Impact of nuclear data uncertainties on neutronics parameters of MYRRHA/XT-ADS

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Abstract

A flexible fast spectrum research reactor MYRRHA able to operate in subcritical (driven by a proton accelerator) and critical modes is being developed in SCK·CEN. In the framework of IP EUROTRANS programme the XT-ADS model has been investigated for MYRRHA. In this study, the sensitivity and uncertainty analysis was performed to comprehend the reliability of the XT-ADS neutronics design. The calculated sensitivity coefficients for neutronics parameters varied significantly between calculation models. The uncertainties deduced from the covariance data strongly depend on the original covariance data. The calculated nuclear data uncertainties could not meet the target accuracy. To improve uncertainties, the integral experiments in adequate conditions are expedient.

Introduction

SCK·CEN, the Belgian Nuclear Research Centre in Mol is designing a Multi-purpose Hybrid Research Reactor for High-tech Applications (MYRRHA) [1]. The Accelerator-Driven System (ADS) concept has been chosen as a basis for this reactor, assuming that it can operate in both sub-critical and critical modes. The design studies for eXperimental demonstration of technical feasibility of Transmutation in an Accelerator-Driven System (XT-ADS) have been conducted in the framework of IP EUROTRANS FP6 project [2].

Recently, the sensitivity and uncertainty (S/U) analysis has been reported aiming to identify target nuclear data accuracies for nuclear systems modelling [3,4], the influence of covariance data on the criticality safety was assessed in [5] and the evaluation of the effect of hypothetical MA-loaded critical experiments on a reduction of the data uncertainty has been performed in [6]. Since uncertainties are calculated by the sensitivity coefficients and covariance data from nuclear data libraries, the reliability of the results in the S/U analysis is based on these two parameters. It has been pointed out [7] that the covariance data contained in JENDL-3.3 [8] may underestimate the uncertainty in the nuclear design of the transmutation systems. It was also mentioned that further discussion on the application of the S/U analysis to the nuclear design is required.

This paper reports the comparison of the sensitivity coefficients calculated for different calculation models and the uncertainties deduced from various covariance data for the discussion on the reliability of XT-ADS neutronics design. Sensitivity analysis is based on the comparison of three-dimensional heterogeneous and two-dimensional RZ calculation models. Three covariance data sets were employed to perform uncertainty analysis. Besides that, the uncertainties were compared with the results calculated by the MCNPX code [9] to discuss the uncertainty reliability.

