TECHNICAL MATERIAL

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# Nuclear data-induced uncertainty quantification of neutronics parameters of accelerater-driven system

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Nuclear data-induced uncertainties for one accelerator-driven system concept designed by the Japan Atomic Energy Agency is quantified. The variance-covariance data provided in the JENDL-4.0 library are used. Uncertainties are quantified for several neutronics parameters such as effective neutron multiplication factor, subcritical neutron multiplication rate, a family of delayed neutron fractions, power peaking and coolant void reactivity, and for several operational states. Inter-cycle and inter-parameter correlation matrices and detailed information such as nuclide-wise and nuclear data-wise uncertainties are also provided.

***Keywords: uncertainty quantification; JENDL-4.0; accelerator-driven system***

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## 1. Introduction

An accelerator-driven system (ADS), or an accelerator-driven sub-critical reactor, is one of future nuclear systems, and is expected to have a role to efficiently and safely burn (or vanish) long-lived minor actinoid (MA) nuclides which are considered to possess a potential risk when they are deposited to deep underground. In order to realize ADS, research and development activities in wide engineering areas have been or are being conducted in the past and now.

Accuracy and reliability of nuclear data, which significantly affect evaluations of neutronics performances and MA burning capability of ADS, are one of major concerns in the ADS development since nuclear fuel loaded to ADS, which is composed of MA nuclides mainly, is quite different from that loaded to conventional nuclear systems. Furthermore, candidate of coolant material of ADS, that is a lead-bismuth eutectic, is also different from the conventional one such as water and sodium. Since measurement data for nuclear data of the MA nuclides and the coolant materials specific for ADS are scarce, uncertainties of the nuclear data of these nuclides are expected much larger than other nuclides which have been considered important historically in the nuclear engineering field.

Nuclear data-induced uncertainty quantification for ADS neutronics parameters is quite important and is beneficial to specify the nuclear data which are dominant in the total uncertainty and should be improved in future through new measurements or advanced nuclear physics modeling developments for nuclear data evaluation. An extensive work on the nuclear data-induced uncertainty quantification for ADS has been carried out by Aliberti et al. in 2004[1]. In their work, nuclear data-induced uncertainties have been quantified for various kinds of neutronics parameters such as effective neutron multiplication factor, coolant void reactivity, effective delayed neutron fraction, reactivity loss during irradiation, decay heat, transmutation potential of MA nuclides and peak power. Although their pioneering work has played a significant role in the ADS development, they have used "low-fidelity" variance-covariance data for nuclear data of the MA nuclides and the coolant materials of ADS because at that time variance-covariance data of these nuclides were scarce in all major nuclear data files.

Recently this situation has been drastically changed and the latest versions of evaluated nuclear data files such as JENDL-4.0[2] contain variance-covariance data for these nuclides. In this technical material, we will quantify nuclear data-induced uncertainty of several neutronics parameters of ADS using the high-fidelity variance-covariance data of nuclear data taken from JENDL-4.0. In the recent design study of ADS, plutonium isotopes are initially loaded to ADS to suppress positive reactivity swing during operation[3]. Thus fuel compositions are significantly dependent on the operation cycle. We will do uncertainty quantification calculations at several operational states of ADS.

Since nuclear data-induced uncertainty quantifications of ADS neutronics parameters with the JENDL-4.0 covariance data have been already conducted by the other research group[4], those presented here are never novel and new. Extensive works for various kinds of neutronics parameters at various operational states conducted in the present work, however, are notable and the authors believe that these information are beneficial for the further advancement of nuclear data relevant to the ADS development.

## 2. Uncertainty Analysis

Since the present uncertainty quantification calculations are based on the well-established numerical procedures, such as adjoint-based uncertainty propagation calculations, deterministic neutron transport (diffusion) calculations, efficient sensitivity calculations with the (generalized) perturbation theory, etc, detailed explanations on each of them are omitted in this technical material.

### 2.1. *Calculation method*

Uncertainty quantification calculations are conducted with the so-called adjoint procedure, which uses sensitivity profiles of target neutronics parameters with respect to nuclear data and variance-covariance information on the nuclear data[5].

The target neutronics parameters in the present work are effective neutron multiplication factor $k_{\mathrm{eff}}$, subcritical neutron multiplication rate $k_{\mathrm{sub}}$, several definitions of delayed neutron fraction, power peaking factors and coolant void reactivity.

The subcritical multiplication factor $k_{\mathrm{sub}}$ is defined as

$$k_{\mathrm{sub}} = \frac{S}{Q+S}, \tag{1}$$

where $Q$ and $S$ are the total external neutron sources and the total fission neutron sources, respectively. This parameter was initially defined by Kobayashi[6] and it can be interpreted as a generation-averaged neutron multiplication rate because the total neutron sources $(Q+S)$ can be written as[7]

$$Q + S = Q + \frac{k_{\mathrm{sub}}}{1-k_{\mathrm{sub}}}Q = Q + Qk_{\mathrm{sub}} + Qk_{\mathrm{sub}}^2 + \cdots . \tag{2}$$

Regarding the delayed neutron fraction, the effective delayed neutron fraction $\beta_{\mathrm{eff}}$ has been usually used in critical reactor core calculations. That is defined as

$$\beta_{\mathrm{eff}} = \frac{\langle \phi^\dagger, F_d\phi \rangle}{\langle \phi^\dagger, F\phi \rangle}, \tag{3}$$

where $\phi^\dagger$ is fundamental mode of the eigenfunctions of the adjoint neutron diffusion equation. On the other hand, Kobayashi has insisted that a different definition for delayed neutron fraction should be used when subcritical systems are considered.[8] Since the proper definition of delayed neutron fraction in ADS is under discussion presently, the following three different definitions are considered in the present work. The first one is defined as

$$\beta_{\mathrm{source}} = \frac{\langle F_d\psi \rangle}{\langle F\psi \rangle}, \tag{4}$$

where $F$ and $F_d$ denote the neutron generation operator and the delayed neutron generation operator, $\psi$ is neutron flux in the subcritical state with external neutron sources, and the brackets denote the integration over the whole phase space. The second one is defined as

$$\beta_{\text{eigen}} = \frac{\langle F_d \phi \rangle}{\langle F \phi \rangle}, \tag{5}$$

where $\phi$ is fundamental mode of the eigenfunctions of the neutron diffusion equation. These delayed neutron fractions, $\beta_{\text{source}}$ and $\beta_{\text{eigen}}$, are referred to as the *physical* delayed neutron fractions in this technical material. The third one is $\beta_{\text{eff}}$.

The power peaking factor is defined as a ratio of power density at a spatial numerical mesh located at the core center to the averaged power density.

The coolant void reactivity $\rho_{\text{void}}$ is defined as

$$\rho_{\text{void}} = \frac{1}{k_{\text{eff,ref}}} - \frac{1}{k_{\text{eff,void}}}, \tag{6}$$

where $k_{\text{eff,ref}}$ and $k_{\text{eff,void}}$ are the effective neutron multiplication factors of the reactor core at the reference state and the coolant-voided state where all the coolant materials in fuel regions are removed from a system.

For the uncertainty propagation calculations, sensitivity profiles of these neutronics parameters with respect to nuclear data are required. Those for $k_{\text{eff}}$, $k_{\text{eff,ref}}$ and $k_{\text{eff,void}}$ are calculated by the perturbation theory, and those for $\rho_{\text{void}}$ are obtained from two sensitivities of $k_{\text{eff,ref}}$ and $k_{\text{eff,void}}$. Those for $k_{\text{sub}}$, $\beta_{\text{source}}$, $\beta_{\text{eigen}}$ and the power peaking factor are calculated by the generalized perturbation theory[9]. Finally those for $\beta_{\text{eff}}$ are calculated by using a procedure based on the so-called k-ratio method[10]. Nuclear data uncertainties also propagate to nuclide number densities during reactor operation, this kind of uncertainties are not considered in the present work.

