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Uncertainty quantification calculations of nuclide number densities of Gd-bearing fuel rods in light water reactors

Go Chiba[1,*]

[1]Hokkaido University, Faculty of Engineering, Kita 13 Nishi 8, Sapporo, Hokkaido 060-8628, Japan

Abstract. The Post-Irradiation Examination (PIE) data are quite useful to validate the evaluated nuclear data. Recently, a new experimental program, REGAL (the Rod-Extremity and Gadolinia AnaLysis), has been proposed and launched. During this program, the PIE data are acquired for the Gd-bearing fuel rods during (or after) the initial Gd burnout. These PIE data would be different from those for the normal UOX or MOX fuel rods from a viewpoint of nuclide transmutation process. In the present work, we attempt to quantify this difference through calculating sensitivity coefficients of nuclide number densities of the Gd-bearing rods using the depletion perturbation theory and performing uncertainty quantification calculations with the sensitivity coefficients and the nuclear data covariance data. Through the numerical analyses, we found that the impact of the uncertainties of the nuclear data of Gd isotopes on the number densities of actinoids is negligible. The nuclear data-induced uncertainties of Gd isotopes number densities are relatively large during the Gd depletion, and those become small after the Gd burnout. After the Gd burnout, the relative standard deviations of Gd-155 and -157 number densities are approximately 6% and 13%, respectively, and the nuclear data of the parent nuclides of these Gd isotopes, Gd-154 and -156, are also important as well as those of Gd-155 and -157.

1 Introduction

The Post-Irradiation Examination (PIE) data are quite useful to validate the evaluated nuclear data, and the PIE data which have been accumulated in the world so far have been utilized in benchmarking the newly-developed evaluated nuclear data files. Recently, a new experimental program, REGAL (the Rod-Extremity and Gadolinia AnaLysis), has been proposed and launched[1]. In this program, the PIE data are acquired for the Gd-bearing fuel rods during (or after) the initial Gd burnout. These PIE data would be different from those for the normal UOX or MOX fuel rods from a viewpoint of nuclide transmutation process since the neutron flux energy spectra in these Gd-bearing rods are somewhat different from those in the normal fuel rods. In the present work, we attempt to quantify this difference through calculating sensitivity coefficients of nuclide number densities of the Gd-bearing rods and the normal fuel rods using the depletion perturbation theory (DPT) and performing uncertainty quantification calculations with the sensitivity coefficients and the covariance data of the nuclear data.

*e-mail: go_chiba@eng.hokudai.ac.jp

2 Brief description of numerical methods and tools

2.1 Sensitivity calculations and uncertainty quantification

The relative sensitivity of the nuclide number density N to nuclear data i, σ_i, is defined as

$$s_i = \frac{dN}{d\sigma_i} \cdot \frac{\sigma_i}{N}. \tag{1}$$

Since quite a large number of nuclear data, such as neutron-induced reaction cross sections, fission yields, decay constants and decay branching ratios, are used in nuclear fuel depletion calculations, numerical differentiation to obtain these sensitivities to all of the relevant nuclear data is unrealistic. DPT is a powerful method to efficiently calculate sensitivities of N with respect to nuclear data during nuclear fuel depletion. The fundamental theory of DPT has been established in many years ago[2, 3], and it has been recently adopted to the fuel depletion problems of the light water fuel assembly containing burnable absorbers[4]. The details of DPT are omitted here, and interested readers are recommended to refer the literatures listed at the end of this paper.

