



Original Article

Validation of spent nuclear fuel decay heat calculation by a two-step method



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ABSTRACT

In this paper, we validate the decay heat calculation capability via a two-step method to analyze spent nuclear fuel (SNF) discharged from pressurized water reactors (PWRs). The calculation method is implemented with a lattice code STREAM and a nodal diffusion code RAST-K. One of the features of this method is the direct consideration of three-dimensional (3D) core simulation conditions with the advantage of a short simulation time. Other features include the prediction of the isotope inventory by Lagrange non-linear interpolation and the use of power history correction factors. The validation is performed with 58 decay heat measurements of 48 fuel assemblies (FAs) discharged from five PWRs operated in Sweden and the United States. These realistic benchmarks cover the discharge burnup range up to 51 GWd/MTU, 23.2 years of cooling time, and spanning an initial uranium enrichment range of 2.100–4.005 wt percent. The SNF analysis capability of STREAM is also employed in the code-to-code comparison. Compared to the measurements, the validation results of the FA calculation with RAST-K are within $\pm 4\%$, and the pin-wise results are within $\pm 4.3\%$. This paper successfully demonstrates that the developed decay heat calculation method can perform SNF back-end cycle analyses.

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1. Introduction

The management of spent nuclear fuel (SNF) is one of the most important issues in South Korea because of the saturation problem of spent fuel pools (SFPs). According to reports, 66–81% storage capacity of the SFP is currently occupied, and Kori nuclear power plant units 1–4 SFP will be fully saturated by 2024 [1,2]. There are two methods to slow down the saturation of SFP. One is to increase the number of high burnup fuel assemblies (FAs) during the design process of commercial reactors because FAs with high discharge burnups can be stored in denser racks. The second is to use dry storage casks. To ensure the safety of management and transportation of SNFs, inventory calculation is important to predict the radiation source terms and its consequences: activity and decay heat, and neutron and gamma intensities.

Various SNF analysis codes have been developed in companies and laboratories globally, including South Korea. In this study, we developed a source term calculation method that maximizes the advantages of the existing codes: STREAM and RAST-K. A strength of STREAM [3] is its high accuracy, which has been validated with

decay heat measurements in previous studies [4,5]. Furthermore, the relative errors are within $\pm 5\%$. However, STREAM performs two-dimensional (2D) depletion calculations using power history information from RAST-K. For the case of a commercial reactor with 121 FAs and 24 axial nodes per FA (i.e., 2904 calculation nodes per cycle), 43,560 min (i.e., about 30 days) are needed to deplete all the nodes in the core using 3D-core operating conditions. This assumes that approximately 15 min are required to deplete each axial node. The developed SNF analysis capability is implemented to reduce the computational time; for the commercial reactor previously mentioned, it would take 1.6 h without cooling time and one day considering cooling. To consider three-dimensional (3D) core operating conditions, the SNF analysis capability is developed and implemented in a nodal code RAST-K. RAST-K accounts for only 36 isotopes that are important for core operation. SNF analysis uses the Lagrange non-linear interpolation with the number density generated by history branch calculation of the lattice code, STREAM. STREAM considers 1640 isotopes in the depletion chain. Therefore, to exploit the advantages of STREAM/RAST-K, the developed SNF analysis has two main features: high accuracy and computational efficiency.

To assess the accuracy of the SNF analysis code system, 58 decay heat measurements of 48 PWR SNF assemblies are used. The FAs

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Abbreviations

1D	one-dimensional
2D	two-dimensional
3D	three-dimensional
BOR	boron concentration
CMFD	coarse mesh finite difference
CRAM	Chebyshev rational approximation method
EOC	end of cycle
FA	fuel assembly
HEDL:	Hanford Engineering Development Laboratory
ND	number density

PCF	power history correction factor
PSM	point energy slowing-down method
PWR	pressurized water reactor
RK	RAST-K v2.0
SFP	spent fuel pools
SNF	spent nuclear fuel
ST	STREAM
TFU	fuel temperature
TH1D	one-dimensional thermal-hydraulic feedback
TMO	moderator temperature
UNM	unified nodal method
XS	cross section

were irradiated and discharged from five PWRs operated in Sweden and United States. The measurements were performed at the Swedish central interim storage facility for SNF (CLAB) [6–8] and United States Hanford Engineering Development Laboratory (HEDL) [6]. The assembly discharged burnups and initial enrichment range from 19 to 51 GWd/MTU and 2.100 to 4.005 wt percent (w/o) of ^{235}U , respectively.