## 2.2. Calculation tools and basic data library

All the numerical calculations except spallation neutron source calculations are performed with a deterministic reactor physics code system CBZ[11], which is being developed at Hokkaido university. Space and energy dependent spallation neutron source is evaluated by Nishihara[12]. Region-wise 70-group effective cross sections are obtained from a JENDL-4.0-based 70-group library and these are supplied to following core calculations. A three-dimensional reactor core is simplified to a two-dimensional cylinder, and fixed-source and eigenvalue neutron diffusion equations of this two-dimensional system are numerically solved by a diffusion solver implemented in CBZ. Whereas a transport solver is also available in CBZ, a diffusion solver is employed in the present work. This is because transport calculations are much more time consuming than diffusion calculations and difference in quantified uncertainties between diffusion calculation and transport calculation is expected insignificant. Depletions of heavy nuclides are taken into account by a detailed burnup chain shown in **Figure 1**.

[Figure 1 about here.]

Note that some MA nuclides such as Cm-247, -248, -249 and Bk-249, which are ignored in conventional burnup chains, are considered. Fission product nuclides are lumped to one fictitious nuclide for each fissile nuclide for simplifications.

The covariance data of JENDL-4.0 are processed by the NJOY-99 code[13] and 70-group covariance data are generated. The covariance data of the following nuclides are considered in the present work: N-15, Cr-52, Fe-56, Ni-58, Pb-204, -206, -207, -208, Bi-209, U-234, -235, Np-237, Pu-238, -239 ,-240, -241, -242, Am-241, -242m, -243, Cm-242, -243, -244, -245, -246, -247, -248, -249 and Bk-249. All the reactions to which the covariance data are given are taken into account.

# 3. Dedicated System for Uncertainty Quantification

## *3.1. System description*

We perform uncertainty quantification calculations for a benchmark problem based on a commercial grade ADS proposed by the Japan Atomic Energy Agency (JAEA)[14]. This benchmark system has a cylindrical geometry as shown in **Figure 2**.

[Figure 2 about here.]

This system uses a lead-bismuth eutectic (LBE) coolant, and is radially divided into two core fuel zones with different initial plutonium loading to flatten a radial power distribution. For the core fuel, mixture of mono-nitride of MA and plutonium with the inert matrix zirconium-nitride is used. A proton beam with 1.5 GeV provided by the LINAC is injected into the core through the beam duct along the core central axis. Flat beam profile with 40 cm in diameter is assumed in this benchmark problem. Although it is considered that spatial distribution and strength of the beam are also uncertain, such uncertainties are not taken into consideration in the present work.

The core thermal power is 800 MW and burnup period is 600 effective full power days. After each burnup cycle, all fuels are removed from the core and reloaded for next burnup cycle after cooling and reprocessing. The time period for the cooling and the reprocessing consists of 3-month unloading, 1.5-year cooling, 6-month refabrication and 3-month reloading. In the refabrication process, the fission products are removed and only MA of equal mass to the burnup fuel is added to the recycled fuel. Plutonium is used as mixture of MA only at the first cycle and is not additionally loaded to the following cycles.

The JENDL-4.0-based library is used in the present work whereas JENDL-3.3 is used in the reference, hence fuel composition is slightly adjusted from that given in the reference. Weight ratio of zirconium-nitride is 48.75 wt%, and the plutonium weight ratios in fuel are 26.9 wt% and 50.0 wt% for inner and outer cores, respectively.

The detailed information on this benchmark problem can be found in the reference[14].

### *3.2. Numerical results of cycle-dependent neutronics parameters*

In this sub-section, numerical results of neutronics parameters which are dependent on operation cycles are provided. Results of $k_{\text{eff}}$ and $k_{\text{sub}}$ are shown in **Figure 3**, those of $\beta_{\text{source}}$, $\beta_{\text{eigen}}$ and $\beta_{\text{eff}}$ are in **Figure 5**, those of power peaking are in **Figure 6**, and those of coolant void reactivity are in **Figure 7**. Since different fuel material loading in the core region is adopted only in the first cycle, neutronics parameters in the first cycle are relatively different from those in the following cycles. After 10-cycle operation, cycle dependence of neutronics parameters becomes almost negligible both at BOC and at EOC.

[Figure 3 about here.]

[Figure 4 about here.]

[Figure 5 about here.]

[Figure 6 about here.]

[Figure 7 about here.]

## 4. Results of Uncertainty Analysis

Since the purpose of the present work is to provide the extensive information on neutronics parameter uncertainties of ADS, detailed interpretations of the quantified uncertainties are omitted.

### *4.1. Cycle-dependent uncertainties*

Neutronics parameters uncertainties are calculated at the beginning of cycle (BOC) and the end of cycle (EOC). Results of $k_{\text{eff}}$ and $k_{\text{sub}}$ are shown in **Figure 8**, those of $\beta_{\text{source}}$, $\beta_{\text{eigen}}$ and $\beta_{\text{eff}}$ are in **Figure 9**, those of power peaking and coolant void reactivity are in **Figure 10**. The uncertainties of $k_{\mathrm{eff}}$ and coolant void reactivity at the first cycle are consistent with the previous study[4] even though the fuel composition of the present work is slightly different from the previous one. After ten-cycle operation, cycle dependence of neutronics parameters uncertainties becomes negligible in all the parameters. It is interesting to point out that the uncertainties in the first cycle are generally smaller than those in the following cycle.

[Figure 8 about here.]

[Figure 9 about here.]

[Figure 10 about here.]

### *4.2. Inter-parameter and inter-cycle correlation matrices*

Inter-parameter correlation matrices are calculated for cycle 1 to cycle 4. Results at BOC are shown in **Figure 11**. Since results at EOC are quite similar, those are omitted here. A strong positive correlation is observed between $k_{\mathrm{eff}}$ and $k_{\mathrm{sub}}$. Strong positive correlations are observed also among a different definition of delayed neutron fractions. A strong negative correlation between power peaking and $k_{\mathrm{eff}}$ (or $k_{\mathrm{sub}}$) is also notable.

[Figure 11 about here.]

Inter-cycle correlation matrices are calculated for six parameters. Results are shown in **Figure 12**. Because of the initially loaded plutonium, correlations between the first or second cycle and the following cycles are relatively weak.

[Figure 12 about here.]

### *4.3. Nuclide-wise and nuclear data-wise uncertainties*

Nuclide-wise uncertainties are calculated at several operational states. Results for $k_{\mathrm{eff}}$ are shown in **Figure 13**, those for $k_{\mathrm{sub}}$ are in **Figure 14**, those for $\beta_{\mathrm{source}}$ are in **Figure 15**, those for $\beta_{\mathrm{eff}}$ are in **Figure 16**, those for power peaking are in **Figure 17** and those for coolant void reactivity are in **Figure 18**. Generally uncertainties induced by plutonium-239, -241 and americium-241 decrease and those induced by plutonium-238, curium-244, -245 and uranium-234 increase as the operation cycle proceeds. At the third cycle and the following cycles, plutonium-238 is the most dominant contributor to the total uncertainty except the coolant void reactivity.

[Figure 13 about here.]