Nuclear data-induced uncertainties of N can be easily quantified by the well-known sandwich rule as

$$\Delta N/N = \sqrt{\sum_i \sum_{i'} s_i s_{i'} \mathrm{cov}(\sigma_i, \sigma_{i'})}, \tag{2}$$

where $\mathrm{cov}(\sigma_i, \sigma_{i'})$ is a relative covariance between σ_i and $\sigma_{i'}$. When we define a sensitivity vector $\mathbf{s}$ as $\mathbf{s} = (s_1 \ \ s_2 \ \ \cdots \ \ s_I)^T$, where T is for vector transposition, $\Delta N/N$ can be rewritten using $\mathbf{s}$ and $\mathbf{V}_\sigma$, which is a covariance matrix covering all the nuclear data considered, as

$$\Delta N/N = \sqrt{\mathbf{s}^T \mathbf{V}_\sigma \mathbf{s}}. \quad (3)$$

2.2 Reactor physics code system CBZ

Numerical calculations of the nuclide number density sensitivities with DPT are generally based on numerical methods for nuclear fuel depletion calculations, which consist of neutron flux distribution calculations by solving the neutron transport equation and nuclides transmutation calculations. In the present study, all these calculations were carried out with a reactor physics code system CBZ[5] which has been developed at Hokkaido University.

At each fuel burnup point, medium-wise 107-group cross section data were generated, and neutron transport calculations with the 107-group cross sections including generalized adjoint neutron flux calculations for DPT were performed with a neutron transport calculation module of CBZ based on the method of characteristics, and reaction rates were calculated for all the nuclear fuel media. Energy structure of the 107-group is that of the SRAC code developed for thermal reactor analyses. Note that angular integration of bilinear functions of neutron flux and generalized adjoint neutron flux in DPT should be carefully carried out in a system containing strong neutron absorbers[4]. Scattering anisotropy was taken into account by the P0 transport approximation.

Nuclides transmutation calculations were carried out with the simplified nuclide chain model consisting of 21 actinoids and 138 fission products (FP). Nuclides transmutation equations including adjoint problems in DPT were solved by the matrix exponential method with the minimax polynomial approximation method[6]. To reduce the time-discretization error, the predictor-corrector method was employed. Only for the normal (or forward) nuclides transmutation calculations, the advanced optimally-weighted predictor-corrector method[7] was used with the coarse burnup mesh of 2.0 GWD/t.

All these calculations were carried out with the JENDL library: JENDL-4.0[8] for neutron-induced reaction cross sections, JENDL/FPY-2011 and JENDL/FPD-2011[9] for fission yield data and decay data of FP. Calculated sensitivities were then used to quantify nuclear data-induced uncertainties of nuclide number densities. The present work focuses on the number densities of actinoids and Gd isotopes, uncertainties of reaction cross sections of actinoids and Gd isotopes were taken into account. In JENDL-4.0, covariance data are evaluated for almost all the important actinides, and those were taken into account in the present study. However, JENDL-4.0 provides no covariance data for reaction cross sections of gadolinium isotopes, and thus we used the covariance data for these nuclear data taken from ENDF/B-VIII.0[10].

3 Problem specification

Sensitivities of nuclide number densities with respect to nuclear data during nuclear fuel depletion were calculated for a 3×3 multicell model which had been used in our previous study[11]. In this model, a Gd-bearing fuel rod whose Gd enrichment is 5.0 wt% is located at the center position and it is surrounded by normal uranium fuel rods whose uranium-235 enrichment is 3.9 wt%. Geometrical and material specifications are taken from a BWR fuel assembly model developed through the OECD/NEA burnup credit benchmark phase-IIIC[12]. Reflective boundary conditions were adopted. As for coolant condition, void fraction of 0% was assumed. The geometrical specification of the 3×3 multicell model is shown in **Fig. 1**.

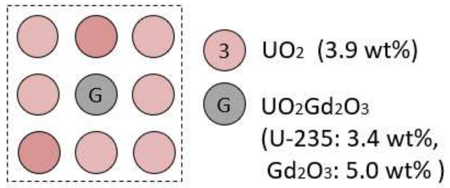

Figure 1. Geometric specification of a 3×3 multicell problem

The infinite neutron multiplication factor during fuel depletion of this 3×3 multicell model is shown in **Fig. 2**. The reactivity peak is observed at around 13 GWD/t. Volume-integrated number densities of U-235, Pu-239, Gd-155, and Gd-157 of the Gd-bearing rod are shown in **Fig. 3**. The Pu-239 build up and the burnout of Gd-155 and -157 can be found. The fuel burnup values corresponding to the burnout of Gd-155 and -157 are approximately 18 and 12 GWD/t, respectively.