The remainder of this paper is organized as follows. Section 2 describes the code system for predicting the SNF isotopic inventory for the calculation of source terms by the two-step method STREAM/RAST-K. Section 3 explains the Lagrange non-linear

interpolation method and power history correction factors implemented in our code system. The power history correction factor is used to correct the decay effect generated at different power levels. Section 4 contains the validation results from the analysis of measured data, sensitivity tests, the effect of power history correction factor, and computational time comparison.

2. Description of the code system

This section describes the code system for isotope inventory prediction. The STREAM/RAST-K v2.0 two-step code system is

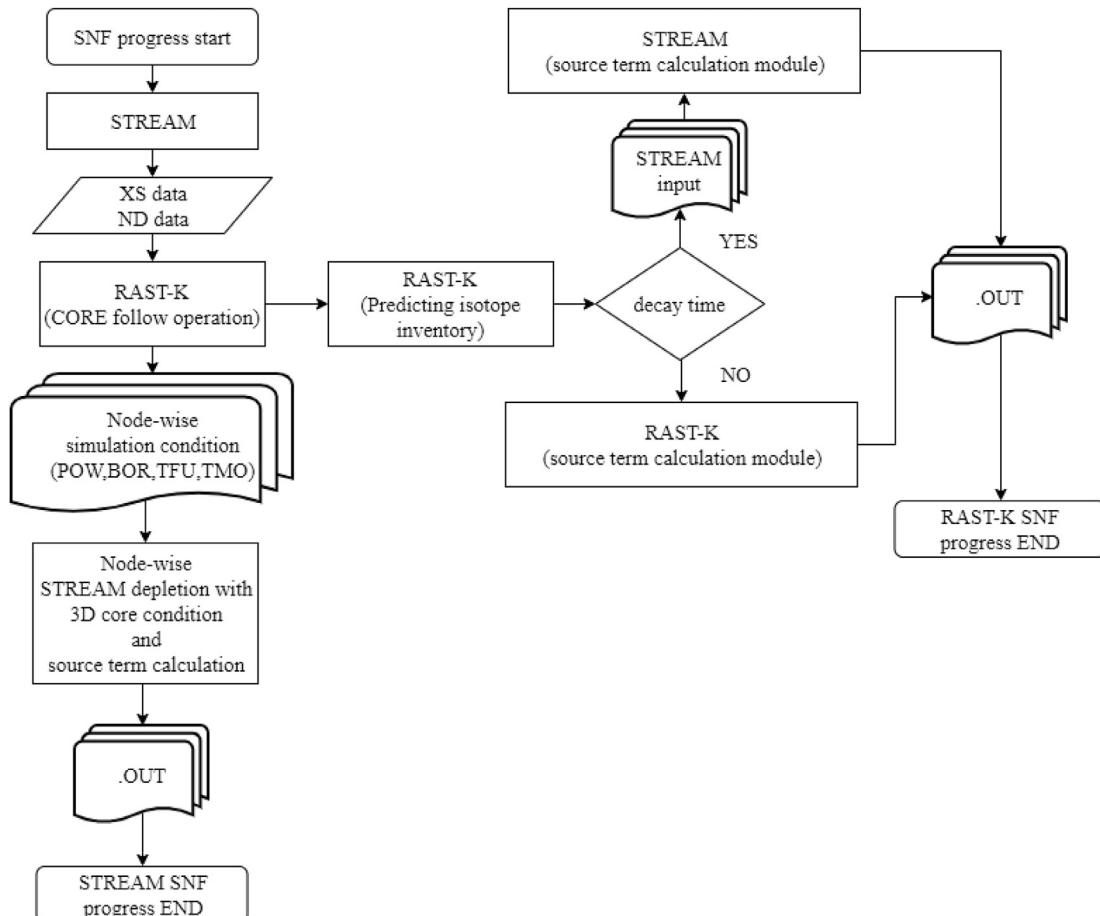


Fig. 1. Flow chart of source term calculation with two-step method.

