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Uncertainty Quantification of Nuclear Reactor Decay Heat

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1. Introduction

The decay heat of fission products is important for safety analyses of nuclear power plants and nuclear waste disposal. It is significant to predict decay heat accurately and to quantify its uncertainty. These attempts contribute to make safety margin rational and then to improve the reliability of design. The objective of this study is to quantify decay heat uncertainty resulting from nuclear data.

The uncertainty quantification of decay heat has been conducted till now [1]. The latest research [2] used updated evaluated decay data which offer enough data used for the summation calculation. It eliminated the most of simplifications or assumptions of the decay heat data. This study improves the result by eliminating approximation in the calculation and calculates decay heat uncertainty in the case of fission pulse and finite irradiation experiment as a step to quantify and evaluate practical cases of decay heat uncertainty quantification.

2. Theory

The decay heat at time t, $DH(t)$, is calculated by integrating the nuclide-wise decay heat by a following equation:

$$DH(t) = \sum_{i=1} \lambda_i N_i(t) E_i, \tag{1}$$

where λ_i is decay constant, N_i is number density, and E_i is mean decay energy of nuclide i. E_i consists of three components: alpha, beta, and gamma energy. We can obtain number densities by solving a following burn-up equation:

$$\frac{d\boldsymbol{N}(t)}{dt} = \boldsymbol{A}(t)\boldsymbol{N}(t), \tag{2}$$

where $\boldsymbol{A}$ and $\boldsymbol{N}$ are a burn-up matrix and a nuclide number density vector respectively. Equation (2) is solved by a new numerical solution of the matrix exponential, a Mini-Max Polynomial Approximation (MMPA) method [3].

The sensitivity coefficients of decay heat *DH(t)* to four nuclear data components: decay energy, independent fission yield, half-life, and branching ratio, are given by

(1) Decay energy

$$S_{E_i}^{DH} = \frac{\partial DH}{\partial E_i} \cdot \frac{E_i}{DH} = \frac{E_i \lambda_i n_i}{DH} \tag{3}$$

(2) Independent fission yield

$$\begin{aligned} S_{y_i}^{DH} &= \frac{\partial DH}{\partial y_i} \cdot \frac{y_i}{DH} \\ &= \left(\frac{E_i \lambda_i \int_0^P \boldsymbol{N}^* \Delta \boldsymbol{A} \boldsymbol{N} dt}{\Delta y_i} \right) \frac{y_i}{DH} \end{aligned} \tag{4}$$

where y_i is a independent fission yield. $\boldsymbol{N}^*$ is an adjoint number density vector. P is end time of burn-up.

(3) Half-life

$$\begin{aligned} S_{\lambda_i}^{DH} &= \frac{\partial DH}{\partial \lambda_i} \cdot \frac{\lambda_i}{DH} \\ &= \frac{E_i \lambda_i n_i}{DH} + \left(\frac{E_i \lambda_i \int_0^P \boldsymbol{N}^* \Delta \boldsymbol{A} \boldsymbol{N} dt}{\Delta \lambda_i} \right) \frac{\lambda_i}{DH} \end{aligned} \tag{5}$$

(4) Branching ratio

$$\begin{aligned} S_{BR_j}^{DH} &= \frac{\partial DH}{\partial BR_j} \cdot \frac{BR_j}{DH} = \\ &= \left(\frac{E_i \lambda_i \int_0^P \boldsymbol{N}^* \Delta \boldsymbol{A} \boldsymbol{N} dt}{\Delta BR_j} \right) \frac{BR_j}{DH} \end{aligned} \tag{6}$$

where BR_j is branching ratio of each branch point.

Here, these sensitivities are obtained by burnup sensitivity calculation based on the general perturbation theory [4].

The uncertainty of decay heat v is derived through the following error propagation equation:

$$v = \boldsymbol{G}^T \boldsymbol{M} \boldsymbol{G} \tag{7}$$

where $\boldsymbol{G}$ is sensitivity coefficient vector and $\boldsymbol{M}$ is relative covariance matrix of nuclear data.

3. Results

The uncertainty quantifications are conducted in the case of fission pulse and finite irradiation experiments. Regarding the fission pulse experiment, U-233, U-235, U-238, Np-237, Pu-239, and Pu-241 are selected as irradiated nuclides. Thermal and fast neutrons are considered for each case. For the finite irradiation experiment, U-235 and Pu-239 thermal neutron fissions are calculated between 10 and 10^5 seconds. The cooling time after irradiation is from 10^{-1} to 10^5 seconds. We use three different yield and decay data from three evaluated nuclear data libraries: JENDL/FPD-2011 and FPY-2011, which we call JENDL-2011 on the paper, ENDF/B-VII.1, and JEFF-3.1.1.

The calculated uncertainties of pulse fission decay heat on JENDL-2011 are shown in Figs.1 and 2 for U-235 and Pu-239. These figures also show four components of uncertainty: decay energy, fission yield, half-life, and branching ratio. Around 10^{-1} to 10^{0} seconds after pulse fission, the uncertainty is about 10% and gradually decreases along the cooling time.

