Review of the Impact on the Heating Rate Calculation ascribed to the Lack of Gamma Production Data in the MCNP Cross-section Library

Jae Kyeong Lim*, Yong IL Kim, Keon Young Bae
Safety Analysis Department, NSSS Division, KEPCO Engineering & Construction Company, Inc.,
269, Hyeoksin-ro, Gimcheon-si, Gyeongsangbuk-do, 39660
*Corresponding author: jklim0820@kepco-enc.com

*Keywords: MCNP, (n, γ) reaction, ENDF/B, heating rate, AIC Control Rod

1. Introduction

The i-SMR NPP design adopts soluble boron-free operational strategy and uses Ag-In-Cd(AIC) alloy as the regulating bank for reactivity control during normal operation. Heat is generated by the interaction of fission neutrons and gamma rays with materials. The calculated heating rate data are used as design input for core thermal-hydraulic analysis.

During the calculation of the heating rate of AIC control rods using the MCNP [1] code and the ENDF/B-VII library, an error described as "lack of gamma production data" was encountered for key constituent nuclides of AIC control rods, Cadmium and Indium. According to Ref. [4], such errors may occur for certain nuclides in the MCNP ENDF/B-VII library. This study was conducted to investigate the impact of the "lack of gamma production data" error on heating rate calculations.

This study constructed a simplified MCNP test model to confirm that, for nuclides dominated by (n,γ) reactions, the lack of gamma production data leads to an overestimation of the heating rate. In addition, the cause of the overestimation in heating rate was identified based on the calculation equations in MCNP code used for heating rate evaluation and the characteristics of nuclides undergoing (n,γ) reactions. Finally, in the i-SMR design, the heating rates of AIC control rods were compared using nuclear data libraries with and without gamma production errors, and a more reliable heating rate was presented based on the results.

2. Methods and Results

To investigate the impact of the "lack of gamma production data" error on heating rate calculations using MCNP, a simplified MCNP test model was simulated as shown in Fig. 1.

2.1 Description of the Test Model

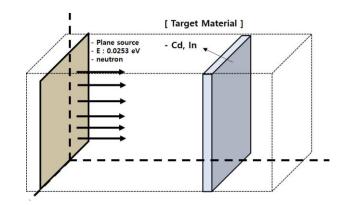


Fig. 1. Simplified MCNP test model to verify (n, γ) reaction

Fig. 1 shows a simplified model in which particles are transported in a mono-direction from a plane thermal neutron source with an energy of 0.0253 eV. Target material with a thickness of 1 cm, composed of either Cadmium or Indium, was placed at a certain distance from the neutron source. Neutron and photon transport calculations were performed to enable gamma-ray production from target materials with high (n,γ) cross sections. The incident neutron source strength was specified as 10^{18} neutrons. The ENDF/B-VII.1 library was used for the nuclear data, and the plane flux was obtained using the f2 tally to measure both neutron and photon fluxes. The results are summarized in the following Tables 1 and 2.

2.2 Result of Test Model

Table 1. Flux and Heating rate of Target Material (Cd) using ENDF/B-VII.1

	Neutron Flux (in)	Neutron Flux (out)	Photon Flux (in)	Photon Flux (out)	Heating rate by neutron (W/cm ³)	Heating rate by photon (W/cm ³)
¹⁰⁶ Cd	6.03x10 ¹⁵	4.79x10 ¹⁵	9.58x10 ¹⁴	9.09x10 ¹⁴	0.01	87.31
¹⁰⁸ Cd	5.78x10 ¹⁵	4.84x10 ¹⁵	0	0	280.41	0
¹¹⁰ Cd	5.45x10 ¹⁵	2.80x10 ¹⁵	0	0	2399.85	0
¹¹¹ Cd	5.75x10 ¹⁵	3.42x10 ¹⁵	6.80x10 ¹⁵	6.01x10 ¹⁵	0.03	544.62
¹¹² Cd	5.96x10 ¹⁵	4.47x10 ¹⁵	0	0	582.70	0
¹¹³ Cd	5.00x10 ¹⁵	0	0	0	7236.34	0
¹¹⁴ Cd	6.24x10 ¹⁵	5.00x10 ¹⁵	0	0	81.27	0
¹¹⁶ Cd	6.11x10 ¹⁵	5.08x10 ¹⁵	0	0	18.47	0

Since Cadmium and Indium have high (n,γ) cross-sections, photon flux should be produced when neutrons are incident on the target.