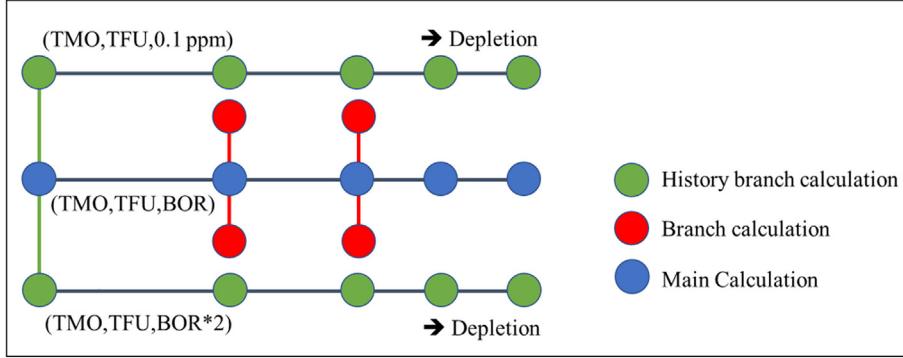


Fig. 2. Description of history branch calculation progress.

Table 1
Description of history branch calculation cases.

INDEX	Moderator temperature	Fuel temperature	Boron concentration
1 ^a	TMO _{ref}	TFU _{ref}	BOR _{ref}
2	TMO _{ref} - 40 K	TFU _{ref}	BOR _{ref}
3	TMO _{ref} - 20 K	TFU _{ref}	BOR _{ref}
4	TMO _{ref} + 20 K	TFU _{ref}	BOR _{ref}
5	TMO _{ref} + 40 K	TFU _{ref}	BOR _{ref}
6	TMO _{ref}	TMO _{ref} - 20 K ^b	BOR _{ref}
7	TMO _{ref}	1500 K	BOR _{ref}
8	TMO _{ref}	TFU _{ref}	0.1 ppm
9	TMO _{ref}	TFU _{ref}	2*BOR _{ref}
10	TMO _{ref}	TFU _{ref}	2400 ppm

^a Reference case.

^b To cover hot zero power condition.

composed of a lattice code STREAM and a nodal code RAST-K v2.0 [9,10].

The lattice code steady state and transient reactor analysis with method of characteristics (STREAM) generates the cross sections and the form functions by two-dimensional (2D) assembly calculation with reflective boundary conditions [3]. The resonance treatment during cross-section generation is based on the pin-based slowing-down method (PSM) [3]. The SNF analysis capability has been added to STREAM and validated with 91 decay heat calorimetric measurements of 52 PWR FAs. The average

calculation-to-experiment decay heat ratio (C/E) of STREAM-SNF is 1.000 ± 0.017 for 71 Swedish decay heat measurement benchmarks and 0.997 ± 0.013 for 20 US measurements [4,5]. Therefore, STREAM is employed for code-to-code comparison [3]. The ENDF/B-VII.0 data library is used for the validation because the STREAM-SNF was validated with this library in previous studies [4,5,11].

RAST-K v2.0 is a nodal code based on the 3D multigroup unified nodal method (UNM) with multigroup coarse mesh finite difference (CMFD) acceleration [9]. RAST-K considers only 36 isotopes (22 actinides, 12 fission products, and 2 burnable poison isotopes) generated by a micro depletion solver [9]. These isotopes have a high sensitivity to power history during the 3D core simulation. In the course of the validation, depletion calculation is performed with one axial node containing four radial nodes. Moreover, the TH1D (one-dimensional thermal-hydraulic feedback) solver in RAST-K is turned off to maintain consistency with the calculation conditions of STREAM-SNF and to consider the fixed temperature conditions given in the benchmark documentations [12–15].

