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Implementation of Fuel Burnup Sensitivity Calculation Capability into a Deterministic Reactor Physics Code System CBZ for Accelerator-Driven System Multi-Cycle Burnup Calculations

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Abstract - *A new capability of calculating fuel burnup sensitivity with the generalized perturbation theory is implemented into a deterministic reactor physics code system CBZ, which is under development at Hokkaido University. This capability is well verified through comparisons with reference sensitivities obtained by numerical differentiation. Nuclear data-induced uncertainties of two neutronics parameters, k_{eff} and coolant void reactivity, of an accelerator-driven system designed by the Japan Atomic Energy Agency are quantified using sensitivities calculated with the new version of CBZ, and effect of burnup term in the sensitivities is also quantified. On both k_{eff} and coolant void reactivity, cancellation between static and burnup components in nuclear data-induced uncertainties is observed; uncertainties become small if the burnup component is taken into account.*

I. INTRODUCTION

An accelerator-driven system (ADS) is one of promising nuclear systems, which has a potential to drastically reduce the burden of nuclear waste disposal by burning minor actinoid (MA) nuclides. Since accurate prediction of neutronics parameters of ADS is essential and important, so much effort have been devoted to quantify and reduce uncertainties of ADS neutronics parameters.

Nuclear data-induced uncertainty is one of dominant contributors to total uncertainty of ADS neutronics parameters. In our previous study, nuclear data-induced uncertainties of neutronics parameters of one specific ADS design are quantified with sensitivity-based uncertainty propagation calculations [1]. Sensitivities used in this study have been calculated with the perturbation theory for static problems, and effects of fuel burnup during operation have not been taken into account. The burnup effects on sensitivities are not negligible generally, so we implement a new capability of calculating fuel burnup sensitivities for multi-cycle ADS burnup calculations into a deterministic reactor physics code system CBZ, which is under development at Hokkaido University.

In the present paper, we describe a fundamental theory of fuel burnup sensitivity calculations for ADS multi-cycle burnup calculations briefly in Sec. II, and detail of ADS dedicated to the present calculations is described in Sec. III. Procedures of numerical calculations and numerical results of sensitivity calculations and uncertainty quantification are presented in Sec. IV, and conclusion is provided in Sec. V.

II. THEORY

The generalized perturbation theory (GPT) for fuel burnup problems has been well established [2, 3], and the fundamental theory and actual implementations are described in the previous paper written by one of the present authors in detail [4]. Some issues specific to the ADS burnup calculations are addressed in the present paper.

One of the main differences is in the neutron transport equation which is solved to obtain neutron flux spatial distribution. In ADS calculations, the following fixed source equation is solved:

$$\boldsymbol{B}_i \boldsymbol{\Phi}_i = \boldsymbol{Q}, \tag{1}$$

where $\boldsymbol{B}_i$ and $\boldsymbol{\Phi}_i$ are the transport operator and neutron flux at t_i, and $\boldsymbol{Q}$ is the external neutron source.

Another specific issue in the ADS burnup calculations is a multi-cycle fuel burnup process. Let us assume that number density changes during processes of fuel discharging, reprocessing and reloading in the ADS cycle are represented with a matrix $\boldsymbol{R}$ and a vector $\boldsymbol{s}$ as

$$\Delta \boldsymbol{n} = \boldsymbol{R}\boldsymbol{n} + \boldsymbol{s}, \tag{2}$$

where $\boldsymbol{n}$ is the number density vector. The size of the vectors $\boldsymbol{n}$ and $\boldsymbol{s}$ is $K \times J$ where K is the total number of nuclides traced by burnup calculations and J is the total number of burnup regions, and $\boldsymbol{R}$ is a $KJ \times KJ$ matrix. With this notation, burnup process in multi-cycle ADS can be written with the following equation:

$$\frac{d\boldsymbol{n}(t)}{dt} = \boldsymbol{M}(t)\boldsymbol{n}(t) + \sum_{l=1}^{L} \delta(t - \tilde{t}_l)\left(\boldsymbol{R}\boldsymbol{n}(t) + \boldsymbol{s}\right), \tag{3}$$

where $\boldsymbol{M}$ is the burnup matrix. It is assumed that number density changes due to the fuel discharging and reloading are conducted simultaneously at $\tilde{t}_l$ ($l = 1, 2, ..., L$).