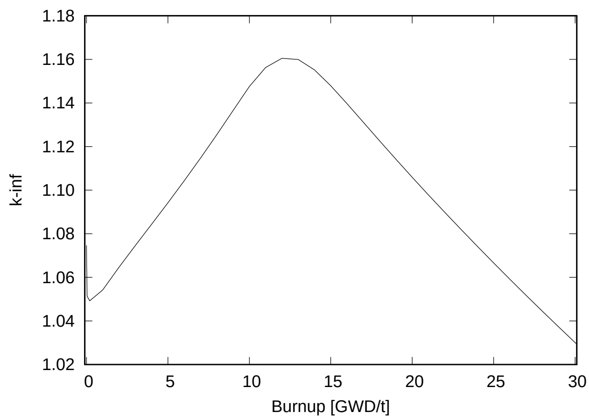

Figure 2. Infinite neutron multiplication factor during fuel depletion

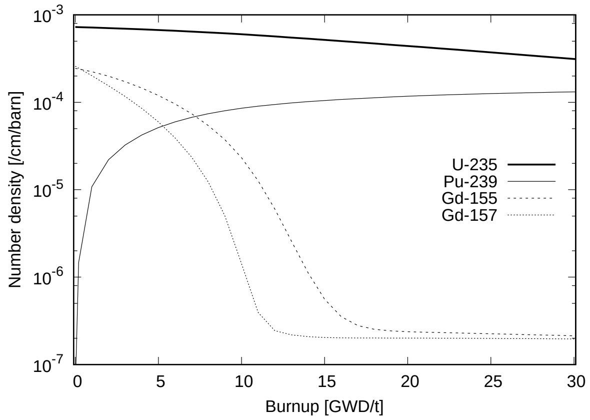

Figure 3. Volume-averaged nuclide number densities in the Gd-bearing rod

4 Numerical results

4.1 Verification of depletion perturbation theory against Gd-bearing fuel rod

The sensitivity calculation capability of CBZ based on DPT has been carefully verified in our previous works[4, 13]. In these works, however, sensitivities of the number densities of nuclides contained in the Gd-bearing fuel rods have never been addressed. In the present work, sensitivities of the nuclide number densities in the Gd-bearing rod at the fuel burnup of 10 GWD/t were calculated with DPT, and those were compared with the reference sensitivities calculated by the direct numerical differencing; the small perturbation of 1% was given to the infinite dilution cross section of specific nuclide, reaction, and energy group, and the change in the nuclide number density was observed. In the calculations with DPT, three different fuel burnup mesh schemes were adopted. **Figure 4** shows sensitivities of U-235 number density to Gd-157 (n,γ) cross section. Sensitivities calculated with the coarse burnup mesh differ from the references, but the good agreement is obtained when the fine burnup mesh of 0.5 GWD/t was adopted. Next, **Figure 5** shows sensitivities of Pu-239 number density to Gd-155 (n,γ) cross section. Better agreements are obtained when finer burnup mesh is adopted similar as Figure 4, but the non-negligible differences are still observed in the resonance energy range. This comes from the implicit effect which is not taken into account in CBZ. The same comparisons were made under the infinite dilution condition where no self-shielding effect was considered during the depletion. **Figure 6** shows sensitivities of Pu-239 number density to Gd-155 (n,γ) cross section under the infinite dilution condition, and the difference observed in the resonance range disappears. From the above comparisons, it is found that the DPT capability of CBZ works properly for the number densities of nuclides in Gd-bearing rods, and that the implicit effect is observed in those to Gd-155 (n,γ) cross sections. Since the contribution of the resonance range to the total capture reaction rate is limited in the Gd-155 (n,γ) reaction, conclusion of our work shown in the following would be unchanged if the implicit effect is properly taken into account.