Fig. 1 shows the workflow of the implemented code system. During RAST-K 3D core calculations, three history indices are generated: 1) boron concentration (BOR) history index, 2) fuel temperature (TFU) history index, and 3) moderator temperature (TMO) history index. The definition of history index is in section 3.1. The number densities (NDs) of 1640 isotopes are calculated via the interpolation method using the history indices. The base files of the number density for the interpolation are generated by STREAM

Table 2
Equation of Lagrange interpolation applied to the code system.

Case	Index*	Equation
Moderator temperature	1–5	$ND_{TMO} = \sum_{i=1}^5 \left(\prod_{j=1, j \neq i}^5 \frac{(h_{TMO} - TMO_j)}{(TMO_i - TMO_j)} \right) (ND_i) \quad (4)$
Fuel temperature	1, 6, 7	$ND_{TFU} = \sum_{i=1}^7 \left(\prod_{j=1, j \neq i, (j < 2 \text{ and } i > 5)}^7 \frac{(h_{TFU} - TFU_j)}{(TFU_i - TFU_j)} \right) (ND_i) \quad (5)$
Boron concentration	1, 8–10	$ND_{BOR} = \sum_{i=1}^{10} \left(\prod_{j=1, j \neq i, (j < 2 \text{ and } j > 7)}^{10} \frac{(h_{BOR} - BOR_j)}{(BOR_i - BOR_j)} \right) (ND_i) \quad (6)$
Total	1–10	$\begin{aligned} ND_{calculated} &= ND_1 + \Delta ND_{TMO} + \Delta ND_{TFU} + \Delta ND_{BOR} \\ &= ND_1 + ND_{TMO} - ND_1 + ND_{TFU} - ND_1 + ND_{BOR} - ND_1 \\ &= ND_{TMO} + ND_{TFU} + ND_{BOR} - 2 * ND_1 \end{aligned} \quad (7)$

*Indices are matched with the indices presented in Table 1.

Table 3

Isotope list calculated by RAST-K micro depletion module.

CASE	Isotope
Actinide (22)	^{234}U , ^{235}U , ^{236}U , ^{237}U , ^{238}U , ^{237}Np , ^{238}Np , ^{239}Np , ^{238}Pu , ^{239}Pu , ^{240}Pu , ^{241}Pu , ^{242}Pu , ^{243}Pu , ^{241}Am , ^{242}Am , ^{243}Am , ^{244}Am , ^{242m}Am , ^{242}Cm , ^{243}Cm , ^{244}Cm
Fission product (12)	^{135}I , ^{137}Xe , ^{147}Nd , ^{148}Nd , ^{149}Nd , ^{147}Pm , ^{148}Pm , ^{149}Pm , ^{148m}Pm , ^{147}Sm , ^{148}Sm , ^{149}Sm
Burnable poison (2)	^{152}Gd , ^{160}Gd

Table 4

Specification of measurements.

Reactor	Measurement facility	Assembly Design	Enrichment (w/o ^{235}U)	Burnup [GWd/MTU]	No. of Assemblies measured	No. of Measurements
Ringhals Unit 2	CLAB	15 × 15	3.095–3.252	34–51	16	20
Ringhals Unit 3	CLAB	17 × 17	2.100–3.103	19.7–41.6	14	18
Turkey Point Unit 3	HEDL	15 × 15	2.557	25.6–28.4	4	6
Point Beach Unit 2	GE-Morris	14 × 14	3.865, 3.996, 4.005	31.9–39.4	6	6
San Onofre Unit 1	GE-Morris	14 × 14	3.397	26.5–28.4	8	8

