5.1. Comparison of k-effective uncertainties

For all test problems, k-effective values and their associated uncertainties due to cross section uncertainty propagation (taking into account all the possible reactions for which there is uncertainty information) are shown in Table 1. In addition, the reactivity values computed in both the forward and adjoint calculations are included, verifying an excellent agreement.

Table 1. Multiplication factors and associated uncertainties (relative standard deviation of k-effective, %Δk/k) for all configurations due to cross-section covariance data

Test problems	k-effective		% Δk/k
Unrodded Fuel Assembly	Forward Calculation: Adjoint Calculation:	1.088974 1.088965	0.5474
Rodded Fuel Assembly	Forward Calculation: Adjoint Calculation:	0.778953 0.778951	0.5950
1-D Assembly/Reflector	Forward Calculation: Adjoint Calculation:	0.620948 0.620942	0.5364
2-D Color-set	Forward Calculation: Adjoint Calculation:	0.943464 0.943460	0.5497

It can be seen that the total uncertainty in k-eff for the unrodded fuel assembly is very similar to the cases where control rod is inserted, or where the environment of the single fuel assembly is modified.

The top eight reaction-nuclide contributors to the uncertainty in k-eff are given in Table 2 in order to identify reactions that contribute most to the uncertainties. The contributions are given in relative std. dev. (%). Only relative contributions larger than 0.05 are included, sorted in descending order only for the unrodded fuel assembly. The square root of the sum of the square rel.std.dev. would provide the total uncertainty in k-eff as rel.std.dev.(%) shown in Table 1.

Table 2. Top eight nuclide-reaction contributors to the uncertainty in k-effective for all test problems

Nuclide-Reaction		Contributions to Uncertainty in k_{eff} (% Δk/k)			
		Unrodded FA	Rodded FA	FA/Reflector	Color-set 2D
^{238}U	*(n,γ)*	0.30457	0.27556	0.31037	0.29392
^{235}U	*ν*	0.26782	0.25007	0.26660	0.26124
^{238}U	*(n,n')*	0.20541	0.31075	0.14342	0.22530
^{235}U	*χ*	0.14316	0.20507		0.15604
^{235}U	*(n,γ)*	0.14202	0.12390	0.13531	0.13470
^{235}U	*(n,f)*	0.12643	0.14358	0.14192	0.13973
^{235}U	*(n,f) (n,γ)*	0.12018	0.11255	0.12105	0.11756
^{238}U	*ν*	0.93636	0.13109	0.10197	0.10723
^{1}H	*(n,n)*			0.14275	

It can be seen that the same cross-sections are the main responsible of k-eff uncertainties for all configurations except the (n,n) reaction of ^{1}H, which becomes one of the main contributors in the assembly/reflector case, whereas is not as important for the other configurations.

5.2. Comparison of sensitivity profiles of k-effective

It is interesting to compare the sensitivity profiles among all configurations. As an example, the sensitivity profiles to ^{238}U (n,γ) *r*eaction cross section are presented in Figure 5 for the four configurations. Differences in sensitivity profiles are found, and the same trend is observed for other isotope-reactions, but they do not lead to large differences in the k-effective uncertainty.

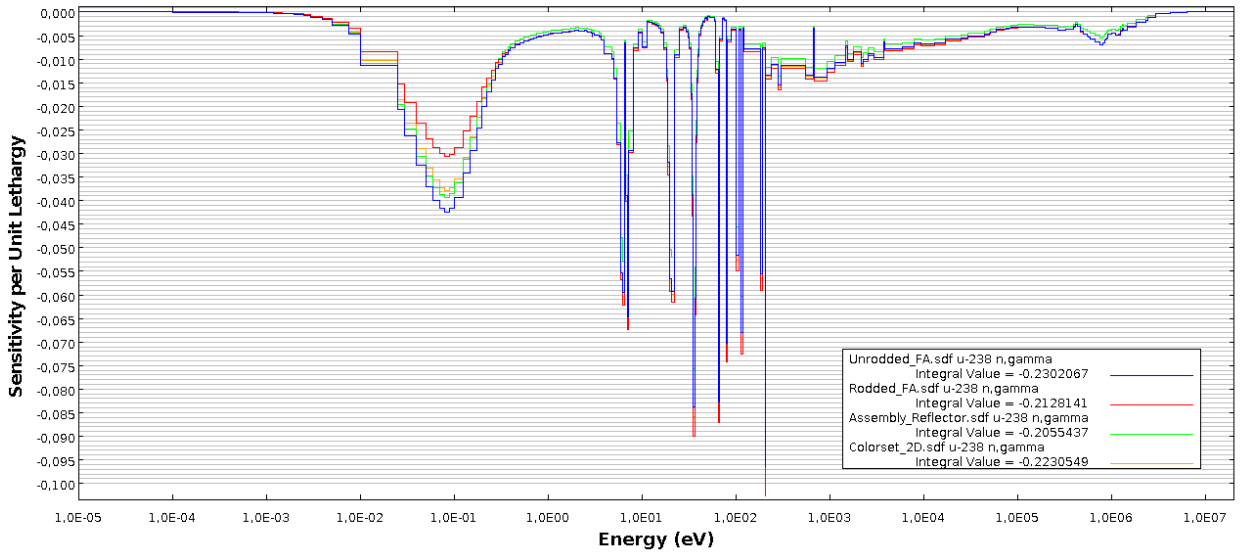

Figure 5. Sensitivity profiles to ^{238}U (n,γ) for all test problems at HFP

5.3. Comparison of homogenized macroscopic cross sections uncertainties

Two-group assembly homogenized macroscopic cross-sections and associated uncertainties are given in Tables 3 and 4, using 0.625 eV as cut-off point. Uncertainties in other parameters of interest for core calculations such us discontinuity factors have not been computed.