Methods

XT-ADS

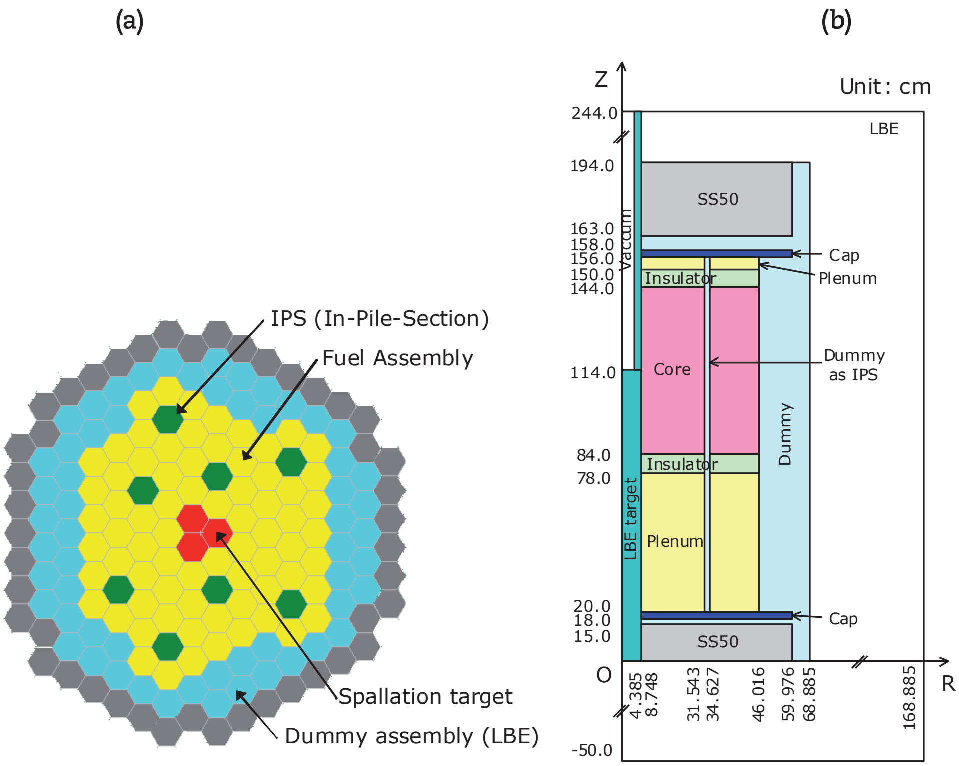
SCK·CEN has been working since 1998 on the design of MYRRHA in order to replace the aging BR2 (Belgian Reactor 2) multi-functional materials testing reactor which operates since 1962. The ADS concept has been chosen as a basis for this reactor, assuming that it can operate in both sub-critical and critical modes. In the framework of PDS-XADS (Preliminary Design Study of an eXperimental ADS) FP5 project, the basic design of installation has been elaborated [1]. The proton accelerator is coupled with multiplying core loaded with MOX fuel cooled by liquid lead-bismuth eutectic (LBE) which serves also as spallation target. The design studies have been continued in the framework of IP EUROTRANS FP6 project. The goal of the project was to develop an advanced design leading to the XT-ADS. The XT-ADS was intended to be a test bench for the main components and irradiation scheme of a full-scale ADS, EFIT (European Facility for an Industrial Transmutation) [10].

Three-dimensional heterogeneous and two-dimensional RZ homogenized models

The XT-ADS is a LBE cooled pool-type 100 MWth subcritical reactor with MOX fuel containing 35 wt.% Pu [11]. The core is driven by the proton accelerator (proton energy 600 MeV, maximum current 2.5 mA). The layout of the XT-ADS core is illustrated in Figure 1, a. Three central assemblies serve as feeders for liquid lead-bismuth spallation target. The core itself contains 72 fuel assemblies and 8 assemblies are used as In-Pile-Section (IPS) dedicated for the irradiation and measurements. There are also dummy assemblies filled with LBE but designed to host control rods and mock-up reflecting stainless steel assemblies on the periphery of the core.

To estimate the difference in the sensitivity coefficients between calculation models, a two-dimensional RZ calculation model for the XT-ADS was also employed. A conceptual diagram of the RZ calculation model is shown in Figure 1, b. Each region was homogenized. SS50 denotes the core support region which was homogenized as fifty-fifty volume ratio of LBE and T91.

Figure 1: a) Three-dimensional heterogeneous calculation model for XT-ADS
b) Two-dimensional RZ homogenized calculation model for XT-ADS



Sensitivity coefficients and uncertainties deduced from covariance data

Generally, the sensitivity coefficient S of a parameter R against parameter Σ is defined as

$$S = \frac{dR}{R} \Big/ \frac{d\Sigma}{\Sigma} \tag{1}$$

Effective neutron multiplication factor k_{eff} plays role of R and microscopic cross-section data for each particular neutron induced reaction are supposed as Σ. Applying the perturbation theory to the Boltzmann transport equation, one can obtain [12]

$$S = \frac{\partial k}{k} \Big/ \frac{\partial \Sigma(r)}{\Sigma(r)} = -k\Sigma(r) \frac{\left\langle \phi^+(\xi) \left(\frac{\partial A[\Sigma(\xi)]}{\partial \Sigma(r)} - \frac{1}{k} \frac{\partial B[\Sigma(\xi)]}{\partial \Sigma(r)} \right) \phi(\xi) \right\rangle}{\langle \phi^+(\xi) B[\Sigma(\xi)] \phi(\xi) \rangle} \tag{2}$$

Here ξ is the phase space vector, ϕ^+ is adjoint neutron flux, *A* is an operator of the left-hand side of the transport equation except fission term and *B* is an operator for the fission term of transport equation.