two-dimensional (2D) fuel assembly (FA) history branch calculation with reflective boundary condition. Fig. 2 shows the differences in the history branch calculation and branch calculation. The branch calculation involves the progress of the cross-section generation through the depletion calculation with different conditions (TMO, TFU, BOR, and control rod) to generate broad-group nodal diffusion data (burnup-dependent physics data; cross section, discontinuity factors, diffusion coefficient, and so on) [16]; the details are described in a previous study [9]. The main difference is in the depletion calculation. History branch calculations use the changed

operating conditions at the burnup of 0 MWd/kg (beginning of the depletion progress) and go through the depletion with the same burnup steps as the main calculation steps. Table 1 describes the conditions of each history branch calculation. The state points are taking from previous study [9]. There are nine history branch conditions for the validation with index 1 as the base condition.

After the inventory calculation, the source terms including the decay heat are calculated by the SNF analysis module. The case without cooling uses the RAST-K SNF stand-alone calculation, and the case with the cooling period employs the RAST-K/STREAM

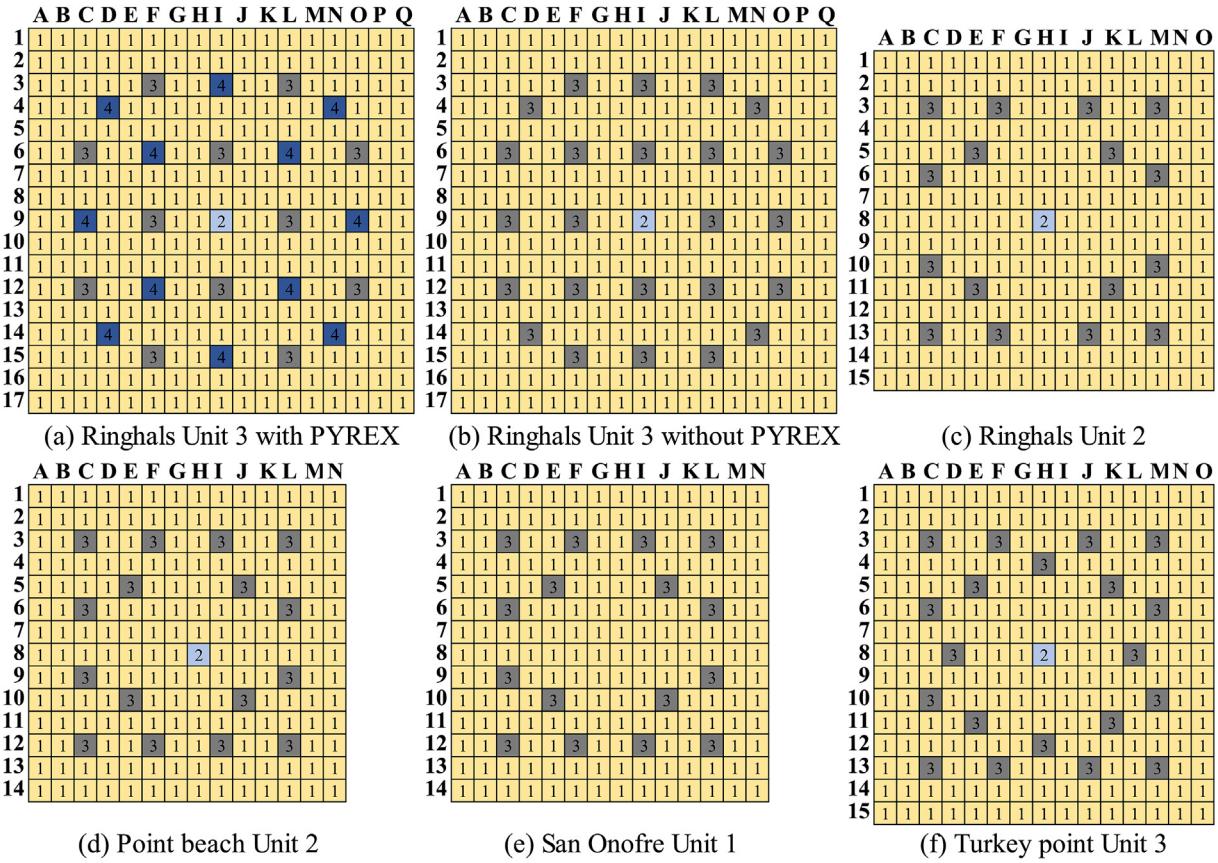


Fig. 3. Radial layouts of measured assemblies.