Sensitivity of number density of nuclide k in region j at t_I, $N_l^j(t_I)$, with respect to nuclear data σ can be calculated with GPT-based procedure described in the previous paper [4], but there is a difference in a definition of adjoint number density $\boldsymbol{w}$. For brevity, we omit the full definition of $\boldsymbol{w}$ and only present a simplified definition without spatial dependence as follows:

$$-\frac{d\boldsymbol{w}(t)}{dt} = \boldsymbol{M}^T(t)\boldsymbol{w}(t) + \sum_{l=1}^{L} \delta(t - \tilde{t}_l)\boldsymbol{R}^T \boldsymbol{w}(t), \tag{4}$$

where the superscript T denotes the matrix transposition. Note that generalized adjoint neutron flux and adjoint power are introduced in actual numerical calculations in order to consider neutron flux spatial and energy distribution effect and power normalization effect on burnup of nuclides.

Sensitivity of a neutronics parameter after fuel burnup, denoted as P, with respect to nuclear data σ can be written as follows [5]:

$$\frac{dP}{d\sigma} = \frac{\partial P}{\partial \sigma} + \left(\frac{\partial P}{\partial \mathbf{\Phi}}\right)^T \left(\frac{d\mathbf{\Phi}}{d\sigma}\right) + \left(\frac{\partial P}{\partial \boldsymbol{n}}\right)^T \left(\frac{d\boldsymbol{n}}{d\sigma}\right). \qquad (5)$$

The first and second terms of the right hand side of Eq. (5) are referred to as a *static term*. The static term can be calculated easily with the perturbation theory or the GPT for static problems. The third term is referred to as a *burnup term* and it is calculated with the new capability.

III. DEDICATED ADS

We treat a benchmark problem based on a commercial grade ADS proposed by the Japan Atomic Energy Agency (JAEA) [6]. 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. In the present calculation, ratio of the zirconium-nitride to the total fuel is set as 48.75 wt%, and ratios of plutonium-nitride (PuN) to the total actinide-nitride (PuN+MAN) are set as 26.9 wt% and 50.0 wt% for inner and outer cores, respectively. Spent fuels, which are loaded in a PWR core till the burnup of 45 GWd/t and are reprocessed after 7-year cooling, are used as sources of MA and Pu fuels in this ADS. The isotopic compositions of MA and Pu are shown in Tables I and II.

TABLE I. Isotopic composition of plutonium fuels.

Nuclide	Weight ratio [%]
U-234	0.04
U-235	0.01
Pu-238	2.41
Pu-239	54.85
Pu-240	24.94
Pu-241	10.84
Pu-242	6.92

A proton beam with 1.5 GeV provided by LINAC is injected into the core through a beam duct along core central axis. Top and side views of this ADS core are shown in Figures 1 and 2.

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 in the next burnup cycle after cooling and reprocessing. The time period for the cooling and reprocessing is 2.5 years in total. In the refabrication process, fission products (FP) are removed and only MA of equal mass to the removed FP is added to the recycled fuel. This is reason why the number density

TABLE II. Isotopic composition of MA fuels.

Nuclide	Weight ratio [%]
Np-237	50.05
Am-241	32.34
Am-242m	0.06
Am-243	13.15
Cm-243	0.03
Cm-244	3.96
Cm-245	0.38
Cm-246	0.04

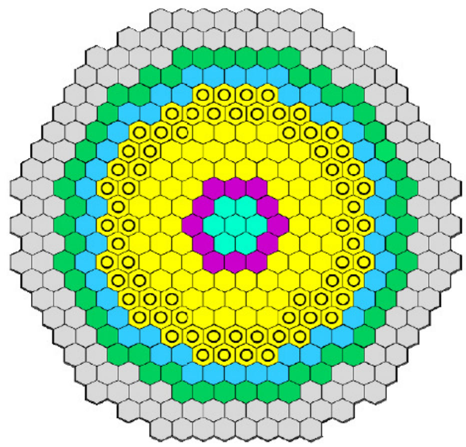

Fig. 1. Top view of JAEA-designed ADS.