The variance for the k_{eff} is determined as [7,12]

$$\sigma^2_{k^{i,j}_{x,y}} = G_{\alpha^i_x} M_{\alpha^i_x \alpha^j_y} G^t_{\alpha^j_y}, \tag{3}$$

where $k^{i,j}_{x,y}$ is 2D-dependence of k_{eff} from *x, y* (reaction type) and *i,j* (nuclide type); $G_{\alpha^i_x}$ and $G^t_{\alpha^j_y}$ are group-wise sensitivity vectors (the latter is transposed one) of length *G* (*G* is the number of energy groups), α is the parameter (cross-section) with respect to which the k_{eff} sensitivity is calculated; $M_{\alpha^i_x \alpha^j_y}$ is $G \times G$ size covariance matrix.

Calculation tool

The SCALE-6 (Standardized Computer Analyses for Licensing Evaluation) [13] code was employed for the S/U analysis. It consists of many calculation modules and utilities for calculations of reactor physics, criticality safety and radiation shielding. For the S/U analysis, the TSUNAMI-3D module was employed. This module performs the calculation of the sensitivity coefficients for the effective neutron multiplication factor by using the forward and adjoint fluxes data. After the sensitivity analysis, this module calculates the uncertainty deduced from the covariance data contained in the nuclear data library. For the neutron transport calculation, the KENO-VI multigroup Monte Carlo transport module was used with a detailed three-dimensional calculation model. In this calculation, the 238 group nuclear data library based on ENDF/B-VII.0 data [14] was employed. For the uncertainty analysis, 44 energy groups, which is a default structure in the TSUNAMI-3D module, was used.

Results

Sensitivity coefficients

The sensitivity analysis with respect to models was performed to reflect the differences in their nature. The RZ calculation model was prepared aiming to match basic integral neutronics parameters calculated with full 3D model taking into account that clear differences will exist between these calculation models. The k_{eff} values calculated for both models reveal ~2000 pcm difference: for 3D heterogeneous model KENO-VI returns k_{eff} = 0.98305±0.00031 while RZ model gives k_{eff} = 0.96234±0.00032. The neutron spectrum in 3D model is harder than in RZ homogenized model [11] thus k_{eff} is higher.

Table 1 and Table 2 show the sensitivity coefficients calculated by the SCALE code with the 3D heterogeneous and RZ homogenized calculation models, respectively. Uranium and Plutonium isotopes, isotopes of LBE (Pb and Bi-209), as well as Fe-56 and O-16 were treated as main objects in the S/U analysis since their sensitivity coefficients dominate among the sensitivity coefficients for the keff of the XT-ADS core. The tables indicate that the total sensitivity of the neutron capture reaction in the RZ model is smaller than that in the 3D heterogeneous model, and coefficients for U-238 and Pu-239 are low enough. On the other hand, the sensitivity coefficients of the neutron induced fission reaction and average neutron release per fission event $\overline{\nu}$ in the 3D heterogeneous calculation model are higher than corresponding coefficients in the RZ model, especially for U-238 and Pu-240. This is also caused by the difference in the neutron spectra.