[Figure 14 about here.]

[Figure 15 about here.]

[Figure 16 about here.]

[Figure 17 about here.]

[Figure 18 about here.]

Finally nuclear data-wise uncertainties are calculated. Results for $k_{\rm eff}$ are shown in **Figure 19**, those for $\beta_{\rm eff}$ are in **Figure 20** and those for coolant void reactivity are in **Figure 21**. Note that uncertainty components from correlations among different reactions are ignored, and that sum of reaction-wise uncertainties (standard deviation) does not correspond to the total uncertainty (standard deviation) for each nuclide.

[Figure 19 about here.]

[Figure 20 about here.]

[Figure 21 about here.]

## 5. Conclusion and Future Perspective

We have quantified nuclear data-induced uncertainties for one ADS concept designed by JAEA. The variance-covariance data provided in the JENDL-4.0 library have been used. The uncertainty quantification has been done for several neutronics parameters such as $k_{\rm eff}$, $k_{\rm sub}$, a family of delayed neutron fractions, power peaking and coolant void reactivity, and for several operational states. Inter-cycle and inter-parameter correlation matrices and detailed information such as nuclide-wise and nuclear data-wise uncertainties have been also provided.

Future perspective on our nuclear data-related researches for ADS is as follows.

We should quantify the required prediction accuracy of the neutronics parameters of ADS from the viewpoint of core design. Then, we will identify nuclear data for which the further improvement can efficiently contribute to the uncertainty reduction of the ADS parameters. Now we are considering to utilize an index of the variance reduction factor[15], which has been proposed by one of the present authors. With the variance reduction factor, we can easily understand further improvement on which reaction and which neutron energy range are required.

Integral experiment data such as the criticality data or the MA sample reactivity worth are also beneficial to reduce the uncertainty. Nuclear data adjustment with such integral data will be carried out, and the prediction accuracy based on all the information presently available will be quantified. If the required accuracy cannot be satisfied even with this, efficient measurements for differential nuclear data or integral properties would be proposed.

The present work has not quantified uncertainties of the burnup-related parameters. These parameters are important to grasp the system capability of MA burning. Uncertainty quantification for the burnup-related parameters is also future subject.

## Acknowledgement

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**Figure Captions**

**Figure 1** Burnup chain for heavy nuclides

**Figure 2** Reactor core specification

**Figure 3** $k_{\mathrm{eff}}$ and $k_{\mathrm{sub}}$ during operation

**Figure 4** Delayed neutron fractions at BOC during operation

**Figure 5** Delayed neutron fractions at EOC during operation

**Figure 6** Power peaking during operation

**Figure 7** Coolant void reactivity during operation

**Figure 8** Cycle-dependent uncertainties of $k_{\mathrm{eff}}$ and $k_{\mathrm{sub}}$

**Figure 9** Cycle-dependent uncertainties of delayed neutron fractions

**Figure 10** Cycle-dependent uncertainties of power peaking and coolant void reactivity

**Figure 11** Inter-parameter correlation matrices of neutronics parameter uncertainties at BOC. “Power” and “Void” stand for power peaking and coolant void reactivity, respectively.

**Figure 12** Inter-cycle correlation matrices of neutronics parameter uncertainties. “1B” and ”1E” stand for BOC and EOC in cycle 1, respectively.

**Figure 13** Nuclide-wise uncertainties of $k_{\mathrm{eff}}$

**Figure 14** Nuclide-wise uncertainties of $k_{\mathrm{sub}}$

**Figure 15** Nuclide-wise uncertainties of $\beta_{\mathrm{source}}$

**Figure 16** Nuclide-wise uncertainties of $\beta_{\mathrm{eff}}$

**Figure 17** Nuclide-wise uncertainties of power peaking

**Figure 18** Nuclide-wise uncertainties of coolant void reactivity

**Figure 19** Nuclear data-wise uncertainties of $k_{\mathrm{eff}}$

**Figure 20** Nuclear data-wise uncertainties of $\beta_{\mathrm{eff}}$

**Figure 21** Nuclear data-wise uncertainties of coolant void reactivity

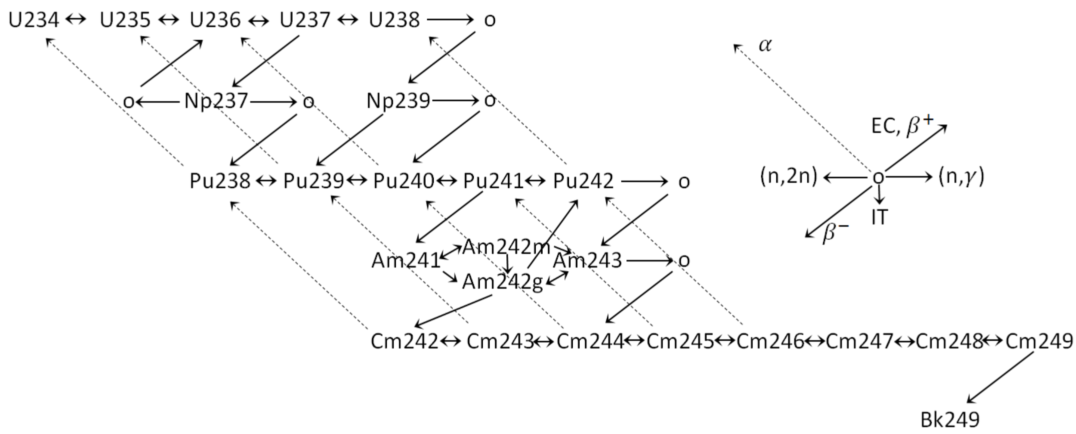


**Figure 1** Burnup chain for heavy nuclides

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Nuclear data-induced uncertainty quantification of neutronics parameters of accelerator-driven system