Table 5
Summary of results.

Reactor	Number of measurements		STREAM-SNF		RAST-K SNF			
			Mean ^{*3}	STD ^{*4}	FA-wise	STD	pin-wise	STD
Ringhals 2	20	C* ¹ /E* ² -1 [%]	0.04	0.95	-0.96	1.31	-0.35	1.56
		C-E [W]	0.27	4.07	-3.95	5.43	-1.40	6.49
Ringhals 3	18	C/E-1 [%]	0.17	1.06	0.25	1.23	0.56	1.23
		C-E [W]	0.87	4.02	0.57	4.62	2.07	4.80
Turkey point Unit 3	6	C/E-1 [%]	0.72	1.04	-1.43	1.40	-0.77	1.76
		C-E [W]	10.99	11.13	-13.35	14.25	-9.83	26.21
Point Beach Unit 2	6	C/E-1 [%]	0.03	0.69	-1.62	0.95	0.78	1.52
		C-E [W]	0.12	6.17	-14.67	8.24	7.83	12.28
San Onofre Unit 1	8	C/E-1 [%]	-0.15	1.00	-0.87	1.04	-0.40	1.06
		C-E [W]	0.52	5.22	-3.64	4.79	-0.02	5.75
Overall	58	C/E-1 [%]	0.13	1.07	-0.69	1.43	0.00	1.59
		C-E [W]	1.58	7.06	-4.59	8.76	-0.05	11.94

^{*1}C is calculation.

^{*2}E is measured data.

^{*3} Mean is the average value of 'C/E-1' or 'C-E'. $Mean = \frac{\sum_{i=1}^N (x_i)}{N}$

^{*4} STD is standard deviation, $STD = \sqrt{\frac{\sum_{i=1}^N (x_i - \bar{x})^2}{N}}$ where, x is value of 'C/E-1' or 'C-E', \bar{x} is mean value, and N is the total number of comparison results.

coupled system. During cooling, STREAM decay input is generated by RAST-K. Although this method seems to be contrary to the main purpose (which is to reduce the computational time), the decay calculation time occupies a small portion of the entire progress. It is therefore negligible. Section 4.6 presents the details of the computation time.

In SNF analysis after core depletion calculation, STREAM-SNF stand-alone calculation can be performed in the following five steps: 1) generation of cross-section by history/branch calculations in STREAM, 2) 3D core simulation with RAST-K, 3) STREAM depletion calculation using history information (BOR, TMO, TFU, and power) from RAST-K, 4) decay of isotope inventory, and 5) decay heat calculation. Therefore, the previous STREAM-SNF method required a longer computation time than the calculation implemented performed here because of the depletion calculation in step 3. In case of the benchmark calculation, steps 1 and 2 are skipped (i.e., STREAM-SNF uses the direct method with on-the-fly method for generation of the cross-section). Therefore, in the benchmark calculation, the total simulation time of STREAM-SNF is shorter than that for RAST-K SNF. The details of this discussion are illustrated in Section 4.6.