However, as shown in Table 1, in the case of Cadmium, photon flux is not observed in most of Cadmium isotopes (108 Cd, 110 Cd, 112 Cd, 113 Cd, 114 Cd, 116 Cd) except for a few specific isotopes. In particular, since no photon flux was generated even in 113 Cd, which has a very high (n, γ) cross section, the impact of the "lack of gamma production data" error mentioned in the introduction can be clearly confirmed. As a result, the heating rate due to photons was evaluated as zero, and the entire heating was attributed to neutrons.

Table 2. Flux and Heating rate of Target Material(In) using ENDF/B-VII.1

		Neutron Flux (in)	Neutron Flux (out)	Photon Flux (in)	Photon Flux (out)	Heating rate by neutron (W/cm³)	Heating rate by photon (W/cm³)
	¹¹³ In	5.36x10 ¹⁵	3.00x10 ¹⁵	0	0	2296.30	0
Ī	¹¹⁵ In	5.02x10 ¹⁵	1.96x10 ¹²	0	0	5416.10	0

As shown in Table 2, no photon flux was generated for any of the Indium isotopes. Consequently, as in the case of Cadmium, the contribution of heating rate by photons was neglected, and all heating was attributed to neutrons.

2.3 Analysis of the Impact of the Lack of Gamma Production Data Error on Heating Rate Calculations

If gamma production reactions are neglected for nuclides in which (n,γ) absorption reactions are dominant, the evaluation of heating rate is overestimated due to the phenomenon described in Section 2.2. This phenomenon can be explained based on the equation used in the MCNP code for calculating the heating tally with the f6 tally [1].

Heating tally(f6) =
$$\frac{f4 \ tally \ (\#/cm^2) \times \sum_{t} (cm^{-1}) \times Heating \ number(\frac{MeV}{Collision})}{Density \ (g/cm^3)}$$
(1)

In the MCNP code, the heating tally is calculated using Eq. (1). The heating numbers by neutron used in the heating tally are shown in Eq. (2) [2].

$$H(E)_{neutron} = E - \sum_{i} p_i(E) [E_{i,out}(E) - Q_i + E_{i,\gamma}(E)],$$
(2)

where

- $p_i(E): \frac{\sigma_i(E)}{\sigma_t(E)} =$ probability of reaction i at neutron incident energy E
- $E_{i,out}(E) =$ average exiting neutron energy for reaction i at neutron incident energy E

- $Q_i = Q$ value of reaction i
- $E_{i,\gamma}(E) =$

average exiting gamma energy for reaction i at neturon incident energy E

By dividing the incident neutron energies into two groups(thermal, fast), the cause of heating rate overestimation for nuclides dominated by (n,γ) reactions is analyzed through a simplification of Eq. (2).

(i) Fast neutron

In the case of fast neutron incidence, scattering reactions become dominant. Thus, Q_i and $E_{i,\gamma}$ are approximately zero. However, due to the relatively small scattering cross-section, E can be approximated as E_{out} . As a result, H(E) is small enough to be neglected.

(ii) Thermal neutron

In the case of thermal neutron incidence, (n, γ) reactions become dominant. Since neutron absorption reactions occur, E_{out} becomes zero. In addition, the energy of the incident neutron is so small that it can be neglected.

Therefore, based on (i) and (ii), the neutron heating number for (n,γ) dominant reactions nuclides (Eq. (2)) can be simplified as shown in Eq. (3).

$$H(E)_{neutron} \approx Q_{n,\nu} - E_{n,\nu}(E)$$
 (3)

When an (n,γ) reaction occurs, gamma rays transport most of the Q-value energy released by the reaction. Gamma rays lose their energy through interactions such as the photoelectric effect, compton scattering, and pair production. The energy lost through these processes is absorbed by the target material. However, due to the high penetrability of gamma rays, some of them escape the target material without being fully absorbed. This can be calculated through the photon heating tally, based on the heating number that accounts for photon transport as described in Eq. (4) [2]. In actual condition, part of the Q-value energy generated from (n,γ) reaction is deposited as heat in the material. The remaining unabsorbed photons, instead, escape from the material.

$$H(E)_{photon} = E - \sum_{i=1}^{3} p_i(E)[E_{i,out}(E)],$$
 (4)

where

- i = 1: inconherent (Compton) *scattering with form factors*
- i = 2: pair production; $E_{i,out}(E) = 2m_0c^2 = 1.022016 \, MeV$
- i = 3: photoelectric absorption; $E_{i,out}(E) = 0$
- $p_i(E) = probability of reaction i at gamma incident energy E$

• $E_{i,out}(E) =$ average exiting gamma energy for reaction i at neturon incident energy E

When there is no gamma production in the target material, the entire Q-value is assumed to be deposited in the material as heat. As a result, heating tallies only by neutrons lead to an overestimation of the total heating rate due to the reasons described above.

