# Objectives and status of neutronics sub-exercises of the oecd/nea Benchmark for Uncertainty Analysis in Modelling for Design, Operation and Safety Analysis of SFRs[[1]](#footnote-2)

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**Abstract**

The OECD/NEA Benchmark for Uncertainty Analysis in Modelling (UAM) for Design, Operation and Safety Analysis of Sodium-cooled Fast Reactors (SFRs) was launched in 2015 to study reactivity feedback coefficients and their uncertainties for a medium-sized 1,000 MWth metallic core and a large 3,600 MWth oxide core. In addition to investigations of full core models, stand-alone multi-scale neutronics analyses of several sub-exercises on the fuel pin and assembly levels were identified to be relevant for a systematic assessment of the influence of nuclear data in fast reactor simulations. When studying simple models, comparisons between computational results using different methods, models, and applied nuclear data libraries can reveal the major drivers of observed differences and calculated uncertainties. For the fuel pin and assembly levels, calculation of nominal values and corresponding uncertainties of the multiplication factor, reactivity effects, and collapsed cross sections are requested. Up to now, 18 contributions to these sub-exercises have been received from 9 international institutions. The preliminary results for nominal metrics values from calculations that were based on the same nuclear data library show good agreement. A similar conclusion was drawn for the comparison of submitted uncertainties: differences in the applied covariance data dominate the cause of differences between results that were obtained using different methods for the neutron transport calculation and uncertainty quantification. This paper provides an overview of the objective and describes the status of the sub-exercises of the standalone neutronics phase for the UAM SFR benchmark. Preliminary comparisons between results submitted by participants are presented and discussed.

## INTRODUCTION

The Organisation for Economic Co-operation and Development (OECD) / Nuclear Energy Agency (NEA) Benchmark for Uncertainty Analysis in Modelling (UAM) for Design, Operation and Safety Analysis of Sodium-cooled Fast Reactors (SFRs) was launched in 2015 to study reactivity feedback coefficients and their uncertainties for a medium-sized 1,000 MWth metallic core and a large 3,600 MWth oxide core [1]. In addition to investigations at the full core level, stand-alone multi-scale neutronics analyses of several sub-exercises on the fuel pin and assembly levels were identified to be relevant for a systematic assessment of the influence of uncertainties in fast reactor simulations. When studying simple models, comparisons between computational results using different methods, models, and applied nuclear data libraries can reveal the major drivers of observed differences and obtained uncertainties. The original benchmark specifications for each of the two reactor designs [1] were therefore amended by neutronics sub-exercise specifications covering a fuel pin cell, a fuel assembly, and a super cell that is a small lattice of assemblies with a central absorber assembly surrounded by fuel assemblies.

Although input uncertainties can arise from multiple sources—such as manufacturing uncertainties and uncertainties associated with methods and modeling approximations utilized—the focus of these sub-exercises is the analysis of the impact of nuclear data uncertainties. Uncertainty analyses are requested for several output quantities of these models using different methods, models, and nuclear data libraries. For some of the requested quantities, the identification of input parameters that contribute most to the observed output uncertainty, i.e. a sensitivity analysis, is requested.

Up to now, 9 international institutions have contributed 18 sets of sub-exercise results based on a wide range of methods and nuclear data libraries. This paper provides a brief description of the sub-exercise specifications, lists the details of the participating institutions, and presents preliminary comparisons between submitted results.

## BENCHMARK Description

The models defined in the sub-exercises are derived from the medium-sized metallic core (MET1000) and the large oxide core (MOX3600) of the UAM SFR specifications, both of which contain fuel at the end of equilibrium cycle [1]. The sub-exercises follow the lines of Phase I of the OECD/NEA UAM Light Water Reactor (LWR) benchmark [2]. Each exercise is defined for both the metallic and the oxide core types. Figures 1–3 show the MOX3600 models.

### Exercise I-1: Fuel pin cell

Exercise I-1 describes an infinite lattice of two-dimensional hexagonal fuel pin cells composed of fuel cylinders surrounded by cladding and cooled by sodium (Figure 1). As leakage effects are not accounted for through this very simple model, the identification of the sources of differences between calculations are not hidden by the interference of various effects as might occur for a complicated geometry, so in this case, identification is more straightforward. Output quantities of interest are the uncertainties of the eigenvalue keff, several 1-group microscopic cross sections (23Na elastic scattering in the coolant, 56Fe elastic scattering in the structural material, 238U inelastic scattering in fuel, and fission and neutron capture (n,g) of 238U and several plutonium isotopes in fuel), and 1-group homogenized macroscopic fuel and absorption cross section of the fuel region.