3. Calculation method

3.1. Inventory calculation

The progress of isotope inventory prediction involves two parts. One is Lagrange non-linear interpolation for isotope inventory prediction. Second is to correct the decay effect and amount of fission product caused by different power levels. The Lagrange non-linear interpolation method is employed for isotope inventory prediction with history indices [6,17]. History index is the time-dependent average of the parameter and is calculated by Eq. (1).

$$h = \frac{\sum_{i=1}^n x_i \Delta t_i}{\sum_{i=1}^n \Delta t_i} \quad (1)$$

where h is the history index, x is a parameter (BOR, TFU, and TMO), i is the time step index, and Δt_i is the time interval between the i th and (i th-1) step. Power history is not considered to avoid repetition because the TFU and TMO contains the effect of power operating conditions. The number density is calculated using Eq. (2) with history index h .

$$ND(h) = \sum_{i=1}^n L_i(h) * x_i \quad (2)$$

where h is from Eq. (1), i is the index, x is the parameter, ND is the number density, and L_i is the Lagrange coefficient of index i presented in Eq. (3).

$$L_i(x) = \prod_{j \neq i}^n \frac{h - x_j}{x_i - x_j} \quad (3)$$

where i and j are indices, and n is the number of parameters. Table 2 demonstrates the equations of Lagrange non-linear interpolation for each case: moderator temperature condition uses the 4th order Lagrange interpolation, 2nd order for fuel temperature, and 3rd order for boron concentration. The calculation points of TFU and BOR are set to consider the cross-section generation points [9]. Calculation points of TMO are generated to avoid extrapolation and to consider the Chebyshev node to reduce the error caused by harmonic function [17]. The total number density is calculated by a combination of number densities from the three different cases: moderator temperature (ND_{TMO}), fuel temperature (ND_{TFU}), and boron concentration (ND_{BOR}). For the moderator temperature case, five different conditions are used for calculation, and the number density is calculated using Eq. (4). The conditions are contained in the 'index' column of Table 2 that can be matched with those of Table 1. ND_{TFU} and ND_{BOR} are calculated in a similar way as ND_{TMO} using Eq. (5) and Eq. (6), respectively. During the calculation, the effects of boron concentration, fuel temperature, and moderator temperature are assumed to be independent of each other. Therefore, the total number density is calculated by summation of the three different effects on the number density of the reference case (presented in index 1 of Table 1) and calculated number densities

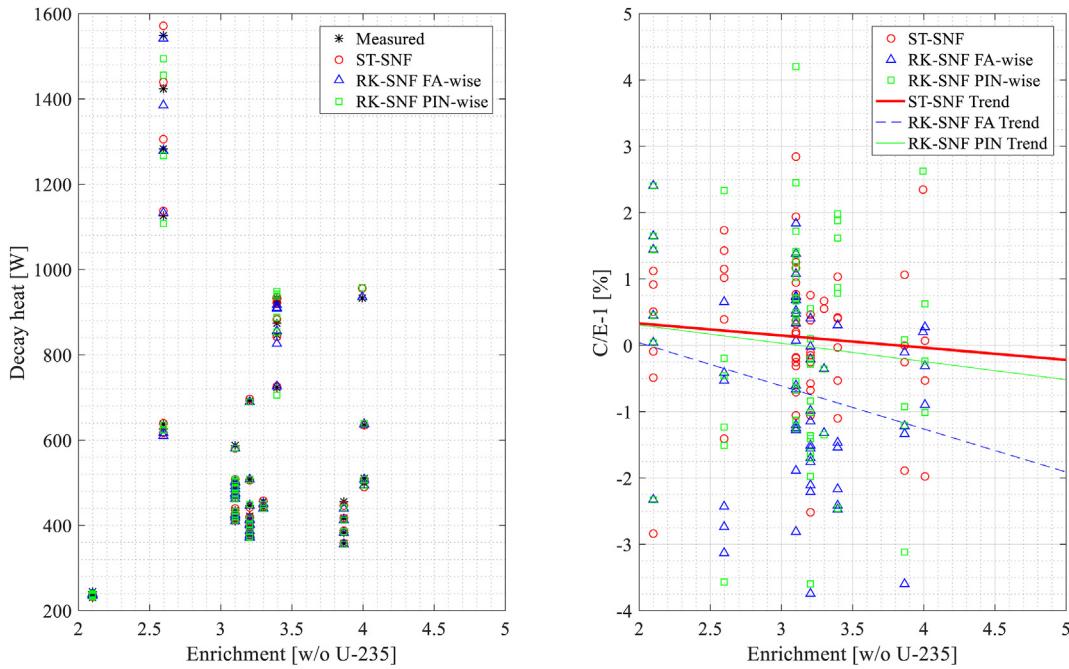


Fig. 4. Decay heat and relative errors as a function of enrichment.