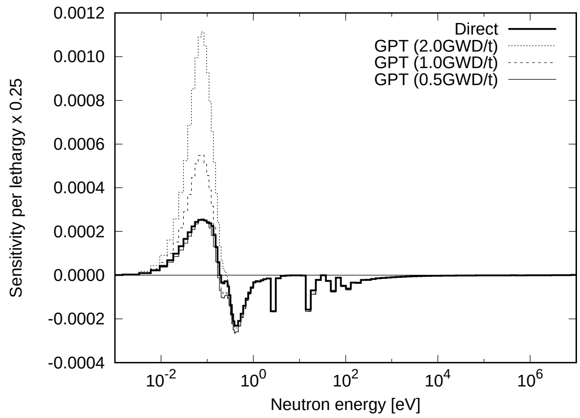

Figure 4. Sensitivities of U-235 number density to Gd-157 (n,γ) cross section

4.2 Uncertainty quantification calculation

Using the sensitivities calculated with the DPT capability of CBZ and the covariance data of the nuclear data, uncertainties of the nuclide number densities can be quantified. **Figures 7** and **8** show nuclear data-induced uncertainties of U-235 and Pu-239 number densities during the depletion. In addition to the uncertainties coming from the all nuclear data considered, those from the Gd-155 and -157 covariance data are presented also in these figures. Relative uncertainties of the nuclide number densities due to the Gd-155 and -157 nuclear data uncertainties are small, and their contributions are negligible in the total uncertainties. The same trends were observed in the uncertainties of number densities of other actinoids, Pu, Am, and Cm isotopes, and the maximum relative uncertainties of 1% were observed in some Am and Cm isotopes around the beginning of the fuel depletion. Correlations in the number densities between the Gd-bearing rod and the non Gd-bearing

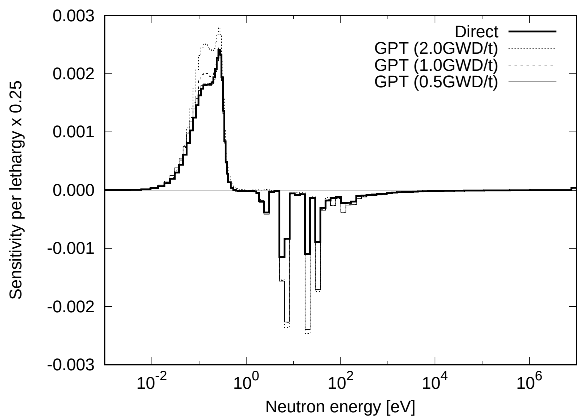

Figure 5. Sensitivities of Pu-239 number density to Gd-155 (n,γ) cross section

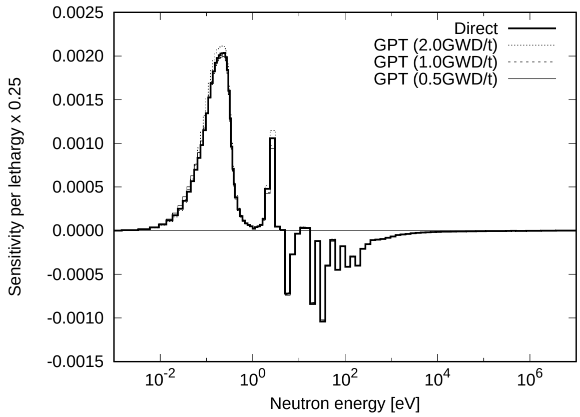

Figure 6. Sensitivities of Pu-239 number density to Gd-155 (n,γ) cross section (infinite dilution condition)

rod, which is neighboring to the central Gd-bearing rod, were also calculated. **Figure 9** shows a correlation matrix of Am-241 number density, and strong positive correlations can be found. The same trends were observed in correlation matrices of number densities of the other nuclides. The above results suggest that the nuclide transmutation process in Gd-bearing fuel rods before and after the Gd burnout are very similar to that in normal fuel rods when the JENDL-5 and ENDF/B-VIII.0 covariance data are used.