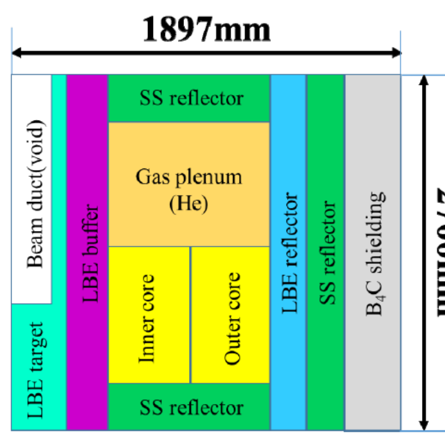

Fig. 2. Side view of JAEA-designed ADS.

changes during the fuel outage period can be represented by Eq. (2). Whereas inner and outer core fuels are reprocessed independently in the original concept of JAEA, these fuels are reprocessed simultaneously in our calculations. Thus this ADS has a homogeneous one-region core after the second cycle. Plutonium is used as mixture of MA only at the first cycle and is not additionally loaded in the following cycles. Figure 3 shows conceptual view of the present nuclear fuel cycle based on ADS.

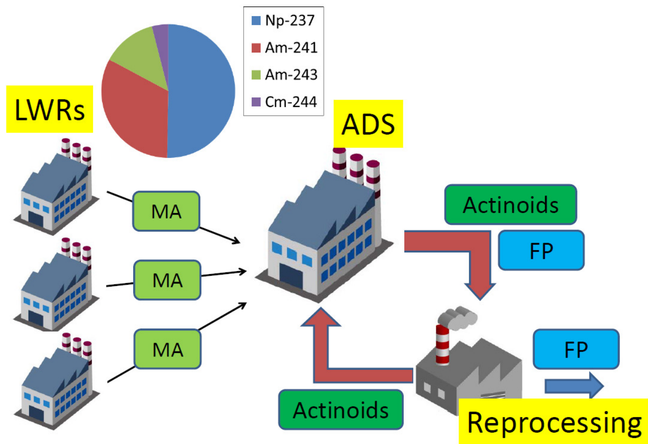

Fig. 3. Conceptual view of nuclear fuel cycle based on ADS.

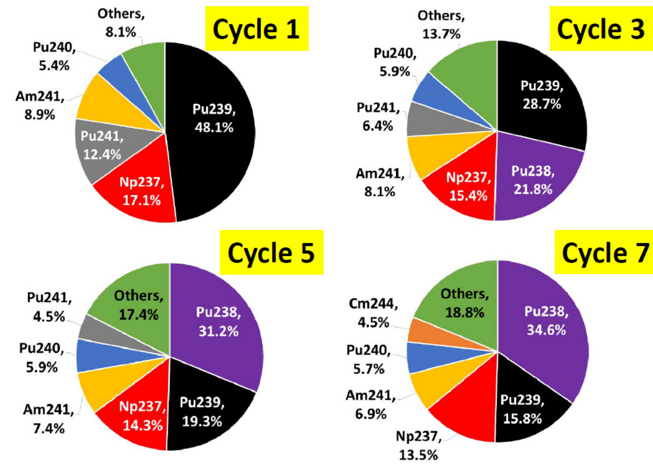

Fig. 4. Nuclide-wise contributions to total fission reactions.

IV. RESULTS AND ANALYSIS

1. Numerical Procedure

All the calculations are carried out with a module named 'FRBurnerRZ' of a deterministic reactor physics code system CBZ. This module has been originally developed to perform multi-cycle burnup calculations of fast reactors, and has been extended to be capable of treating ADS cores. The present ADS core is simplified to two-dimensional cylinder geometry and spatial distributions of neutron flux are calculated with a diffusion theory-based solver. For simplicity it is assumed that all the heat energy is generated by fission reactions. External neutron sources are calculated by the PHITS code [7]. Details of numerical procedures can be found in our previous paper [1].