### Exercise I-2: Fuel assembly

Exercise I-2 describes an infinite lattice of two-dimensional fuel assemblies that contain 271 fuel pin cells enclosed in a duct composed of structural material (Figure 2). The analysis at the assembly level is especially important because these models are often used to generate lattice physics parameters for full-core simulations. Output quantities of interest are the uncertainties of the eigenvalue keff, the Doppler constant KD, and the sodium void coefficient DrNa. For the Doppler constant, the fuel temperature for the perturbed state is doubled compared to its nominal value, as commonly used for such calculations for SFRs; for the sodium void worth calculation, all sodium is removed from the model to simulate a loss of coolant. Furthermore, the uncertainties of the following homogenized macroscopic 4-group cross sections are requested (see Table 4 for the group structure): total cross section Stot, absorption cross section Sabs, the fission cross section multiplied by the number of neutrons released per fission event nSfis, and the total scattering cross section Ss (i.e., the total scattering from an individual energy group to all other groups).

### Exercise I-3: Supercell

Exercise I-3 describes an infinite lattice of a two-dimensional hexagonal primary control assembly surrounded by fuel assemblies (Figure 3). Such a supercell model is sometimes used to generate the lattice’s physics parameters for non-multiplying assemblies in which fuel assemblies provide a representative neutron flux spectrum. The control assembly includes an outer and an interior duct. The absorber rods are included in the interior duct, and they consist of tubes made of structural materials that contain boron carbide pellets. Output quantities of interest are the uncertainties of the eigenvalue, as well as the control rod worth DrCR in the form of the reactivity difference between the nominal model and a model in which the primary control assembly is removed. Uncertainties of homogenized macroscopic 4-group cross sections are requested similar to that of the fuel assembly level.

|  |  |  |
| --- | --- | --- |
| *FIG. 1. MOX3600 pin cell [1].* | *FIG. 2. MOX3600 assembly [1].* | *FIG. 3. MOX3600 super cell [1].* |

## Calculation methodologies

Nine participating institutions have provided results for at least one of the exercises or one of the reactor designs, and additional participants might contribute in the future. A wide variety of calculation methods were used, as summarized in Table 1. Most of the participants used the ENDF/B-VII.1 cross section library [3]. Other applied libraries were JEFF 3.1 [4], JEFF 3.2 [5], JEFF 3.3 [6], ENDF/B-VII.0 [7] and ENDF/B-VIII.0 [8]. Nuclear data uncertainty and correlation data were mostly from SCALE’s ENDF/B-VII.1-based covariance library [9] and the COMMARA 2.0 library, which is a predecessor of ENDF/B-VII.1 [10]. Other applied covariance libraries were COMAC 1.0, COMAC 2.0 [11], ENDF/B-VII.1 [3], and SCALE’s ENDF/B-VIII.0–based library [8]. Both deterministic and Monte Carlo methods were used for the neutron transport calculations. For uncertainty and sensitivity analyses, participants used a variety of methods based on perturbation theory and random sampling.

TABLE 1. Overview of participating institutions and applied codes and methodologies.[[2]](#footnote-3)

|  |  |  |
| --- | --- | --- |
| Institution | Neutron transport code and method | Uncertainty analysis code and method |
| **CEA** | ERANOS [12], SN BISTRO (S8) | ERANOS [12], sensitivity calculation (exact perturbation) + sandwich formula |
|
|
| **NCSU** | Serpent [13], CE-Monte Carlo | Serpent [13], perturbation theory (sandwich rule) |
| **ANL/ NCSU** | ARC codes through Workbench/PyARC (MC2-3 [14], DIF3D/VARIANT [15]) | PERSENT [16], generalized perturbation theory/ direct perturbation |
| **HZDR** | Serpent [13], Monte Carlo | Serpent [13], perturbation theory (sandwich rule) |
| **NECP** | SARAX [17], UFG-collision probability method + 3D Nodal SN method | UNICORN [18], DNPM + sandwich rule |
| **UNIST** | MCS [19], Monte Carlo | MCS [19], generalized perturbation theory |
| **GRS/ ORNL/ EPFL** | SCALE/NEWT [9], 2D deterministic SN | SCALE/TSUNAMI [20], perturbation theory (sandwich rule) |
| XSUSA [21], random sampling |
| SCALE/Sampler [22], random sampling |
| **GRS** | MCNP [23], CE-Monte Carlo | – |
| SCALE/NEWT [9], 2D deterministic SN | XSUSA-LR [24], random sampling |
| **ORNL** | SCALE/NEWT [9], 2D deterministic SN | SCALE/TSUNAMI [20], perturbation theory (sandwich rule) |
| SCALE/Sampler [22], random sampling |