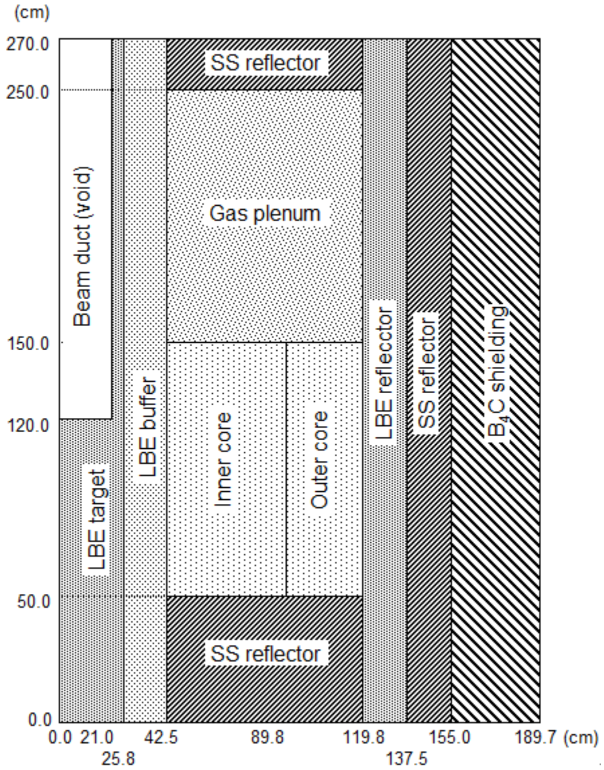


**Figure 2** Reactor core specification

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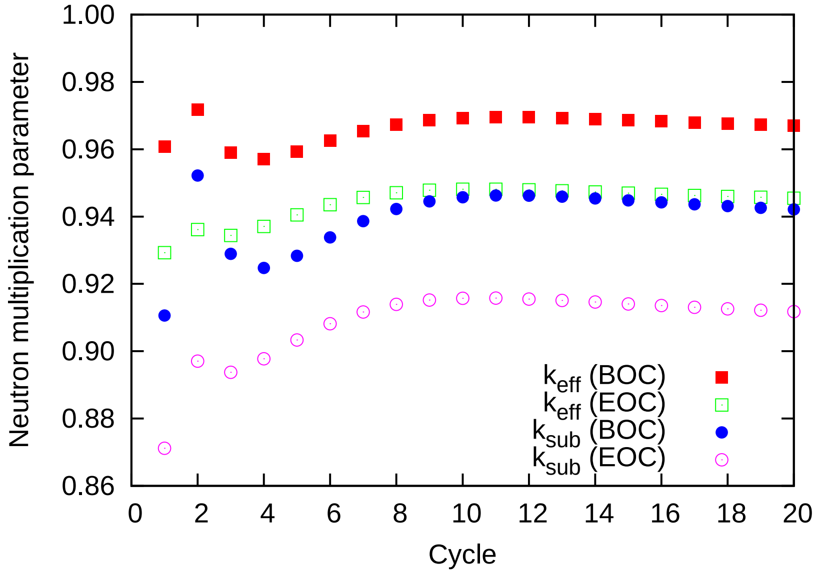


**Figure 3** $k_{\rm eff}$ and $k_{\rm sub}$ during operation

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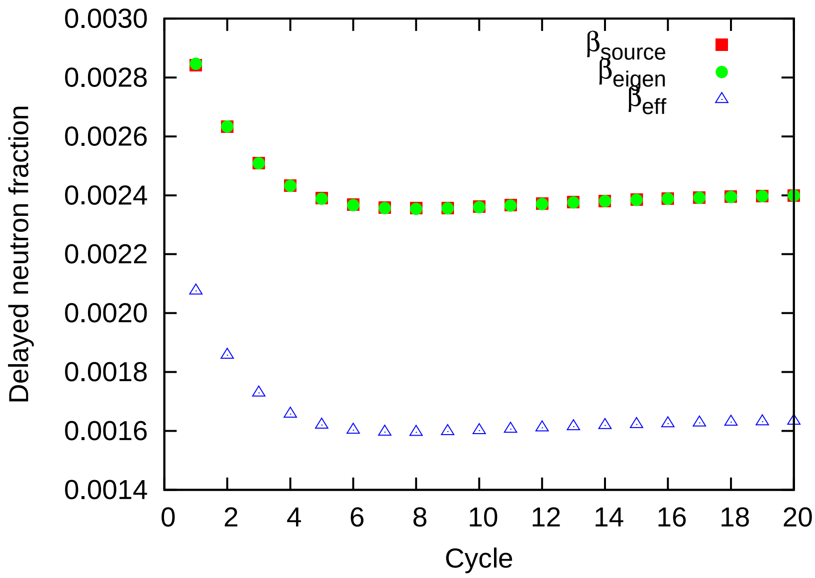


**Figure 4** Delayed neutron fractions at BOC during operation

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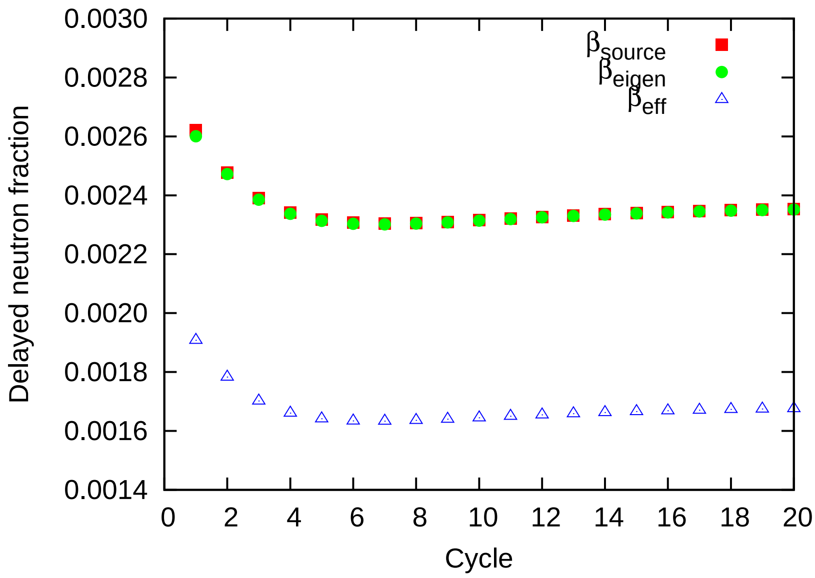


**Figure 5** Delayed neutron fractions at EOC during operation

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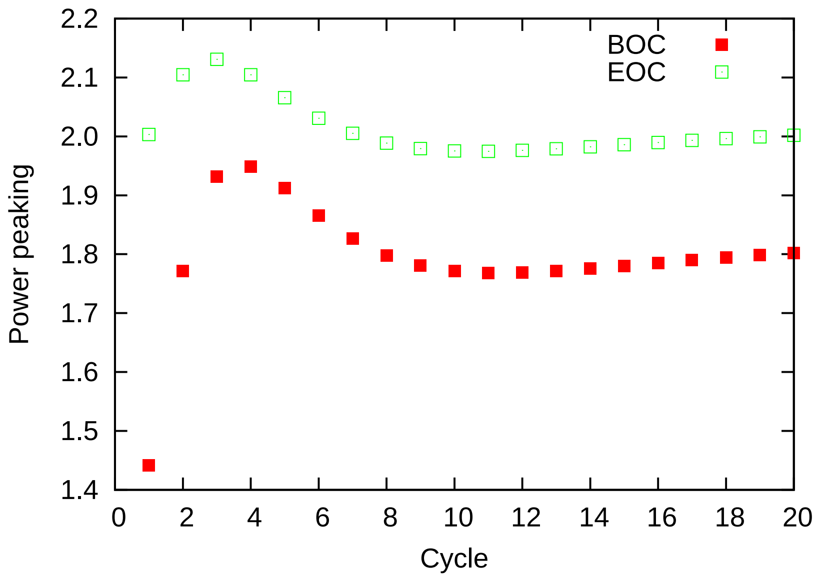


**Figure 6** Power peaking during operation

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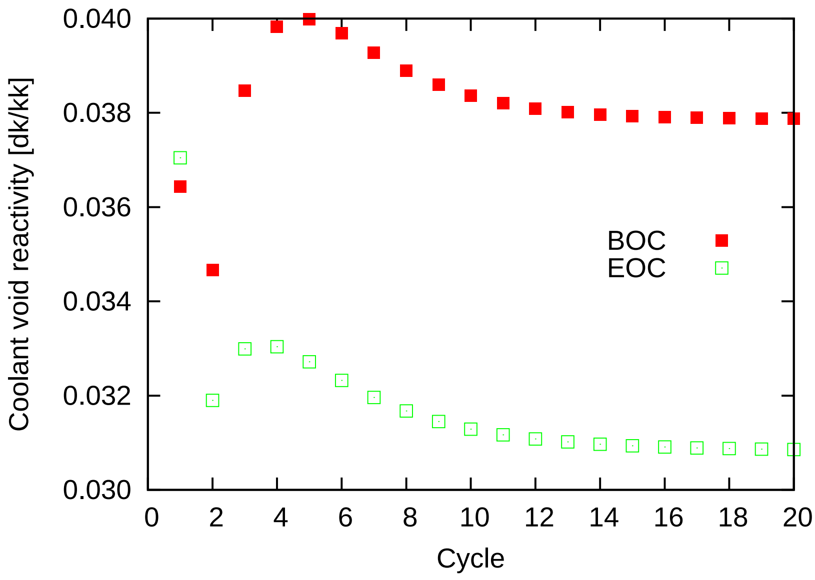