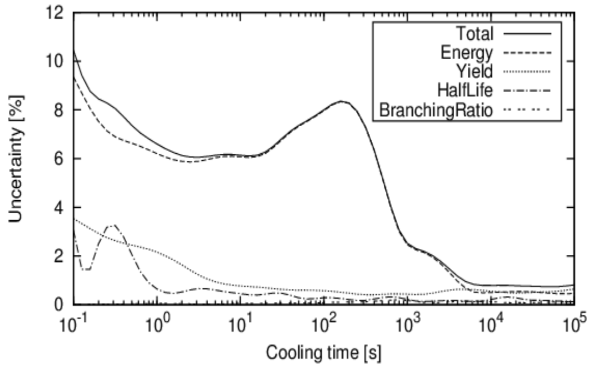

Fig. 1. Decay heat uncertainty of U-235 thermal neutron pulse fission using the JENDL.

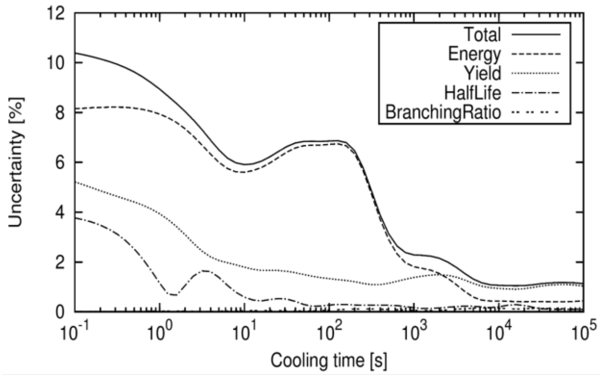

Fig. 2. Decay heat uncertainty of Pu-239 thermal neutron pulse fission using the JENDL.

Figures 3 and 4 show the calculated uncertainties using the JENDL-2011 after 10^3 and 10^5 seconds finite irradiation. It indicates that longer finite irradiation makes the uncertainty of decay heat smaller compared to the case of fission pulse. In a practical situation such as fuel pin in a light water reactor, the uncertainty of decay heat is around 3% around 10^{-1} seconds of cooling time [5].

Then, numerical results of decay heat with uncertainty are compared with experimental data. Those data due to the fast system were taken at Yayoi [6,7,8] experimental reactor at the University of Tokyo. Thermal system data were taken by or at Lowell [9], Oak Ridge National Laboratory [10,11] (ORNL), Tobias [12], and Uppsala [13].

Figure 5 shows the comparison in the case of gamma decay heat of thermal pulse fission on U-235. Almost all data are within the uncertainty through the cooling time.

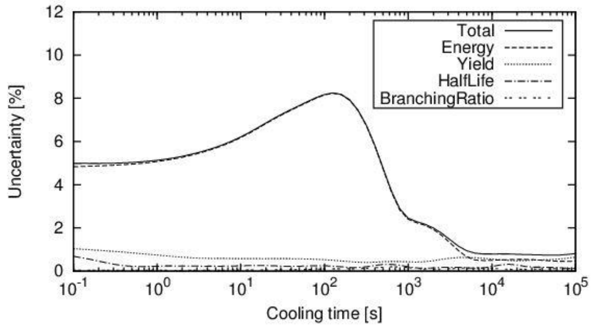

Fig. 3. Decay heat uncertainty of U-235 after 10^3 seconds finite irradiation of thermal neutron using the JENDL.

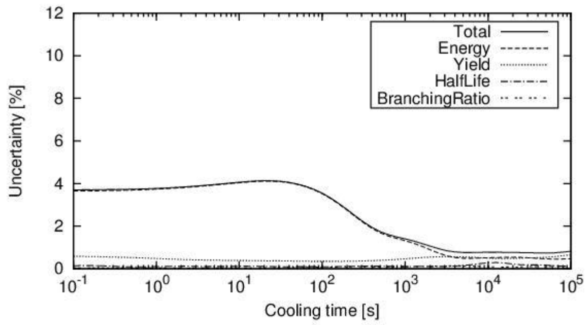

Fig. 4. Decay heat uncertainty of U-235 after 10^5 seconds finite irradiation of thermal neutron using the JENDL.

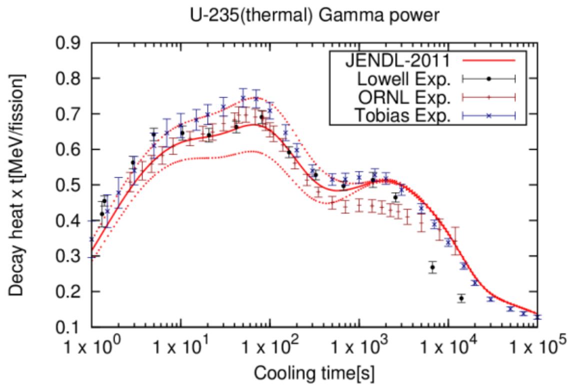

Fig. 5. Gamma decay heat power by a thermal pulse fission on U-235.