## Preliminary results

The major differences between participants’ results were caused by the application of different nuclear data libraries. Therefore, the presented results here are distinguished according to the applied cross section library for the nominal values and the applied covariance library for the uncertainty results. The uncertainty results labelled *ENDF/B-VII.1****+*** refer to SCALE’s ENDF/B-VII.1–based covariance library This library is mainly based on ENDF/B-VII.1 data, but it also contains additional data to fill in gaps such as missing fission spectrum uncertainties [9]; furthermore, data for 1H, 235U and 239Pu were taken from a pre-release of ENDF/B-VIII.0. Correspondingly, *ENDF/B-VIII.0****+*** refers to SCALE’s ENDF/B-VIII.0–based covariance library that contains the same additional data as the ENDF/B-VII.1–based library to fill in missing data.

Tables 1–3 provide the average nominal values and average uncertainties (arithmetic mean) determined from all contributed results. In the calculation of the average nominal results, multiple results with the same transport code based on the same library were only considered once. Many contributed results were based on transport codes, uncertainty analysis codes, and libraries of SCALE, so the average results are biased to some extent. Given the page limit, detailed results are only provided for the MOX3600 models (see figures provided in the Appendix).

### Exercise I-1: Fuel pin cell

Table 1 presents the average results for both the MET1000 and the MOX3600 fuel pins. The eigenvalue uncertainties of 1.40 and 1.53% are clearly above the typical LWR eigenvalue uncertainties of ~0.5% [25]. While one of the major contributors of LWR eigenvalue uncertainty is the neutron multiplicity of 235U, the uncertainty of the fast-spectrum SFR system is mostly driven by inelastic scattering of 238U, which shows a large uncertainty in the fast energy range. The differences in the uncertainty of this cross section for the different covariance libraries result in different eigenvalue uncertainties as shown in Figure 5. Since the major driver of the investigated 1-group microscopic cross section uncertainties is in most cases the reaction itself and a major contribution originates from 238U inelastic scattering (for example, the major contributors to the 1-group microscopic 56Fe elastic scattering reaction are 56Fe elastic scattering and 238U inelastic scattering), differences in the uncertainties between the covariance libraries for the particular reaction and 238U inelastic scattering dominate the observed output uncertainty differences. The large uncertainty of the 1-group microscopic cross section of the 241Pu capture reaction is mainly caused by the uncertainty of this reaction itself in the fast energy range. While the COMMARA and ENDF/B-VII.1 results are in good agreement as expected since much of the covariance data between the two libraries is consistent, the COMAC and ENDF/B-VIII.0 results show clear differences. As an example, the 238U inelastic scattering uncertainty is compared between the different covariance libraries in Figure 4.

TABLE 1. Average fuel pin cell results: Nominal values and uncertainties due to nuclear data. Microscopic cross sections are provided in barn, macroscopic cross sections in cm-1.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  |  | MET1000 | | MOX3600 | |
|  | **Output** | **Nominal** | **Uncertainty** | **Nominal** | **Uncertainty** |
| keff | Eigenvalue | 1.36293 | 1.40% | 1.19293 | 1.53% |
| 1-group microscopic cross section | Coolant, Na23 el. | 4.01E+00 | 5.66% | 4.81E+00 | 4.82% |
| Cladding, 56Fe el. | 3.52E+00 | 5.90% | 4.19E+00 | 5.53% |
| Fuel, 238U inel. | 1.05E+00 | 5.70% | 9.28E-01 | 5.76% |
| Fuel, 238U fission | 3.40E-02 | 7.07% | 4.21E-02 | 7.13% |
| Fuel, 239Pu fission | 1.62E+00 | 0.59% | 1.75E+00 | 0.60% |
| Fuel, 240Pu fission | 3.48E-01 | 3.90% | 3.58E-01 | 3.98% |
| Fuel, 241Pu fission | 2.10E+00 | 1.02% | 2.47E+00 | 1.07% |
| Fuel, 242Pu fission | 2.45E-01 | 5.15% | 2.50E-01 | 5.26% |
| Fuel, 238U n,g | 2.08E-01 | 1.81% | 2.78E-01 | 1.70% |
| Fuel, 239Pu n,g | 2.95E-01 | 6.61% | 4.77E-01 | 5.77% |
| Fuel, 240Pu n,g | 3.62E-01 | 4.24% | 4.95E-01 | 3.55% |
| Fuel, 241Pu n,g | 3.22E-01 | 17.89% | 4.39E-01 | 12.56% |
| Fuel, 242Pu n,g | 2.98E-01 | 4.38% | 4.34E-01 | 4.48% |
| 1-group macroscopic cross section | Fuel, fission | 5.31E-03 | 1.47% | 5.22E-03 | 1.47% |
| Fuel, absorption | 1.12E-02 | 0.95% | 1.26E-02 | 0.86% |