Table 1: Sensitivity coefficients calculated by SCALE-6 for 3D model

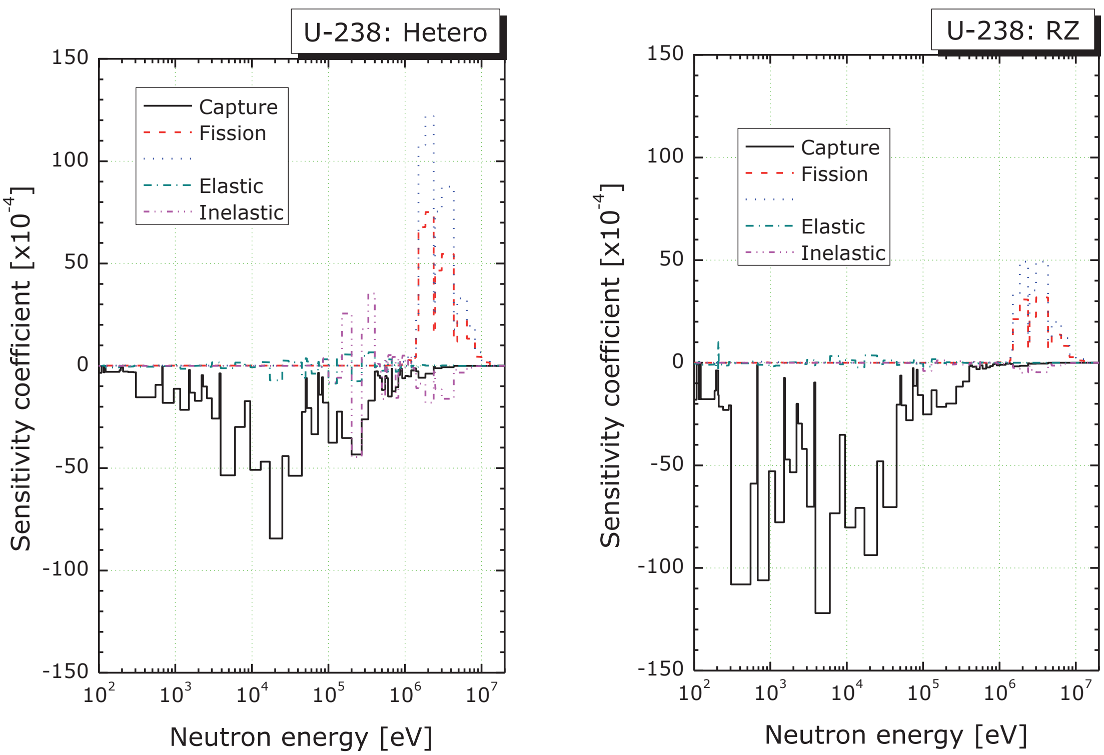
Nuclide	Capture	Fission	$\overline{\nu}$	Elastic	Inelastic	(n,2n)	Total
O-16	-1.23E-03			1.66E-02	-1.31E-04	-2.37E-10	1.53E-02
Fe-56	-1.97E-02			-6.71E-03	-4.92E-03	3.39E-06	-3.13E-02
Pb-204	-2.23E-03			5.17E-04	-9.79E-05	1.63E-06	-1.81E-03
Pb-206	-3.82E-03			3.05E-03	-1.57E-03	3.92E-05	-2.31E-03
Pb-207	-2.82E-03			2.14E-03	-1.32E-03	8.35E-05	-1.92E-03
Pb-208	-5.39E-04			4.53E-03	-8.81E-04	1.19E-04	3.23E-03
Bi-209	-8.82E-03			1.50E-02	-4.08E-03	3.17E-04	2.42E-03
U-235	-1.67E-03	8.60E-03	1.43E-02	1.28E-06	-3.43E-05	2.82E-06	2.12E-02
U-238	-1.02E-01	3.46E-02	5.53E-02	7.01E-05	-7.41E-03	4.79E-04	-1.90E-02
Pu-238	-3.70E-03	1.35E-02	1.99E-02	3.98E-06	-3.59E-05	1.60E-06	2.97E-02
Pu-239	-5.98E-02	4.71E-01	7.06E-01	-4.66E-04	-7.66E-04	3.48E-05	1.12E+00
Pu-240	-2.71E-02	5.68E-02	8.38E-02	1.11E-03	-5.74E-04	1.01E-05	1.14E-01
Pu-241	-6.06E-03	6.89E-02	1.04E-01	-3.86E-06	-7.96E-05	2.33E-05	1.67E-01
Pu-242	-6.79E-03	1.17E-02	1.72E-02	1.02E-04	-1.96E-04	7.90E-06	2.20E-02
Total	-2.46E-01	6.65E-01	1.00E+00	3.59E-02	-2.21E-02	1.12E-03	1.43E+00