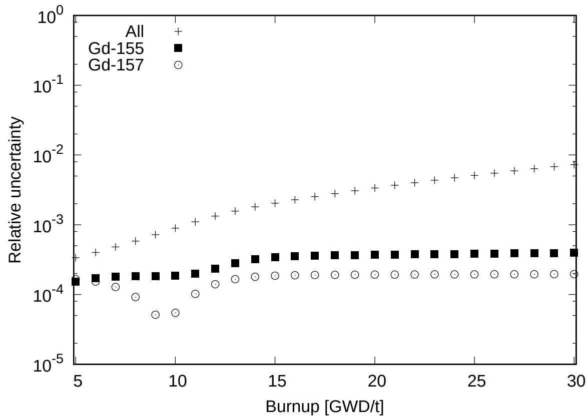

Figure 7. Nuclear data-induced uncertainty in U-235 number density during burnup

Figures 10 and **11** show nuclear data-induced uncertainties of Gd-155 and -157 number densities during the depletion. In these figures, contributions of the nuclear data of the parent nuclide, Gd-154 for Gd-155 and Gd-156 for Gd-157, are presented. Before the Gd burnout, the principal contributor is the concerned Gd isotope itself, but after the burnout, the contribution of the parent nuclide becomes also significant. The nuclear data-induced uncertainties of the number densities of Gd-155 and -157 after the burnout are 6% and 13%, respectively. The PIE data of Gd-bearing rods before and after the Gd burnout would be useful to validate the nuclear data of the Gd isotopes.

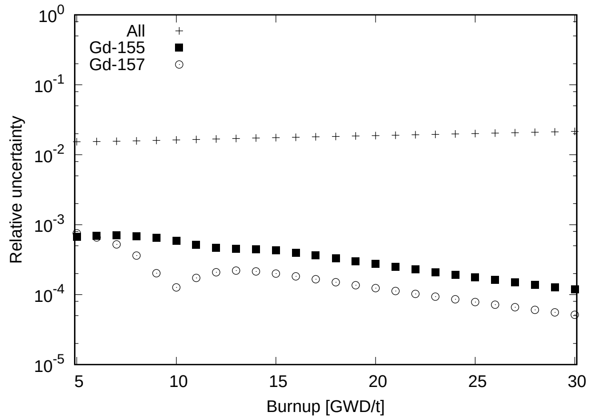

Figure 8. Nuclear data-induced uncertainty in Pu-239 number density during burnup

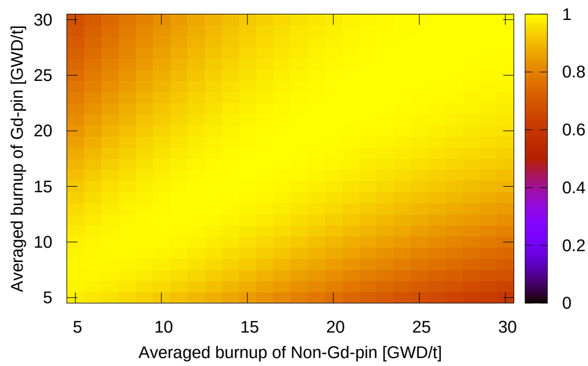

Figure 9. Correlation matrix of Am-241 number density uncertainty between the Gd-bearing and non Gd-bearing rods

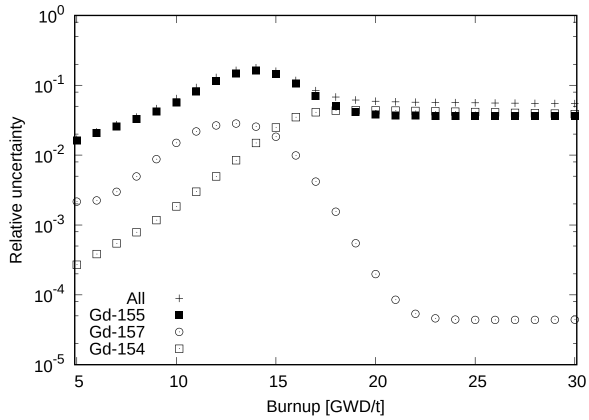

Figure 10. Nuclear data-induced uncertainty in Gd-155 number density during burnup