The new capability of burnup sensitivity calculations is implemented into the FRBurnerRZ module. At present, burnup sensitivities with respect to capture, fission and (n,2n) reaction cross sections of actinoid nuclides are calculated. For simple implementation, perturbation on leakage terms in the diffusion equation is not considered in the burnup sensitivity calculations.

In order to understand burnup characteristics of the present ADS, nuclide-wise contributions to total fission reactions at several cycles are shown in Figure 4. At the initial cycle, contributions of plutonium-239 and -241 are significant, but in the following cycles contributions of these nuclides become small and plutonium-238 contribution becomes dominant.

2. Sensitivities of Number Densities to Cross Sections

Tables III and IV show energy-integrated sensitivities of nuclide number densities after 5 cycles with respect to fission and capture cross sections. In these tables, number densities at two spatial positions are considered; one is at the core center region and the other is at the core peripheral region. Two values are given to each sensitivity; the top one is obtained with GPT calculation, and the bottom one is obtained with direct numerical differentiation in which 0.1% perturbations are given to cross sections of all the energy groups.

These tables show that results obtained with GPT calculations agree well those of the direct calculations, so the present implementation of GPT into CBZ is verified here.

Sensitivities of number density of a nuclide with respect to fission and capture cross sections of the nuclide itself are generally negative. This reason is easily understood since increases of neutron absorption cross sections decrease the number density of the nuclide itself.

It is interesting to point out that there are large differences in the same sensitivities at different spatial positions. Let us consider sensitivities of number densities of neptunium-237 and americium-241 to fission cross sections of plutonium-238 and -239, which are shown as bold characters in these tables. These plutonium isotopes are dominant fissile nuclides in this core, so increase of these fission cross sections makes neutron flux level lower under the fixed power condition. This decrease of neutron flux level moderates transmutations of nuclides, such as neptunium-237 and americium-241, which are supplied from the out of the fuel cycle. Thus sensitivities of number densities of neptunium-237 and americium-241 to plutonium fission cross sections become positive. In addition, we have to consider effect via neutron flux spatial distribution. If fission cross section increases, the system becomes close to the critical state; neutron flux spatial distribution becomes close to the fundamental mode. Thus peak of the neutron flux around the neutron sources becomes smaller and the neutron flux level in the core peripheral region becomes higher. Nuclide transmutation in the core center region is more moderated and that in the core peripheral region is enhanced. This is the reason why the sensitivities in the core center region is much larger than those in the core peripheral region.

3. Uncertainty Quantification of Neutronic Parameters

Sensitivities of neutronic parameters at end of cycles to nuclear data are calculated, and nuclear data-induced uncertainties of these parameters are quantified with these sensitivities and covariance data of nuclear data given in JENDL-4.0 [8]. Covariance data of the following nuclides are considered: uranium-233, -234, -235, -238, neptunium-237, plutonium-238, -239, -240, -241, -242, americium-241, -243, curium-242,

TABLE III. Energy-integrated sensitivities of nuclide number densities after 5 cycles at core center region. The first and second lines correspond to GPT results and direct numerical differentiation results, respectively.

	Fission cross section					Capture cross section				
	Np-237	Pu-238	Pu-239	Am-241	Cm-244	Np-237	Pu-238	Pu-239	Am-241	Cm-244
Np-237	+0.102	**+0.842**	**+0.294**	+0.222	+0.136	*-0.752*	+0.003	-0.112	+0.199	+0.071
	+0.102	+0.833	+0.291	+0.223	+0.138	-0.745	+0.002	-0.113	+0.201	+0.072
Pu-238	-0.027	*-0.322*	+0.097	+0.017	+0.027	+0.284	-0.260	-0.024	+0.134	+0.005
	-0.024	-0.324	+0.098	+0.019	+0.028	+0.290	-0.263	-0.024	+0.133	+0.006
Pu-239	+0.012	-0.159	*-0.863*	+0.021	+0.020	+0.253	+0.526	-0.255	+0.112	-0.001
	+0.014	-0.155	-0.871	+0.021	+0.020	+0.245	+0.540	-0.258	+0.110	-0.001
Am-241	+0.384	**+0.867**	**+0.288**	+0.015	+0.139	+0.307	-0.001	-0.109	*-0.957*	+0.071
	+0.385	+0.857	+0.285	+0.017	+0.141	+0.313	-0.002	-0.111	-0.954	+0.072
Cm-244	+0.001	-0.053	+0.025	-0.006	-0.246	-0.033	-0.008	+0.005	+0.013	*-0.275*
	+0.000	-0.050	+0.025	-0.006	-0.250	-0.036	-0.008	+0.006	+0.011	-0.279