Table 2: Sensitivity coefficients calculated by SCALE-6 for RZ model

Nuclide	Capture	Fission	$\overline{\nu}$	Elastic	Inelastic	(n,2n)	Total
O-16	-7.06E-04			3.34E-03	-7.42E-05	-3.44E-11	2.56E-03
Fe-56	-2.25E-02			4.01E-03	-1.74E-03	3.74E-06	-2.02E-02
Pb-204	-1.66E-03			2.24E-04	-4.10E-05	1.47E-06	-1.48E-03
Pb-206	-2.20E-03			8.45E-04	-6.25E-04	3.45E-05	-1.95E-03
Pb-207	-2.27E-03			6.41E-04	-3.87E-04	6.88E-05	-1.95E-03
Pb-208	-1.91E-04			1.06E-03	-5.65E-04	1.10E-04	4.14E-04
Bi-209	-6.66E-03			5.15E-03	-2.08E-03	2.67E-04	-3.32E-03
U-235	-2.99E-03	1.14E-02	1.91E-02	-1.60E-06	-1.65E-05	1.77E-06	2.75E-02
U-238	-1.73E-01	1.55E-02	2.41E-02	3.23E-04	-2.70E-03	3.20E-04	-1.35E-01
Pu-238	-6.70E-03	1.07E-02	1.58E-02	-4.80E-06	-1.40E-05	1.05E-06	1.98E-02
Pu-239	-1.34E-01	5.00E-01	7.62E-01	-8.46E-04	-2.96E-04	2.19E-05	1.13E+00
Pu-240	-5.27E-02	2.36E-02	3.46E-02	2.21E-03	-2.23E-04	6.66E-06	7.49E-03
Pu-241	-1.10E-02	9.18E-02	1.38E-01	-2.58E-05	-6.85E-05	1.42E-05	2.29E-01
Pu-242	-1.23E-02	3.91E-03	5.66E-03	1.80E-04	-8.35E-05	5.08E-06	-2.63E-03
Total	-4.29E-01	6.57E-01	1.00E+00	1.72E-02	-8.91E-03	8.30E-04	1.24E+00

The sensitivity coefficients of U-238 in the 3D heterogeneous and RZ homogeneous calculation models are shown in Figure 2 for the sake of comparison. The sensitivity due to neutron capture reaction dominates in the RZ model. However, in the 3D heterogeneous model, the contribution of the neutron capture reaction decreases and the sensitivities of the fission and $\overline{\nu}$ in the upper energy region (above 1 MeV) increases. The sensitivity of the inelastic scattering reaction also increased in the 3D heterogeneous calculation model. This is due to the spectrum is harder than in the RZ model.

Figure 2: Sensitivity coefficients for U-238



Uncertainty analysis

The uncertainty analysis was performed using the sensitivity coefficients shown in Table 1 and Table 2. Three calculation cases were prepared. The first case employed the SCALE 44-group covariance data and the sensitivity coefficients calculated in the 3D heterogeneous calculation model. The SCALE 44-group covariance data are constructed on the basis of covariance data from various libraries, including ENDF/B-VII, ENDF/B-VI, JENDL-3.3 and approximate uncertainties [13]. The second case dealt with the covariance data from TENDL-2009 library [15]. In the third case the SCALE 44-group covariance data and the sensitivity coefficients calculated in the RZ calculation model were used.

SCALE 44-group covariance data contain all data for all nuclides and reactions of interest listed in Table 1 and Table 2, while TENDl-2009 lacks χ (fission spectrum covariance) and $\overline{\nu}$. Enhancement of correlation between other reactions such as Capture-Fission is the feature of TENDL-2009 covariance data.