Table 3 contains values for the unrodded and rodded fuel assembly homogenized over the assembly. Table 4 contains values for the assembly/reflector and 2-D color-set, homogenized over the fuel assembly and over the reflector in the first configuration, and over the unrodded and rodded assembly in the second one.

It can be seen that uncertainties in the analyzed few-group cross-sections are lower than 1.5% for all configurations and homogenization regions. In addition, uncertainties in the cross-sections homogenized over the fuel assembly exhibit very slight differences among the four configurations, that is, contributions are very similar independently on the assembly environment.

Table 3. Two-group homogenized macroscopic cross-sections and uncertainties for the unrodded and rodded fuel assemblies

Reaction	Unrodded FA		Rodded FA	
	Σ (cm^{-1})	$\Delta\Sigma/\Sigma$ (%)	Σ (cm^{-1})	$\Delta\Sigma/\Sigma$ (%)
Absorption 1	6.7846E-3	0.85	9.2300E-3	0.87
Absorption 2	5.2333E-2	0.22	7.4123E-2	0.20
Nu-fission 1	4.7086E-3	1.08	4.6012E-3	1.06
Nu-fission 2	6.6870E-2	0.45	7.4958E-2	0.45
Scattering 1→2	1.4396E-2	1.24	1.1322E-2	1.29
Scattering 2→1	9.3617E-4	0.33	1.3409E-3	0.33

Table 4. Two-group homogenized macroscopic cross-sections and uncertainties for the assembly/reflector and for the 2-D color-set

	1-D Assembly/Reflector				2-D Color-set			
Reaction	Unrodded FA		Reflector		Unrodded FA		Rodded FA	
	Σ (cm^{-1})	$\Delta\Sigma/\Sigma$ (%)	Σ (cm^{-1})	$\Delta\Sigma/\Sigma$ (%)	Σ (cm^{-1})	$\Delta\Sigma/\Sigma$ (%)	Σ (cm^{-1})	$\Delta\Sigma/\Sigma$ (%)
Absorption 1	6.3897E-3	0.81	3.7851E-4	1.19	6.6981E-3	0.81	9.3502E-3	0.92
Absorption 2	5.2396E-2	0.21	1.0452E-2	0.49	5.2293E-2	0.21	7.3132E-2	0.19
Nu-fission 1	4.6890E-3	1.19	-	-	4.6966E-3	1.10	4.6134E-3	1.02
Nu-fission 2	6.7195E-2	0.45	-	-	6.6826E-2	0.45	7.4326E-2	0.45
Scattering 1→2	1.2955E-2	1.11	4.4891E-2	1.37	1.3982E-2	1.17	1.1814E-2	1.39
Scattering 2→1	7.8688E-4	0.34	2.6621E-4	0.23	9.6142E-4	0.32	1.2740E-3	0.33

6. CONCLUSIONS

The propagation of cross section uncertainties in criticality calculations for the different BWR configurations at HFP proposed in Exercise I-2 of UAM benchmark has been performed using SCALE6.1 code package. Those configurations are unrodded fuel assembly, rodded fuel assembly, 1-D assembly/reflector and 2-D color set.

First, the uncertainties in k-effective have been calculated, obtaining very similar uncertainty values, lower than 0.6%, for all test problems. The most important contributors are the same in the four cases: $^{238}U(n,\gamma)$, ^{235}U-ν and ^{238}U (n,n'). Additionally, the sensitivity profiles have been compared and although some differences are found, they do not lead to important differences in the k-effective uncertainty.

Second, the uncertainties in some few-group homogenized cross sections have been computed. Very similar uncertainties for the assembly-homogenized cross sections can be found, independently on the assembly environment. That means that the assembly environment does not play a major role in the evaluation of few-group homogenized cross sections uncertainties. Consequently, the standard model for fuel assembly cross-section generation in LWR analysis (single assembly calculations with reflective boundary conditions) can be used to compute few-group cross-sections libraries and their uncertainties, which are to be propagated to core calculations in Exercise I-3 of UAM.

Further calculations are in progress to assess the uncertainties in discontinuity factors and other parameters for core simulators. Also, in order to address the uncertainties in the depletion calculation, extension to Exercise II-2a of UAM will be performed.

ACKNOWLEDGMENTS

This work is partially funded by the Spanish Nuclear Safety Council (CSN), within the agreement with the Universidad Politécnica de Madrid in the area of Propagation of Uncertainties for Neutronic Calculations (P110530207).

REFERENCES

[1] K. Ivanova, M. Avramova, S. Kamerow et al., *Benchmark For Uncertainty Analysis in Modeling (UAM) For Design, Operation and Safety Analysis of LWRs*, NEA/NSC/DOC (2012)

[2] Oak Ridge National Laboratory, "SCALE: a comprehensive modeling and simulation suite for nuclear safety analysis and design," ORNL/TM-2005/39, version 6.1, Radiation Safety