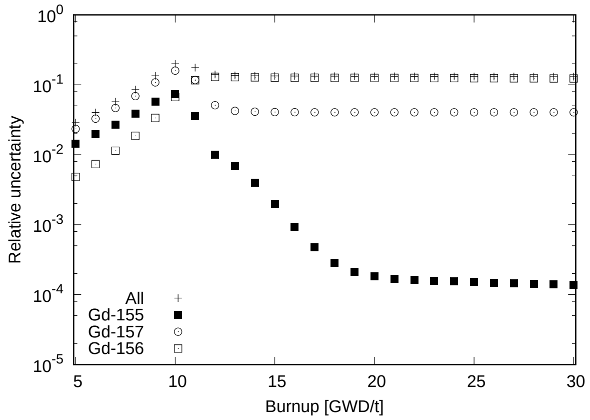

Figure 11. Nuclear data-induced uncertainty in Gd-157 number density during burnup

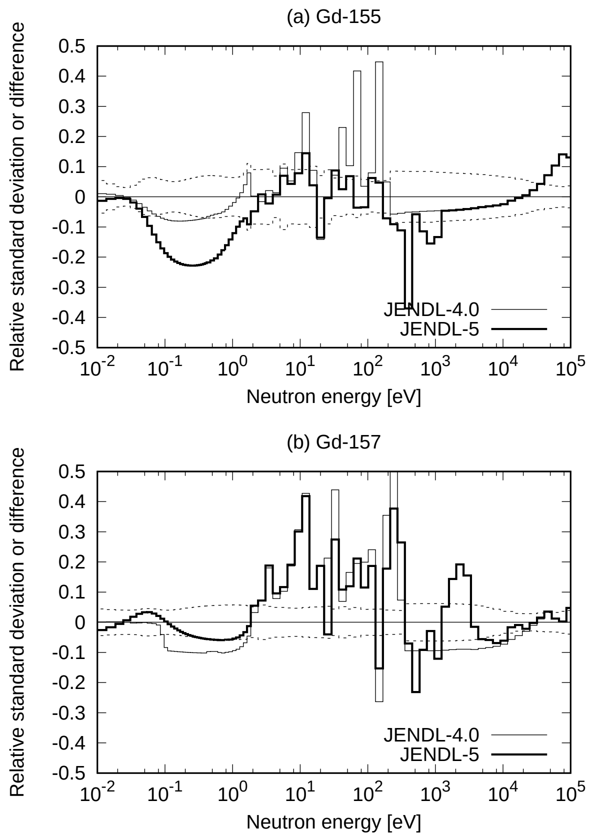

Figure 12. Relative difference in group-wise (n,γ) cross section of Gd-155 and -157 from the ENDF/B-VIII.0 evaluation

It would be useful to observe the covariance data of the Gd-155 and -157 (n,γ) cross sections and to compare them with the differences of these nuclear data among the different evaluations. **Figure 12** shows relative difference in group-wise (n,γ) cross sections of Gd-155 and -157 from the ENDF/B-VIII.0 evaluation. In these figures, dotted lines represent relative standard deviations given in the ENDF/B-VIII.0 evaluation. It is interesting to point out that the difference in the Gd-155 (n,γ) cross section between ENDF/B-VIII.0 and JENDL-5 is significantly large in comparison with the covariance data in ENDF/B-VIII.0.

5 Conclusion

In order to observe and quantify the difference in the nuclide transmutation process between Gd-bearing and non Gd-bearing fuel rods, sensitivities of nuclide number densities of Gd-bearing and non Gd-bearing rods were calculated with DPT, and by using them nuclear data-induced uncertainties of these number densities were quantified. Numerical results suggested that the nuclide transmutation process in Gd-bearing fuel rods before and after the Gd burnout are very similar to that in normal fuel rods. After the Gd burnout, the relative standard deviations of Gd-155 and -157 number densities were estimated at approximately 6% and 13%, respectively, and it was found that the nuclear data of the parent nuclides of these Gd isotopes, Gd-154 and -156, are also important as well as those of Gd-155 and -157.

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