Uncertainty quantification of decay heat in spent nuclear fuel by STREAM/RAST-K with stochastic sampling

Jaerim Jang, Bamidele Ebiwonjumi, Chidong Kong, Yunki Jo, Wonkyeong Kim, Jinsu Park and Deokjung Lee*

Department of Nuclear Engineering, Ulsan National Institute of Science and Technology, 50 UNIST-gil, Ulsan, 44919, Republic of Korea *Corresponding author. Email: <u>deokjung@unist.ac.kr</u>

1. Introduction

This paper deals with uncertainty quantification (UQ) of developed decay heat calculation module. Presented calculation module is developed with in-house two-step codes, a lattice code STREAM and a nodal diffusion code RAST-K. In previous work, this method has been validated with 58 decay heat samples discharged from five different pressurized water reactors (Ringhals-2, Ringhlas-3, Turkey Point-3, Point Beach-2, and San Onofre-1) and relative errors are within $\pm 4.3 \%$ [1].

Uncertainty quantification is essential for licensing

analysis and to determine design margin of developed code system. Decay heat result is affected by many kinds of parameters: for instance, neutronic data (number density data, cross section data, and covariance data), operating condition (moderator temperature, power density, and fuel temperature) and design parameters (UO₂ density, UO₂ enrichment, and pellet radius). To investigate behavior of those parameters in decay heat uncertainty, various kinds of uncertainty quantification studies are performed with Turkey Point-3 Fuel assembly (FA).

2. Methods

The code system is developed in previous work [1] and adapted in in-house two step code system. STREAM is a transport code [2]. Stochastic sampling method is used for uncertainty calculation with Stamm'ler's equivalance two-step method. STREAM perturbs the neutronic data based on reference [3]. ENDF/B-VII.0 covariance data and ENDF/B-VII.1 covariance data are used for sensitivity study [4]. ENDF/B-VII.0 decay library is used for calculation. The calculation progress is performed as follows three steps: 1) evaluate covariance by NJOY, 2) perturbed cross section libraries (72 group), 3) generate neutronic data (cross section data and number density file) as 2 group for nodal diffusion code system.

RAST-K is nodal diffusion code and Lagrange nonlinear interpolation is adapted to predict isotope inventory with three history indices (moderator temperature, fuel temperature, and boron concentration) [1]. Figure 1 shows the flow chart of uncertainty calculation progress. A total of 500 cross section libraries and a total of 500 number density files are used for calculation. The number of 500 comes from previous decay heat uncertainty calculation [5].



3. Specification of fuel assembly

This section details the fuel assembly used in this sensitivity study and describes design uncertainty.

Figure 2 shows the layout of fuel assembly. The sample name is B-43 discharged from Turkey Point-3. Operating conditions are set according to reference [6].

Table 1 contains the specification of fuel assembly (FA). Table 2 presents the design uncertainties and those values are used for sensitivity study to investigate the uncertainty behavior follows each design parameters. There are six values are selected and details are described in reference [5]. One σ of Table 2 is used for stochastic sampling to generate perturbed modeling parameters. In this study, it assumes that the parameters have independent relationship with other parameters. While this progress, sampling progress uses the random values followed the normal distribution. Section 4 contains the histogram and shows whether this sampling progress produces decay heat results according to normal distribution or not.



 Table 1 Specification of FA

Plant	FA type	Enrichment (w/o)	Burnup [GWd/MTU]	Cooling Time [years]
Turkey Point-3	15x15	2.6	25.6	4.88

 Table 2 Uncertainty of modeling parameters

Parameter		1σ	unit
Fuel	Enrichment	0.0167	wt%
design	UO ₂ density	0.0417	g/cm3
parameter	Pellet radius	0.025	cm
Operating data	Specific power	1.67	%
	Coolant density	3.33	%
	Fuel temperature	3 33	0/2

4. Results

This section presents the results of sensitivity study. Five different sensitivity studies are performed: 1) neutronics data (ENDF/B-VII.0 covariance data and ENDF/B-VII.1 covariance data), 2) effect of number density files, 3) effect of cross section libraries, 4) manufacturing data (UO₂ density, UO₂ enrichment, and pellet radius), and 5) operating condition (moderator temperature, power density, fuel temperature).