**Figure 7** Coolant void reactivity during operation

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Nuclear data-induced uncertainty quantification of neutronics parameters of accelerator-driven system

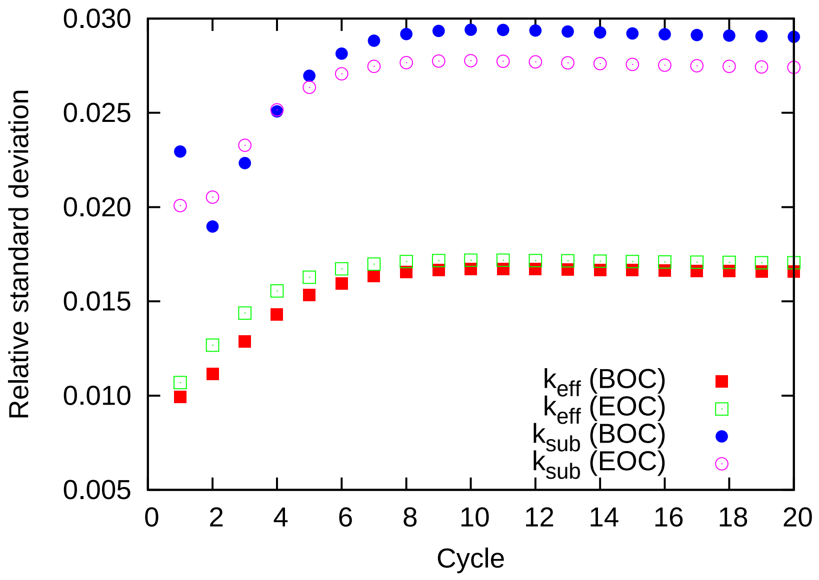


**Figure 8** Cycle-dependent uncertainties of $k_{\mathrm{eff}}$ and $k_{\mathrm{sub}}$

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Nuclear data-induced uncertainty quantification of neutronics parameters of accelerator-driven system

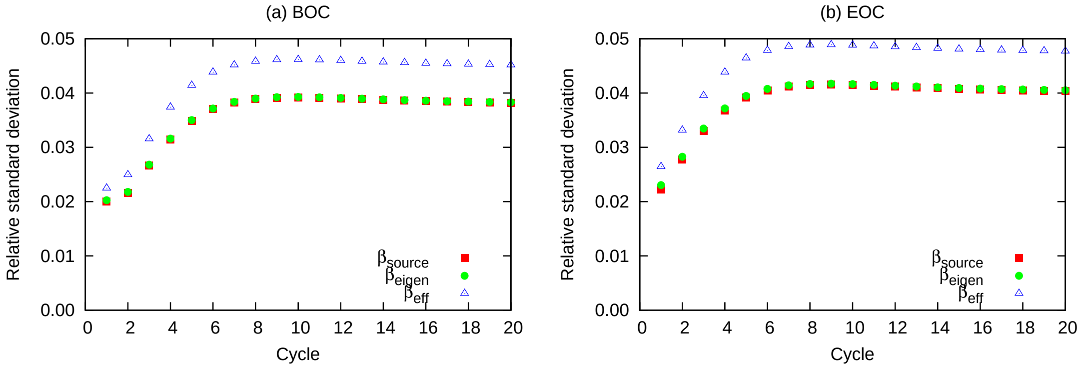


**Figure 9** Cycle-dependent uncertainties of delayed neutron fractions

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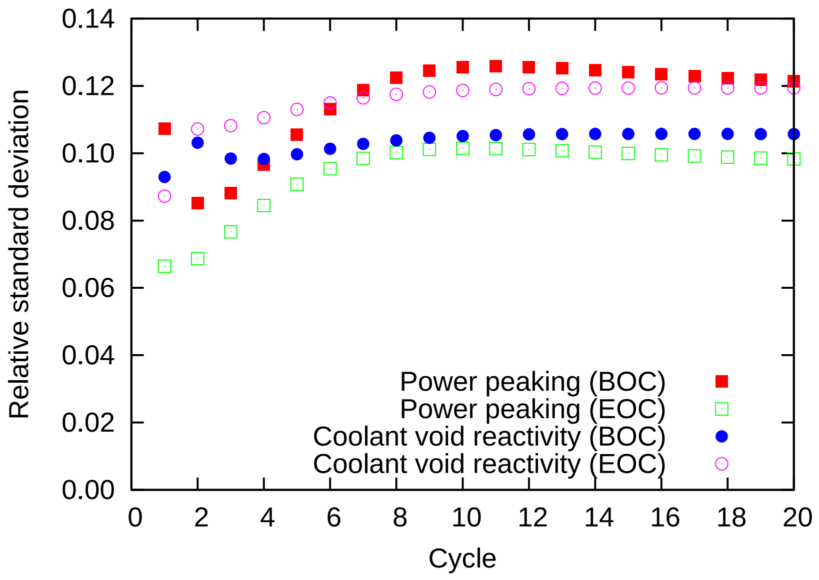


**Figure 10** Cycle-dependent uncertainties of power peaking and coolant void reactivity

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Nuclear data-induced uncertainty quantification of neutronics parameters of accelerator-driven system

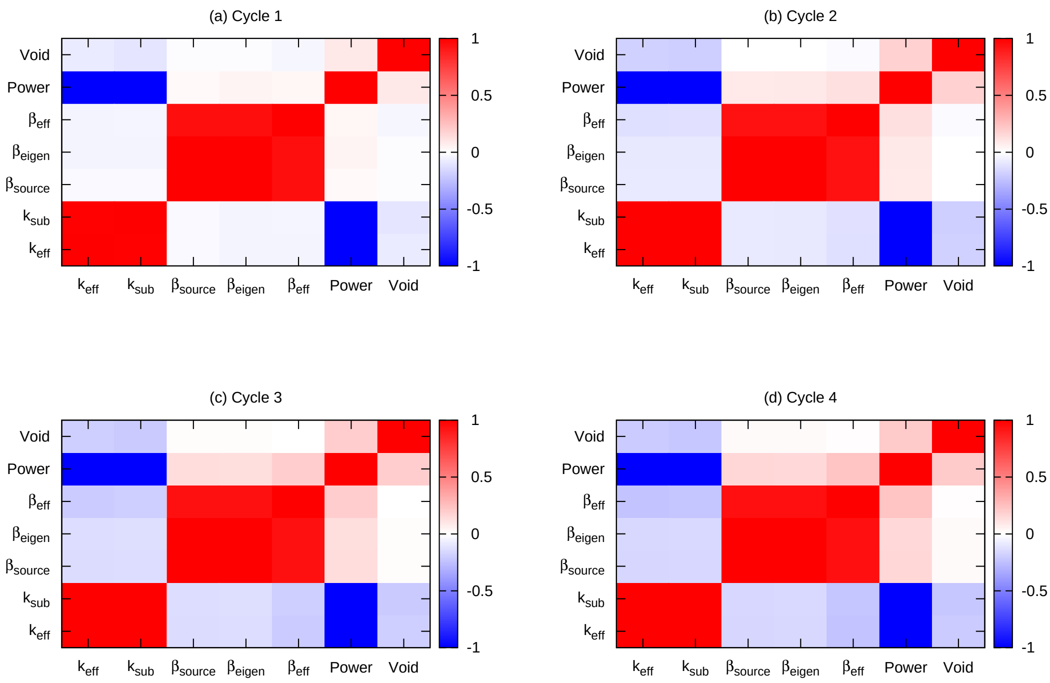


**Figure 11** Inter-parameter correlation matrices of neutronics parameter uncertainties at BOC. “Power” and “Void” stand for power peaking and coolant void reactivity, respectively.