TABLE IV. Energy-integrated sensitivities of nuclide number densities after 5 cycles at core peripheral region. The first and second lines correspond to GPT results and direct numerical differentiation results, respectively.

	Fission cross section					Capture cross section				
	Np-237	Pu-238	Pu-239	Am-241	Cm-244	Np-237	Pu-238	Pu-239	Am-241	Cm-244
Np-237	-0.071	**+0.173**	**+0.174**	+0.052	+0.030	*-0.525*	+0.041	-0.129	+0.105	+0.021
	-0.072	+0.173	+0.173	+0.051	+0.030	-0.523	+0.041	-0.127	+0.105	+0.021
Pu-238	-0.063	*-0.347*	+0.042	-0.017	+0.003	+0.300	-0.202	-0.007	+0.126	-0.007
	-0.062	-0.349	+0.043	-0.017	+0.003	+0.302	-0.204	-0.006	+0.125	-0.007
Pu-239	+0.004	-0.118	*-0.854*	+0.005	+0.008	+0.226	+0.425	-0.232	+0.108	-0.001
	+0.005	-0.116	-0.856	+0.005	+0.008	+0.221	+0.432	-0.233	+0.106	-0.001
Am-241	+0.099	**+0.168**	**+0.164**	-0.083	+0.029	+0.147	+0.040	-0.007	*-0.626*	+0.019
	+0.098	+0.168	+0.163	-0.083	+0.029	+0.148	+0.040	-0.006	-0.625	+0.019
Cm-244	+0.002	-0.032	+0.005	-0.001	-0.183	-0.050	-0.018	-0.001	-0.012	*-0.210*
	+0.001	-0.030	+0.005	-0.001	-0.185	-0.053	-0.018	-0.001	-0.014	-0.212

-244, -245, -246, nitride-15, iron-56, lead-206, -207, -208, -209, bismuth-209.

A. Effective neutron multiplication factor k_{eff}

Cycle-dependent k_{eff} uncertainties are shown in Figure 5. Total uncertainties are decomposed into those evaluated by only static or burnup term of sensitivity, and these component-wise uncertainties are also presented. The k_{eff} uncertainties become small if the burnup term in the sensitivities is taken into account. This is because of cancellation between the static and burnup components. This can be understood by considering importances of nuclides and their neutron reaction cross sections on neutronics parameters. With respect to k_{eff}, fission and capture cross sections have positive and negative importances, respectively. On nuclides, fissile nuclides such as plutonium-238 and -239 have positive importance and others such as neptunium-237, americium-241 and curium-244 have negative importances. Thus if sensitivities of number density of fissile nuclides to fission cross section are negative or sensitivities to capture cross section are positive, cancellation between the static and burnup terms occurs. The same thing can be said if sensitivities of number density of non-fissile nuclides to capture cross sections are negative. From Tables III and IV we can see large negative sensitivities of plutonium number densities to plutonium fission cross sections, and large negative sensitivities of non-fissile nuclide number densities to capture cross sections of neptunium-237 and americium-241, which are presented in italic. From this interpretation, it can be said that there is cancellation between these two components and total uncertainties become smaller than those due to only the static component in k_{eff} of ADS.

Figure 6 shows component- and nuclide-wise nuclear data-induced uncertainties of k_{eff}. As already presented in our previous study, nuclear data of plutonium-238 is dominant source in the k_{eff} uncertainty via the static component [1]. It is interesting to point out that the burnup components are compatible with the static components in the uncertainties of neptunium-237 and americium-241.