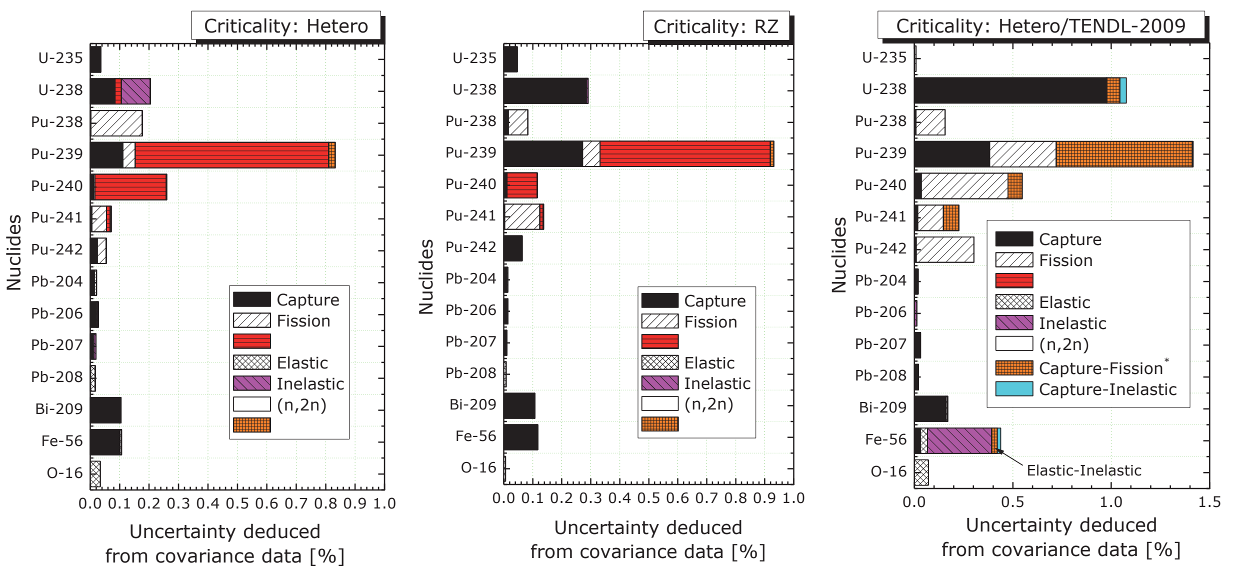
Table 3 shows the uncertainties deduced from covariance data with 1σ confidence. The uncertainty in the 3D heterogeneous model is slightly smaller than uncertainty in the RZ model. The main reason of this difference could be attributed to a decrease of the sensitivity coefficients for the neutron capture reaction in the 3D heterogeneous model. On the other hand, the SCALE-6 / TENDL-2009 result is about twice larger than other uncertainties. Thus the uncertainty for the same calculation model and tool strongly depends on covariance data used.

Table 3: Uncertainty deduced from covariance data

Model	Covariance data	Uncertainty (%)
3D heterogeneous	SCALE-6 44-group	0.94
3D heterogeneous	TENDL-2009	1.9
RZ homogeneous	SCALE-6 44 group	1.0

The contributions of each nuclide and reaction to the uncertainty are plotted on Figure 3. The contribution of neutron capture reaction in the 3D heterogeneous model is smaller than in case of the RZ model, especially for fuel nuclides (U and Pu). On the other hand, due to hardness of the spectrum, the contributions of neutron induced fission and $\overline{\nu}$ increases in 3D model, especially for Pu-238, Pu-240 and Pu-242. It is seen from the Figure 3 that the effect of inelastic scattering for U-238 is large in 3D model.

Figure 3: Uncertainties deduced from covariance data



Significant differences are observed when comparing SCALE-6 44-group and TENDL-2009 covariance data. For example, the neutron capture reaction dominates for U-238 with the covariance data from TENDL-2009, while the contribution of capture reaction in the SCALE-6 44-group case is not so large. There are substantial differences for Pu isotopes and Fe-56. The contribution of correlations between other reactions is not negligible as it could be seen from TENDL-2009 case.

Comparison with MCNPX results

The MCNPX calculation of k_{eff} was performed for detailed 3D heterogeneous model. Although the discussion on uncertainty should normally be related to experimental data, there are no integral experimental data for a LBE-cooled core with MOX fuel. Thus MCNPX calculation results play role of experimental data in this case.

The results of SCALE-6 and MCNPX calculations with 3D model are shown in Table 4. Three nuclear data libraries were used with MCNPX to estimate the influence of data library choice.