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Nuclear data-induced uncertainty quantification of neutronics parameters of accelerator-driven system

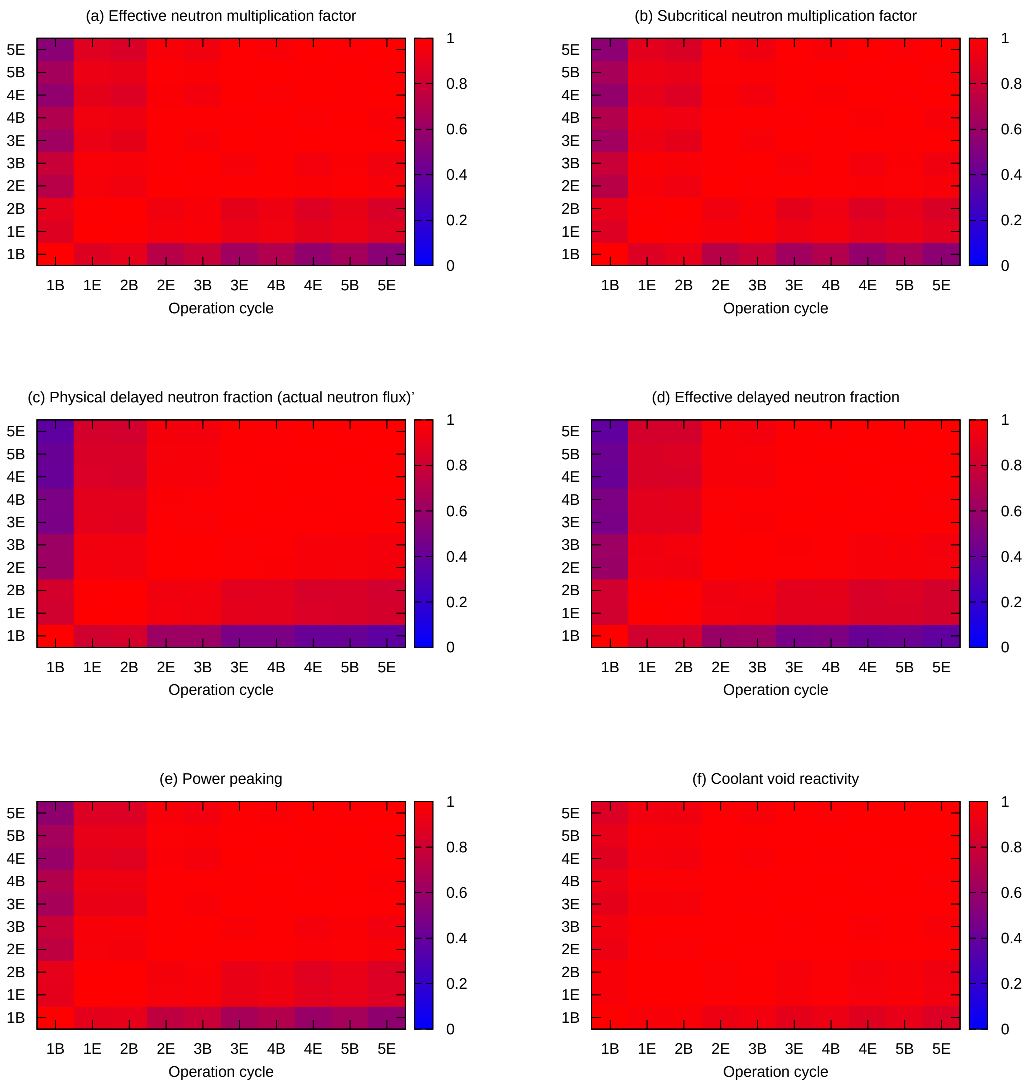


**Figure 12** Inter-cycle correlation matrices of neutronics parameter uncertainties. “1B” and ”1E” stand for BOC and EOC in cycle 1, respectively.

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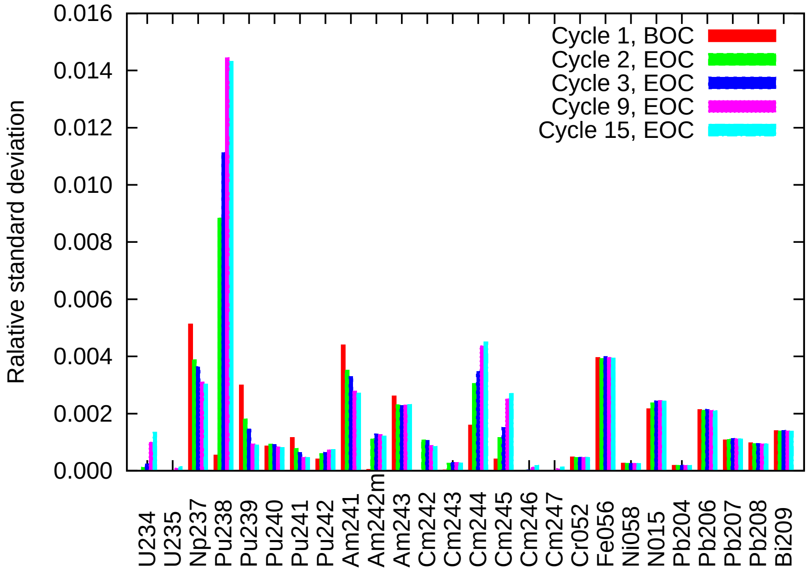


**Figure 13** Nuclide-wise uncertainties of $k_{\text{eff}}$

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Nuclear data-induced uncertainty quantification of neutronics parameters of accelerator-driven system