Note that our previous study has shown that nuclear data-induced uncertainty of k_{eff} has strong positive correlations to that of subcritical multiplication factor k_{sub}, which is a different physical quantity to describe neutron multiplication in sub-critical systems [1].

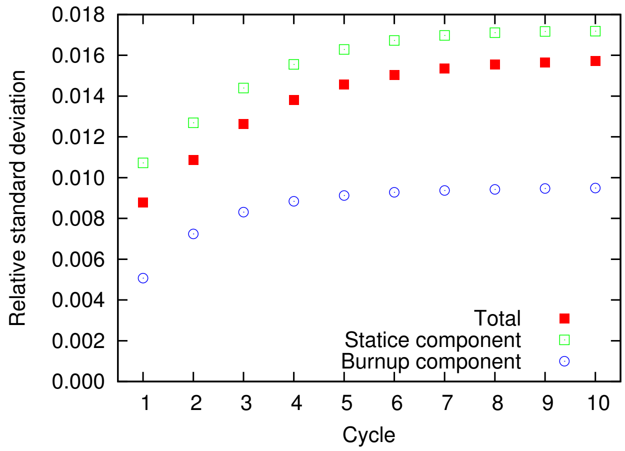

Fig. 5. Nuclear data-induced uncertainties of k_{eff} at the end of cycles.

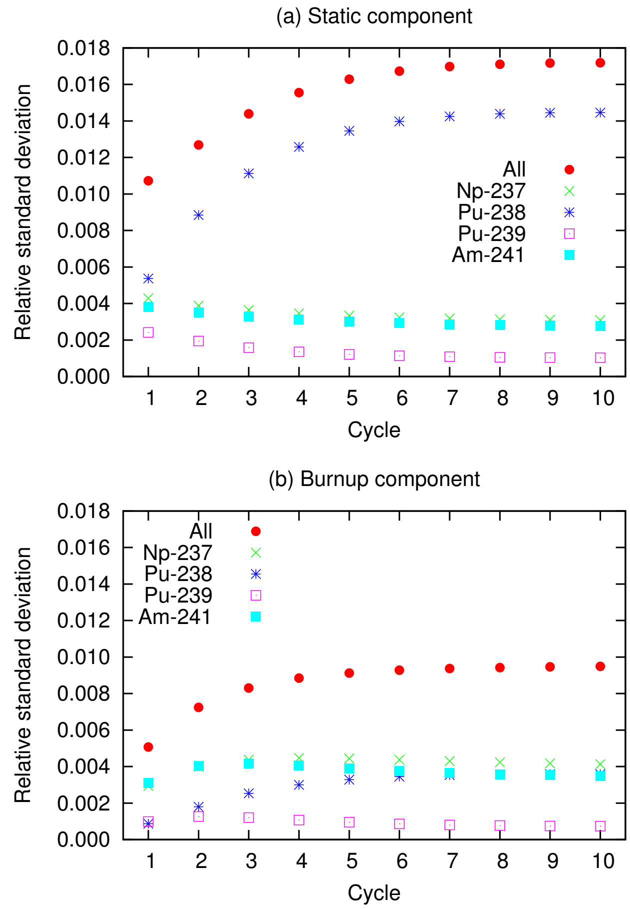

Fig. 6. Component- and nuclide-wise nuclear data-induced uncertainties of k_{eff}.

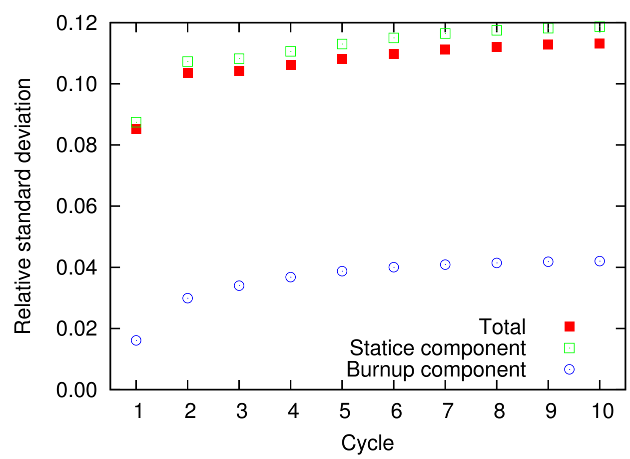

Fig. 7. Nuclear data-induced uncertainties of coolant void reactivity at the end of cycles.