4.1. Decay heat sensitivity study with different covariance data set

This section details the results of sensitivity study with different covariance data. Two of covariance data set are used for calculation: ENDF/B-VII.0 and ENDF/B-VII.1 covariance data set. Table 5 presents the calculation specification of sensitivity study. A total of 500 cross section data and a total of 500 number density files are used for calculation. Table 6 contains the summary of calculation result compared with measurement [6]. The calculation model has about -3% relative errors in both cases and ENDF/B-VII.1 case has larger uncertainty (standard deviation of decay heat calculation result distribution) than ENDF/B-VII.0 case.

 Table 3 Calculation specification with different covariance data

Parameter	Value		
Discharge burnup	25.6 GWd/MTU		
Cooling time	4.88 years		
Decay heat library	ENDF/B-VII.0		
Number of parturbed data set	500 (XS file)		
Number of perturbed data set	+ 500 (ND file)		
Perturbed parameter	Cross section		
CASE: ENDF/B-VII.0 covariance			
Cross section library	ENDF/B-VII.0		
Covariance data	ENDF/B-VII.0		
Number of Perturbed isotopes	25		
CASE: ENDF/B-VII.1 covariance			
Cross section library	ENDF/B-VII.1		
Covariance data	ENDF/B-VII.1		
Number of Perturbed isotopes	185		

Table 4	Uncertainty	depending	on covariance	data

Case	Relative errors [%]	Uncertainty [W]
ENDF/B-VII.0	-3.148	0.006
ENDF/B-VII.1	-3.219	4.000

4.2. Decay heat sensitivity study as a function of cooling period

Table 5 summarizes the calculation specification with cooling time. A total of 500 cross section (XS) data set for nodal calculation and a total of 500 number density (ND) file set for prediction of isotope inventory are used for calculation. Figure 3 and Figure 4 shows the contribution of decay heat and uncertainty as a function of cooling time. Uncertainty is defined as one standard deviation of calculation result set. The discharge burnup is 25.6 GWd/MTU as described in Table 1. The contribution of ²⁴¹Am, ^{137m}Ba, and ⁹⁰Y are dominant in total decay heat. The isotope of ²⁴¹Am and ²³⁸Pu are dominant at total decay heat uncertainty in B43 sample.

Parameter	Value
Discharge burnup	25.6 GWd/MTU
Cooling range	0-100 years
Data point interval	10 years
Decay heat library	ENDF/B-VII.0
Cross section library	ENDF/B-VII.1
Covariance data	ENDF/B-VII.1
Number of Perturbed isotopes	185
Number of parturbad data gat	500 (XS file)
Number of perturbed data set	+ 500 (ND file)
Perturbed parameter	Cross section

Table 5 Calculation specification with cooling time





4.3. Sensitivity study of design parameters

Table 6 presents the calculation specification of design parameter and Table 7 shows the perturbed parameter of each calculation case. Figure 5, Figure 6, and Figure 7 present the behavior of manufacturing parameters and operating condition in total uncertainty. One σ of Table 2 is used for generation of a total of 500 inputs. Figure 5 presents the distribution of decay heat to recognize whether the distribution satisfies the normal distribution or not. Shapiro-Wilk test is used and Figure 5 shows that the distribution is within the criterion of normal distribution (p-value is more than 0.05). The test case is mixed case as shown in Figure 6. Mixed case means case that uses perturbed three parameters (moderator temperature, power density, and fuel temperature). Figure 6 shows the uncertainty contribution of moderator temperature case and mix case are larger than power density case. The isotope of

²⁴¹Am, ²⁴⁴Cm, and ²³⁸Pu are dominant in perturbed operating condition cases. Figure 7 presents the uncertainty contribution by manufacturing parameters. Three parameters are compared: UO₂ density, UO₂ enrichment, and pellet radius. Pellet radius is most sensitive parameter compared with other two parameters. The isotope of ¹³⁷mBa and ⁹⁰Y are dominant in case of UO₂ density and pellet radius. Isotope of ²⁴⁴Cm and ⁹⁰Y are dominant in case of UO₂ enrichment.