For quantitative comparison, we calculate χ^2 by a following equation.

$$\chi^2 = (\boldsymbol{C}-\boldsymbol{E})^t(\boldsymbol{V}_e+\boldsymbol{V}_m)^{-1}(\boldsymbol{C}-\boldsymbol{E}) \qquad (8)$$

where $\boldsymbol{C}$ and $\boldsymbol{E}$ are calculated results vector and experimental data vector respectively. $\boldsymbol{V}_e$ and $\boldsymbol{V}_m$ are variance-covariance matrix for experimental data and calculated results. Here, the correlation coefficient of $\boldsymbol{V}_e$ is set 0.7 because small errors in each experimental data can be assumed that there is correlation between each plot to some extent.

Table I and II show χ^2 values over degree of freedom n in the case of fission pulse and finite irradiation experiments.

Table I. χ^2/n of Tobias Finite irradiation Experiments

Nuclide	Energy	Exp.*	Irradiation time	χ^2/n Nuclear Data JENDL	JEFF	ENDF
U-235	Thermal	Tobias	1.0E+01	8.13	4.84	6.92
			1.0E+02	10.42	5.93	9.08
			1.0E+03	11.64	8.46	10.54
			1.0E+04	9.42	6.09	8.44
			1.0E+05	7.67	4.98	7.36
Pu-239	Thermal	Tobias	1.0E+01	1.64	1.14	1.50
			1.0E+02	2.26	4.17	2.23
			1.0E+03	2.95	6.63	3.13
			1.0E+04	3.43	8.59	3.87
			1.0E+05	4.37	10.20	4.83

Table II. χ^2/n of Fission Pulse Experiments

Nuclide	Energy	Exp.*	χ^2/n Nuclear Data JENDL	JEFF	ENDF
U-233	Fast	Yayoi(b)	0.44	0.42	0.43
		Yayoi(g)	0.19	0.30	0.11
		Yayoi(t)	0.38	0.36	0.30
U-235	Thermal	Lowell(b)	0.58	0.61	0.50
		Lowell(g)	7.87	7.97	6.75
		ORNL(b)	0.32	0.32	0.36
		ORNL(g)	1.64	1.08	1.60
		ORNL(t)	0.51	0.38	0.54
		Tobias(b)	0.18	0.18	0.13
		Tobias(g)	0.57	0.68	0.34
		Tobias(t)	0.76	0.54	0.52
	Fast	Yayoi(b)	0.29	0.26	0.27
		Yayoi(g)	0.30	0.35	0.16
		Yayoi(t)	0.28	0.20	0.14
U-238	Thermal	Lowell(b)	0.51	0.57	0.66
		Lowell(g)	11.10	7.46	4.92
	Fast	Yayoi(b)	0.65	0.64	0.62
		Yayoi(g)	0.48	0.38	0.31
		Yayoi(t)	0.54	0.42	0.45
Pu-239	Thermal	Lowell(b)	1.60	1.42	1.01
		Lowell(g)	7.29	7.88	5.20
		ORNL(b)	0.10	0.09	0.35
		ORNL(g)	0.09	0.44	0.06
		ORNL(t)	0.18	0.36	0.15
		Tobias(b)	0.26	0.21	0.26
		Tobias(g)	0.23	0.65	0.19

Pu-239	Fast	Yayoi(b)	0.31	0.33	0.28
		Yayoi(g)	0.19	0.50	0.18
		Yayoi(t)	0.28	0.42	0.24
Pu-241	Thermal	ORNL(b)	0.38	0.35	0.39
		ORNL(g)	0.20	0.46	0.18
		ORNL(t)	0.38	0.36	0.31

*b,g,t mean beta, gamma, total respectively.

Since the values are less than about 1.4 for the most cases in the fission pulse, numerical results match well with experiment. Some experimental data such as the gamma power of Lowell show higher value. They are caused by large discrepancy around 1×10^4 seconds cooling time. Few number of experimental data is also affect higher χ^2/n value. In the case of finite irradiation, there are not negligible gaps between experimental data and numerical results. In addition to uncertainty of numerical results are low, finite irradiation experimental data are quite different in the specific time region, for example around 1×10^5 seconds cooling time in the case of 1×10^5 seconds irradiation has large discrepancy. Hence it leads to the high value of χ^2/n. Since there is only one finite irradiation experimental data with many experimental data, Tobias, we need more data for the accurate discussion.

6. Conclusions

The uncertainties of fission products' decay heat have been quantified in the case of fission pulse and finite irradiation experiments. These analyses have been carried out by the decay data and fission yield data from the latest JENDL, JEFF, and ENDF files. Decay energy is dominant component of uncertainty and finite irradiation can reduce the uncertainty. From the value of χ^2, calculation results can be considered accurate for fission pulse experiments.

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