Chart

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*FIG. 4. Uncertainty of 238U inelastic scattering compared between different covariance libraries.*

### Exercise I-2: Fuel assembly

Table 2 presents the average results for the MET1000 and MOX3600 fuel assemblies. The same observations were made regarding the eigenvalue uncertainty and the different output uncertainties when using different covariance libraries that were made for the fuel pins. For the macroscopic absorption cross sections, the uncertainty of neutron capture in 238U and in several Pu isotopes plays an increased role; for the macroscopic fission cross sections, naturally the uncertainty of 239Pu provides a major contribution to the output uncertainty, and for the scattering cross sections, elastic scattering in 23Na (coolant), 56Fe (structure), and 238U play an import role. The Doppler constant uncertainty is driven by 238U inelastic scattering and not by 238U neutron capture, as in thermal spectrum systems. The uncertainty of the sodium void coefficient is naturally driven by scattering on 23Na.

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| TABLE 2. Average fuel assembly results: Nominal values and uncertainties due to nuclear data. Reactivity coefficients are provided in pcm, macroscopic cross sections in cm-1.   |  |  |  |  |  |  |  | | --- | --- | --- | --- | --- | --- | --- | |  | | MET1000 | | | MOX3600 | | | Output | **Nominal** | | **Uncertainty** | **Nominal** | | **Uncertainty** | | keff | 1.2825 | | 1.30% | 1.1455 | | 1.39% | | Stot, 1 | 1.73E-01 | | 1.46% | 1.99E-01 | | 1.12% | | Stot, 2 | 2.17E-01 | | 1.97% | 2.68E-01 | | 1.32% | | Stot, 3 | 2.79E-01 | | 2.05% | 3.26E-01 | | 1.57% | | Stot, 4 | 3.98E-01 | | 1.76% | 4.42E-01 | | 1.21% | | Sabs, 1 | 5.83E-03 | | 0.70% | 6.50E-03 | | 0.74% | | Sabs, 2 | 3.14E-03 | | 0.94% | 3.29E-03 | | 0.94% | | Sabs, 3 | 5.40E-03 | | 0.95% | 5.85E-03 | | 0.96% | | Sabs, 4 | 1.24E-02 | | 1.29% | 1.49E-02 | | 1.14% | | nSfis, 1 | 1.50E-02 | | 1.05% | 1.66E-02 | | 1.00% | | nSfis, 2 | 4.82E-03 | | 0.61% | 5.11E-03 | | 0.57% | | nSfis, 3 | 4.70E-03 | | 0.61% | 5.00E-03 | | 0.59% | | nSfis, 4 | 7.75E-03 | | 1.19% | 9.33E-03 | | 1.02% | | Ss, 1 | 1.67E-01 | | 1.59% | 1.94E-01 | | 1.26% | | Ss, 2 | 2.17E-01 | | 1.99% | 2.68E-01 | | 1.33% | | Ss, 3 | 2.80E-01 | | 2.09% | 3.26E-01 | | 1.60% | | Ss, 4 | 3.98E-01 | | 1.62% | 4.37E-01 | | 1.11% | | KD | -339 | | 5.81% | -772 | | 4.94% | | DrNa | 5953 | | 4.44% | 3017 | | 5.00% | | TABLE 3. 4-group structure.   |  |  | | --- | --- | | Group | Upper Energy (eV) | | 1 | 20 MeV | | 2 | 820 keV | | 3 | 110 keV | | 4 | 15 keV | |

### Exercise I-3: Supercell

Table 4 presents the average results for the MET1000 and MOX3600 supercells. Similar observations were made for the fuel assembly. The uncertainty of the control rod worth is driven by 238U inelastic scattering, not as may have been expected by the reactions of the absorber material. Other relevant reactions for this uncertainty are the scattering in 56Fe and 23Na.