Table 4: Comparison of keff calculated by SCALE-6 and MCNPX

Code	Library	k_{eff}
SCALE-6	ENDF/B-VII.0	0.98305±0.00031
MCNPX	JEFF-3.1.1	0.98297±0.00027
MCNPX	JENDL-3.3	0.97578±0.00026
MCNPX	ENDF/B-VII.0	0.98046±0.00026

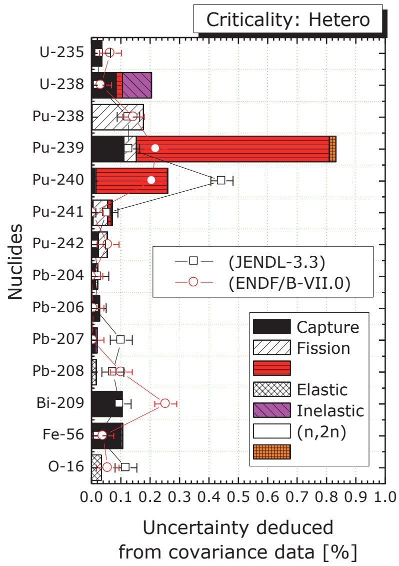
The use of JENDL-3.3 and ENDF/B-VII.0 with MCNPX results in 0.73% and 0.26% lower k_{eff} value than JEFF-3.1.1, accordingly. It is however less than uncertainty margins shown in Table 3. This means that uncertainty deduced from covariance data covers the differences in k_{eff} due to data library variation in MCNPX calculation.

To investigate the "weight" of each nuclide in keff calculated with MCNPX, the variation of data library was employed for each particular nuclide. JEFF-3.1.1 library always served as reference. The black open rectangles on Figure 4 correspond to the use of JENDL-3.3 for each particular nuclide while JEFF-3.1.1 was used for other nuclides shown on the plot. The red open circles denote the use of ENDF/B-VII.0. Uncertainties deduced from covariance data from Figure 3 (obtained with SCALE-6 44-group calculation, left-hand plot) are shown for the sake of comparison. It is seen from Figure 4 that uncertainties deduced from covariance data do not cover the difference caused by data library variation in MCNPX calculation for U-235, Pu-240, Pb-207, Pb-208, Bi-209 and O-16. This may indicate that covariance data are underestimated.

As it is seen in Figure 3, the uncertainties deduced from the covariance data varied significantly with the change of covariance data. Although the uncertainties deduced from the covariance data ensured the differences in the MCNPX calculation, the contribution of each nuclide and reaction was different in each covariance data set. These results indicate that the covariance data of the nuclear data libraries is an open issue to discuss the reliability of the neutronics design.

The target accuracy for the fast reactor nuclear design is discussed in [16] where 0.3%Δk (1σ confidence) was proposed as limiting value for k_{eff} uncertainty. The uncertainties deduced from the covariance data for XT-ADS do not meet this criterion. The uncertainties will obviously be reduced by performing the integral experiments in LBE or Pb moderated environment with MOX or Uranium fuel. The reduction of uncertainties of U-238 neutron capture and inelastic scattering, Pu-238 fission, Pu-239 neutron capture and $\overline{\nu}$, Pu-240 $\overline{\nu}$, Bi-209 and Fe-56 neutron capture is required.

Figure 4: Uncertainties deduced from covariance data by SCALE-6 44-group and difference in MCNPX calculation by data library variation



Conclusions

The sensitivity and uncertainty analysis was performed to confirm the reliability of the calculated effective neutron multiplication factor for the XT-ADS neutronics model.

The obtained sensitivity coefficients differ substantially between the 3D heterogeneous and RZ homogenized calculation models. The uncertainties deduced from the covariance data strongly depend on the covariance data variation. The covariance data of the nuclear data libraries is an open issue to discuss the reliability of the neutronics design. The uncertainties deduced from the covariance data for XT-ADS are 0.94% and1.9% by the SCALE-6 44-group and TENDL-2009 covariance data, accordingly. The uncertainties exceed the 0.3%Δk (confidence level 1σ) target accuracy level. To achieve this target accuracy, the uncertainties should be improved by experiments under adequate conditions such as LBE or Pb moderated environment with MOX or Uranium fuel.

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