2.4 Comparison of Heating Rates in the AIC Control Rod Dependent on Nuclear Data Library

The MCNP calculation model used to evaluate the heating rate of the AIC control rod is shown in Fig. 2 below. The heating rate was calculated for the condition in which all AIC control rods are inserted during normal operation of the i-SMR. Based on a fixed source problem, the heating rate was calculated by separately evaluating the contributions from prompt and delayed particles and summing their values [5].

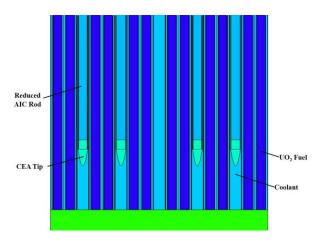


Fig. 2. Calculation Model of Heating Rate in i-SMR (Vertical View).

Based on this calculation model, the heating rates were compared for the main materials of the AIC control rods (Ag, In, Cd) using nuclear data libraries both with and without the "lack of gamma production data" error. The nuclear data for the AIC alloy were taken from ENDF/B-VII.1, ENDF/B-VII.0, ENDF/B-VI, and mixed nuclear data libraries [3]. The mixed nuclear data libraries refer to a combination of nuclear data sets selected to ensure that gamma production reactions are not neglected, particularly for Silver(Ag), Indium and Cadmium. Silver(Ag) data were taken from ENDF/B-VII.1, Indium from ENDF/B-VI and Cadmium from ENDL92, respectively. In Figure 3, the heating rate calculation results for each library are compared.

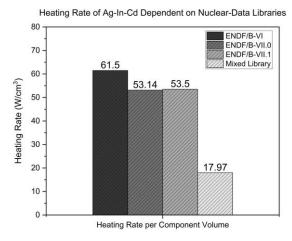


Fig. 3. Comparison of AIC Alloy Heating Rate Dependent on Nuclear Data Library.

In the ENDF/B-VI library, gamma production reactions are neglected for Silver(Ag) and Cadmium. In the ENDF/B-VII.0 and ENDF/B-VII.1 libraries, gamma production reactions are neglected for Indium and Cadmium. As a result, due to the reasons mentioned in Section 2.3, the total heating rates are overestimated.

When a mixed library is used, gamma production reactions are considered for all isotopes of the target material. Consequently, the heating rate evaluated with mixed nuclear data libraries is approximately 3.4 and 3 times lower than those evaluated using ENDF/B-VI and ENDF/B-VII, respectively. This is because the gamma rays generated in the AIC control rods interact with electrons during gamma transport, and the remaining gamma rays escape from the target material. As a result, the heating rate calculated with the mixed nuclear data libraries is significantly lower than with other nuclear data libraries which occur "lack of gamma production data" error.

In actual conditions, when (n,γ) reactions occur, neutrons are absorbed by the nuclides and gamma rays are produced. Some of these gamma rays interact with electrons, while others escape the material. Thus, the results calculated with the mixed nuclear data libraries are regarded as the most reliable.

3. Conclusions

In the MCNP code, if the "lack of gamma production data" error occurs for nuclides dominated by (n,γ) reactions in certain nuclear data libraries, gamma production and transport are ignored, which can lead to an overestimation of the heating rate calculation. Furthermore, considering the high penetration ability of gamma rays, the thinner the target material in which the heating rate is to be calculated, the greater the expected degree of overestimation.

While many of these errors were corrected in the update from ENDF/B-VI to ENDF/B-VII, a few nuclides still don't have gamma production data. To ensure accurate heating rate calculations for nuclides dominated by (n,γ) reactions, it is important to check for the presence of gamma production data and select proper nuclear data libraries that explicitly include gamma production.

REFERENCES

- [1] Los Alamos National Laboratory, "MCNP user's Manual Code version 6.2," LA-UR-17-29981, 2017.
- [2] Los Alamos National Laboratory, "MCNP 5.1.40 RISCC Release Notes," LA-UR-05-8617, 2005.
- [3] Los Alamos National Laboratory, "Listing of Available ACE Data Tables," LA-UR-17-20709, 2017.
- [4] Los Alamos National Laboratory, "New Ace-Formatted Neutron and Proton Libraries Based on ENDF/B-VII.0," LA-UR-08-1999, 2017.
- [5] Y.I Kim, "Evaluation of Heating Rates for CEA, ICI and NSA for KSNP," Proceeding of the Korean Nuclear Society Spring Meeting, Korea, 2002.