TABLE 4. Average supercell results: Nominal values and uncertainties due to nuclear data. Reactivity coefficients are provided in pcm, macroscopic cross sections in cm-1.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | MET1000 | | MOX3600 | |
| Output | **Nominal** | **Uncertainty** | **Nominal** | **Uncertainty** |
| keff | 1.0871 | 1.44% | 1.0768 | 1.47% |
| Stot, 1 | 1.46E-01 | 1.66% | 1.53E-01 | 1.72% |
| Stot, 2 | 2.02E-01 | 1.98% | 2.12E-01 | 1.92% |
| Stot, 3 | 2.70E-01 | 1.85% | 2.85E-01 | 1.83% |
| Stot, 4 | 4.08E-01 | 1.55% | 3.75E-01 | 1.45% |
| Sabs, 1 | 1.54E-03 | 1.10% | 1.89E-03 | 1.05% |
| Sabs, 2 | 4.97E-03 | 0.70% | 5.72E-03 | 0.69% |
| Sabs, 3 | 1.30E-02 | 0.31% | 1.48E-02 | 0.33% |
| Sabs, 4 | 3.45E-02 | 0.36% | 3.70E-02 | 0.36% |
| Ss, 1 | 1.45E-01 | 1.67% | 1.45E-01 | 1.74% |
| Ss, 2 | 1.97E-01 | 2.03% | 1.99E-01 | 1.97% |
| Ss, 3 | 2.57E-01 | 1.94% | 2.56E-01 | 1.93% |
| Ss, 4 | 3.74E-01 | 1.69% | 3.64E-01 | 1.61% |
| DrCR | 12,429 | 2.57% | 4,995 | 2.40% |

## Summary and PRELIMINARY Conclusions

An overview of the objective and the specifications from the sub-exercises for the standalone neutronics phase of the UAM SFR benchmark were provided. The sub-exercises include fuel pin and assembly level exercises to allow for a straightforward identification of the drivers causing the differences between results obtained using different methods, models, and applied nuclear data libraries. The analysis covers nominal values and corresponding uncertainties of the eigenvalue, reactivity coefficients, and collapsed cross sections on the different levels of modelling.

Based on the 18 contributions to these sub-exercises from 9 international institutions, the results were discussed, and preliminary conclusions were drawn. Good agreement was found in the calculated nominal results for calculations based on the same nuclear data library. A similar conclusion was drawn for the comparison of submitted uncertainties: differences in the applied covariance data dominate the cause of differences between results obtained using different methods for the neutron transport calculation and uncertainty quantification. In particular, the uncertainties in 238U inelastic scattering were driving the uncertainties of many of the investigated output quantities. Other relevant reactions were 239Pu fission and the scattering reactions of 56Fe in the structure and 23Na in the coolant, originating in the combination of a significant sensitivity of the output quantities and a significant uncertainty of these reactions.

Particular differences between results were observed when using the COMAC or ENDF/B-VIII.0 covariance library compared to COMMARA and ENDF/B-VII.1 libraries. The uncertainties were in good agreement in many cases, but the ranking of the top contributors to the uncertainties showed significant differences in some cases. A more in-depth study with respect to the approach for the calculation of top contributors, as well as uncertainty comparisons between the library, are needed to improve the understanding of these differences.

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APPENDIX

Besides the eigenvalue keff, the Doppler constant, sodium void worth and control rod worth, results are compared for collapsed 1-group microscopic or macroscopic cross sections. The labels of these cross sections specify material (if not averaged over the geometry), type (microscopic “mic” or macroscopic “mac”), reaction, nuclide (for microscopic cross sections).

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*FIG. 5. MOX3600 pin cell: Uncertainty analysis results.*

A picture containing text, writing implement, stationary, pencil

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*FIG. 6. MOX3600 fuel assembly: Uncertainty analysis results.*

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*FIG. 7. MOX3600 supercell: Uncertainty analysis results.*

Chart

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*FIG. 8. MOX3600 pin cell: Relative difference of individual uncertainty results to corresponding mean value.*

Chart

Description automatically generated

*FIG. 9. MOX3600 fuel assembly: Relative difference of individual uncertainty results to corresponding mean value.*

Chart, waterfall chart

Description automatically generated

*FIG. 10. MOX3600 supercell: Relative difference of individual uncertainty results to corresponding mean value.*

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