Table 6 Calculation specification of design parameter

Parameter	Value	
Discharge burnup	25.6 GWd/MTU	
Decay heat library	ENDF/B-VII.0	
Cross section library	ENDF/B-VII.1	
Number of perturbed	500	
data set	(per each parameter)	

 Table 7 Perturbed parameter of each case

Case	Perturbed parameter		
Moderator temperature	Moderator temperature		
Power density	Power density		
	Moderator temperature,		
Mix	Power density, Fuel		
	temperature		
Density	UO ₂ density		
Enrichment	UO ₂ enrichment		
Radius	Pellet radius		



Figure 5 Histogram of decay heat of B43 discharged from Turkey Point-3



Figure 6 Isotope decay heat uncertainty with operating parameters



4.4. Sensitivity studies with B43 of Turkey Point-3

Figure 8 and Table 8 summarize the uncertainty contribution according to each parameter: 1) ENDF/B-VII.0 case uses ENDF/B-VII.0 covariance data, 2) ENDF/B-VII.1 case is calculated with ENDF/B-VII.1 covariance data, 3) number density (ND) case means only uses perturbed number density files to calculate decay heat, 4) cross section (XS) case means only uses perturbed cross section libraries, 5) density uses perturbed UO₂ density, 6) enrichment employs perturbed UO₂ enrichment, 7) pellet radius uses perturbed pellet radius, 8) TMO case is calculated with perturbed moderator temperature condition, 9) power uses perturbed power density, and 10) mix employs perturbed three operating conditions (moderator temperature, fuel temperature and power density). In case of ND and XS, ENDF/B-VII.1 covariance data is used. ENDF/B-VII.1, ND and pellet radius are dominant parameters to affect decay heat uncertainty.



Figure 8 Decay heat uncertainty of parameters

Tuble o cheertainty depending on parameters			
Parameter	Uncertainty [W]	Parameter	Uncertainty [W]
ENDF/B- VII.0	0.00628	Enrichment	0.28
ENDF/B- VII.1	4.00	Pellet radius	3.28
ND	3.45	ТМО	0.15
XS	1.68	Power	0.13
Density	1.29	MIX	0.30

Table 8 Uncertainty depending on parameters

5. Conclusion

This paper evaluates the decay heat uncertainty caused by ten parameters: 1) ENDF/B-VII.0 covariance data, 2) ENDF/B-VII.1 covariance data, 3) number density files, 4) cross section libraries, 5) UO₂ density, 6) UO₂ enrichment, 7) pellet radius, 8) moderator temperature, 9) power density, and 10) Mix (total effect of operating condition). The calculation model is Turkey Point-3 fuel assembly (B-43). The sensitivity studies recognize the dominant parameters are ENDF/B-VII.1 (0.66 % uncertainty of total decay heat), ND (0.56 %) and pellet radius (0.54 %).

In case of contribution of decay heat and uncertainty as a function of cooling time, contribution of ²⁴¹Am, ^{137m}Ba, and ⁹⁰Y are dominant in decay heat. The isotope of ²⁴¹Am and ²³⁸Pu are dominant at decay heat uncertainty.

Furthermore, the uncertainty sensitivity study will be performed with other nuclear fuel assemblies that were calculated in previous study: fuel assemblies discharged from Ringhals-2, Ringhals-3, Point Beach-2, and San Onofre-1.

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