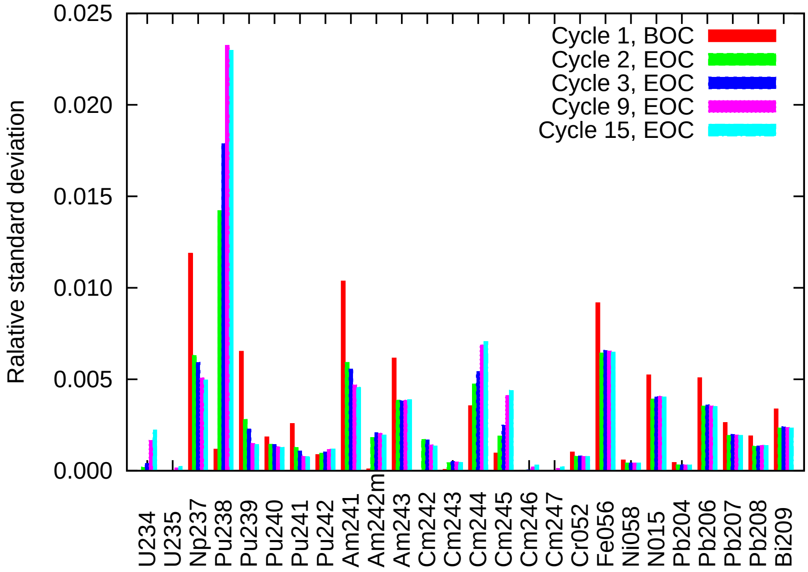


**Figure 14** Nuclide-wise uncertainties of $k_{\mathrm{sub}}$

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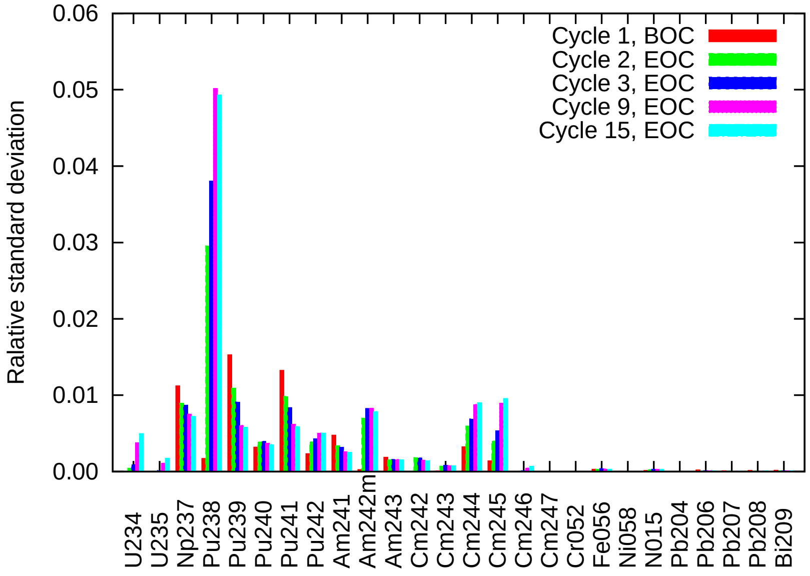


**Figure 15** Nuclide-wise uncertainties of $\beta_{\text{source}}$

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Nuclear data-induced uncertainty quantification of neutronics parameters of accelerator-driven system

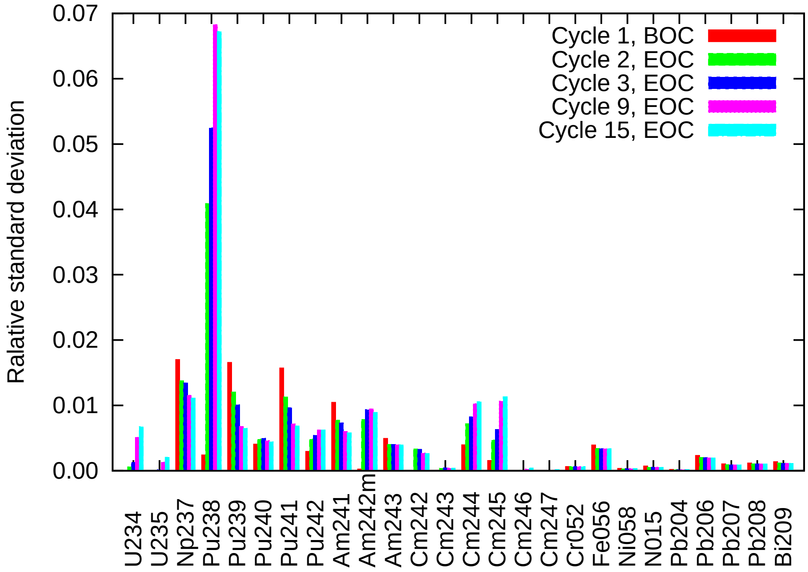


**Figure 16** Nuclide-wise uncertainties of $\beta_{\rm eff}$

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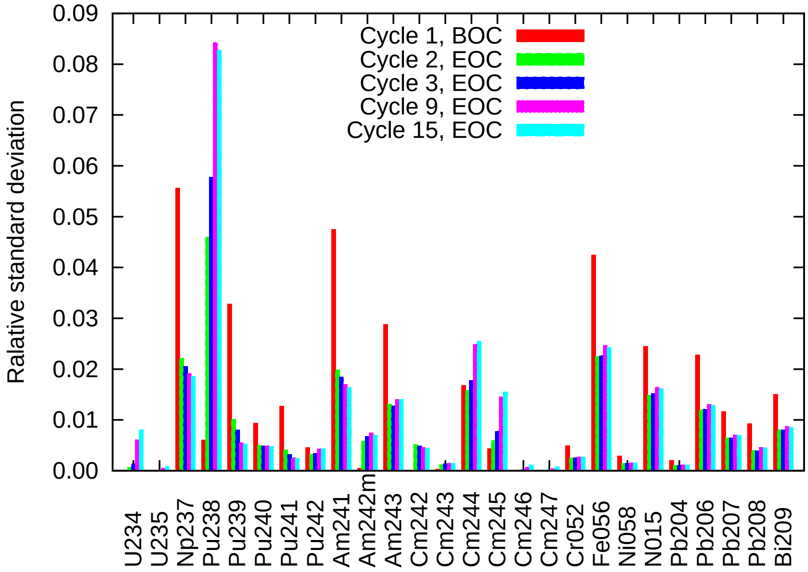


**Figure 17** Nuclide-wise uncertainties of power peaking

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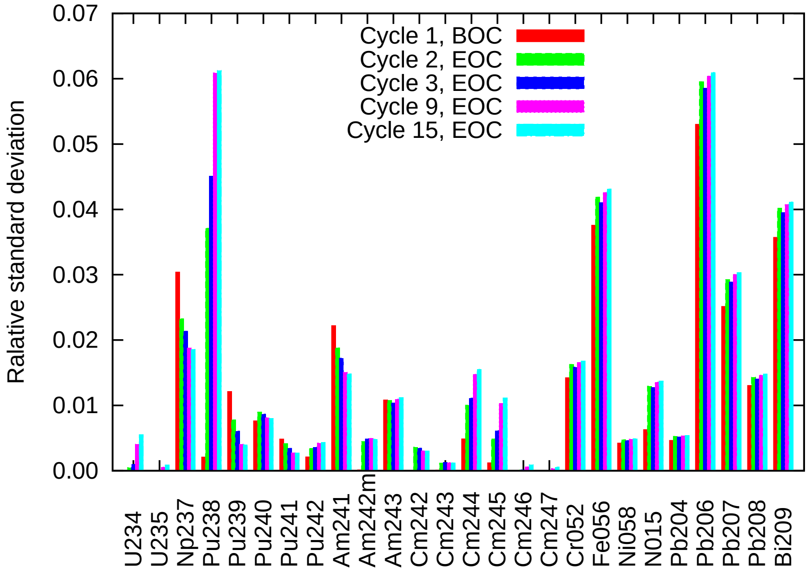