B. Coolant Void Reactivity

Coolant void reactivity is one of important neutronics parameters of ADS. Coolant voiding hardly occurs in the loss of coolant accidents of ADS since boiling temperature of LBE is significantly high, but there is possibility of void insertion into coolant due to some types of accidents such as primary loop rupture.

Sensitivities of coolant void reactivity, which is inserted to the core when all the coolant materials are removed in the core fuel region, at end of cycles are calculated. Each of these sensitivities is calculated from two sensitivities of k_{eff} at reference state and at coolant-voided state. With these sensitivities, nuclear data-induced uncertainties are quantified. Cycle-dependent uncertainties of the coolant void reactivity are shown in Figure 7. As the k_{eff} uncertainties, cancellations between the static and burnup components are observed, but these are less significant than the k_{eff} uncertainty.

Figure 8 shows component- and nuclide-wise nuclear data-induced uncertainties of the coolant void reactivity. Note that uncertainties due to nuclear data of medium-heavy nuclides such as iron, lead and bismuth also contribute to the coolant void reactivity uncertainties [1].

V. CONCLUSIONS

A new capability of calculating fuel burnup sensitivity with GPT has been implemented into a deterministic reactor physics code system CBZ, which is under development at Hokkaido University. This capability has been well verified through comparisons with reference sensitivities obtained by numerical differentiation. Nuclear data-induced uncertainties of two neutronics parameters, k_{eff} and coolant void reactivity, for the JAEA-designed ADS have been quantified using the sensitivities calculated with the new version of CBZ, and the effect of the burnup term in the sensitivities has also been quantified. On both k_{eff} and coolant void reactivity, cancellation between the static and burnup components in nuclear data-induced uncertainties has been observed; the uncertainties have become small if the burnup component is taken into account.

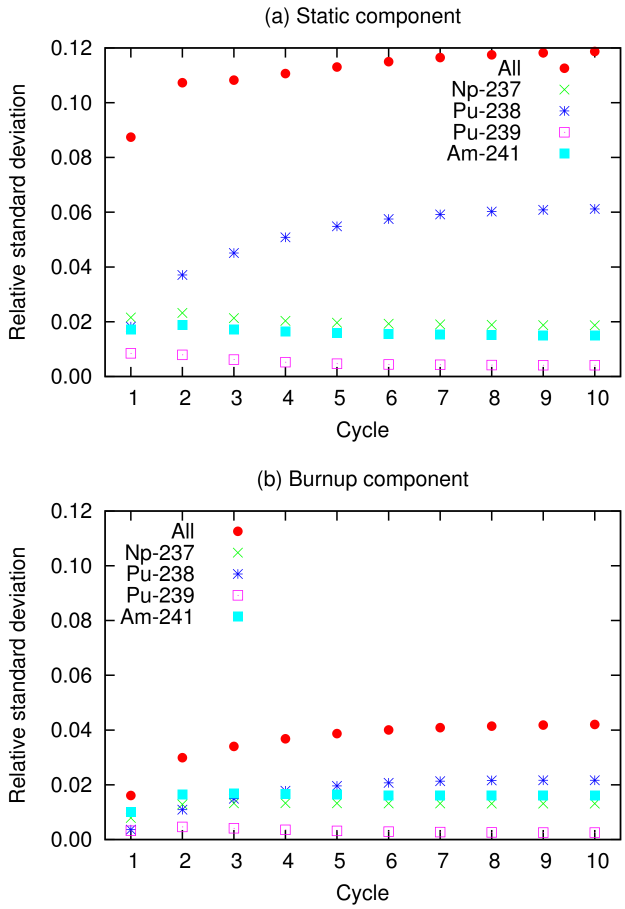

Fig. 8. Component and nuclide-wise nuclear data-induced uncertainties of coolant void reactivity

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