**Figure 18** Nuclide-wise uncertainties of coolant void reactivity

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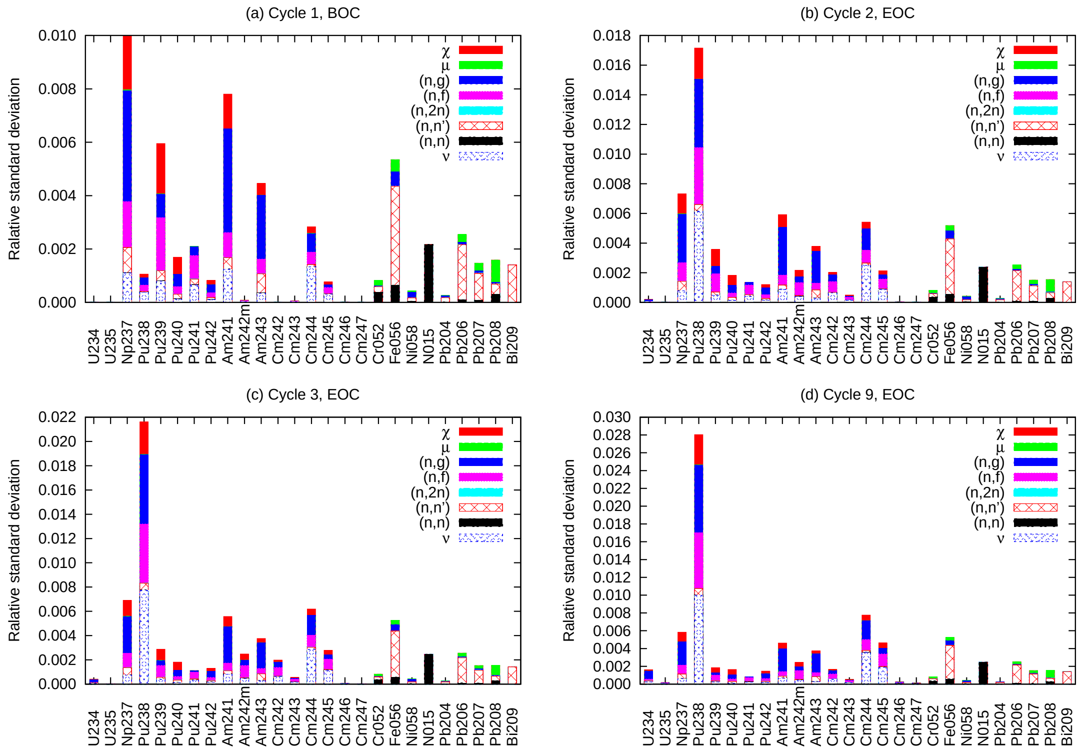


**Figure 19** Nuclear data-wise uncertainties of $k_{\mathrm{eff}}$

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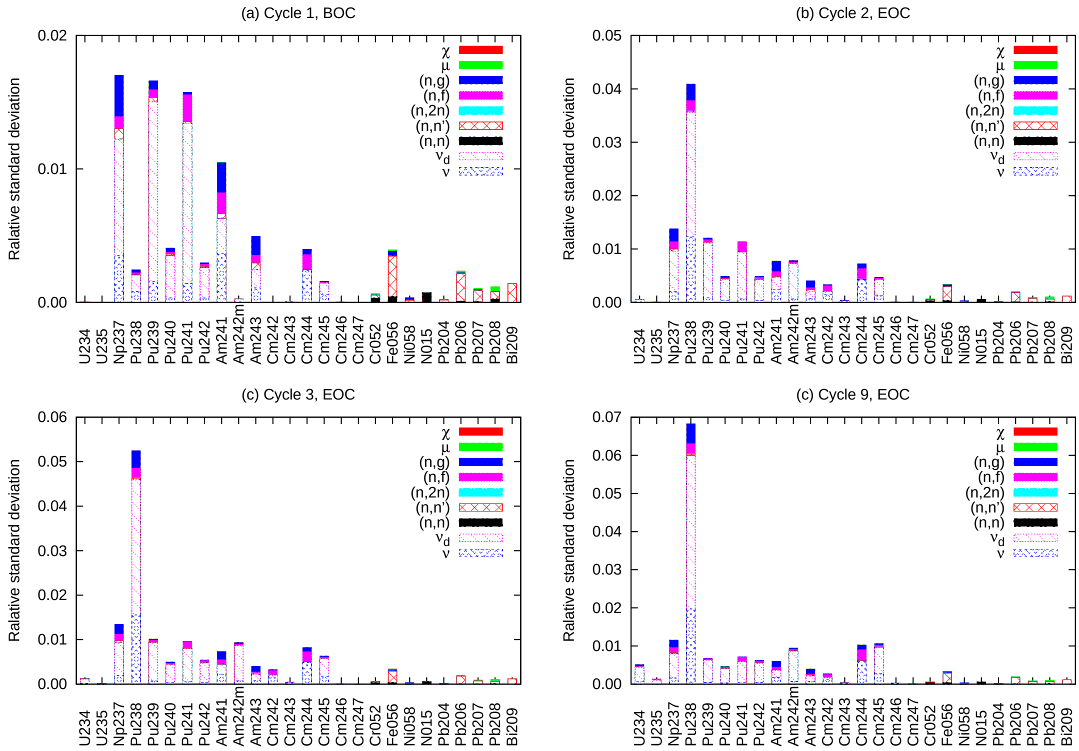


**Figure 20** Nuclear data-wise uncertainties of $\beta_{\mathrm{eff}}$

G.Chiba

Nuclear data-induced uncertainty quantification of neutronics parameters of accelerator-driven system

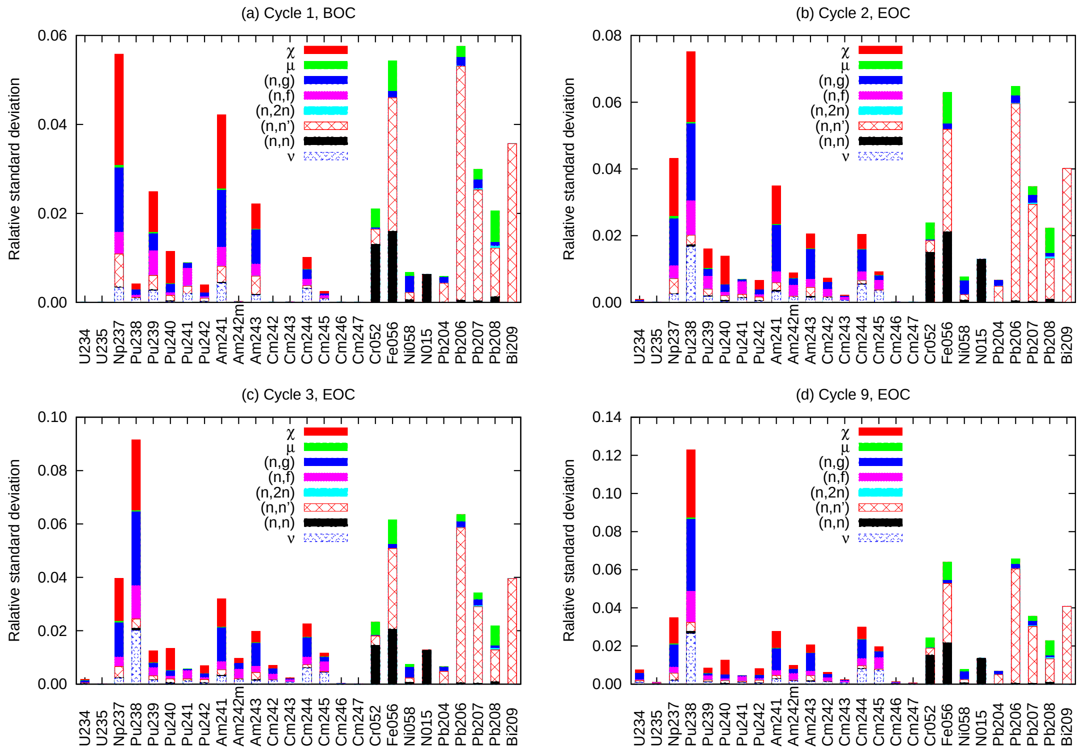


**Figure 21** Nuclear data-wise uncertainties of coolant void reactivity

G.Chiba

Nuclear data-induced uncertainty quantification of neutronics parameters of accelerator-driven system