Table 6
Error trend analysis with linear least square method.

Parameter (x)	Method	Trend ¹	R ²
Enrichment	ST	-1.83e-01*x + 0.695	0.00698
	RK FA-wise	-6.49e-01*x + 1.336	0.04905
	RK PIN-wise	-2.74e-01*x + 0.852	0.00705
Discharged burnup	ST	3.88e-03*x - 0.003	0.00052
	RK FA-wise	-3.22e-01*x + 0.385	0.01978
	RK PIN-wise	1.51e-02*x - 0.502	0.00349
Decay time	ST	-3.05e-05*x + 0.285	0.00525
	RK FA-wise	1.45e-04*x - 1.440	0.06549
	RK PIN-wise	1.69e-05*x - 0.089	0.00072

¹ Calculated by method of linear least square [21].

² The more R² approaches 1, the better the fit of the data to the linear equation [22].

(ND_{TMO}, ND_{TFU} and ND_{BOR}). Eq. (7) calculates the total number density at a given burnup step, which is implemented in our code system.

h_{TMO}, h_{TFU}, and h_{BOR} are history indices. i and j are indices. ND_{calculated} is the result of number density. ND₁ is the number density of the reference case. In addition, the power history correction factor (PCF) shown in Eq. (1) of [18–20] is used for calculation to correct the decay effect generated by different power levels. The effect of the PCF is shown in Section 4.5. The number density corrected by PCF is presented in Eq. (8) as implemented in the code.

$$ND_{corrected}^{j,i,k} = ND_{calculated}^{j,i,k} * PCF^{j,i,k} \quad (8)$$

where ND_{corrected}^{j,i,k} is the final solution of number density, ND_{calculated}^{j,i,k} is the number density generated by Eq. (7), and PCF^{j,i,k} is the power correction factor with indices i, j, and k. Index i is the time step, j is the node index, and k is the isotope index. Before our current implementation, RAST-K previously provided the number density of 36 isotopes, as shown in Table 3.

3.2. Decay heat calculation

The decay heat is proportional to the isotope number density, decay constant, and total recoverable energy per decay [5]. The decay heat results of STREAM-SNF have been validated with 91 measurements [11], and RAST-K employs the same decay heat calculation method as STREAM-SNF. The decay heat is calculated by the summation method in Eq. (9) [5],

$$H = \sum N_i \lambda_i Q_i \quad (9)$$

where H is the decay heat, i is the isotope index, N_i is the number of isotope i, λ is the decay constant, and Q is the total recoverable energy per decay [5].

4. Validation of decay heat calculation of spent nuclear fuels

4.1. Description of measured data

This section details the measured decay heat data used to validate the implementation of the equations presented in the previous section. Table 4 illustrates the discharged burnup and enrichment details of the measured assemblies, number of assemblies, number of measurements, the reactors, and measurement laboratories. Additionally, it should be noted that multiple measurements are performed on some of the assemblies, as will be shown at different decay times in the results section. Ringhals-2 and Ringhals-3 PWRs are operated in Sweden, and from these reactors, 38 decay heat measurements on 30 discharged FAs are performed at the Swedish interim storage facility, CLAB [12–14].

In addition, 20 decay heat measurements on 18 FAs discharged from three US PWRs are used for validation. The US assemblies are measured at the Hanford Engineering Development Laboratory (HEDL) and General Electric Morris Operations (GM-Morris). On the US assemblies, please note that Turkey Point and Point Beach assembly spacer grids contain stainless steel, and San Onofre fuel rods use the clad of stainless steel [14]. Fig. 3 shows the radial layout of

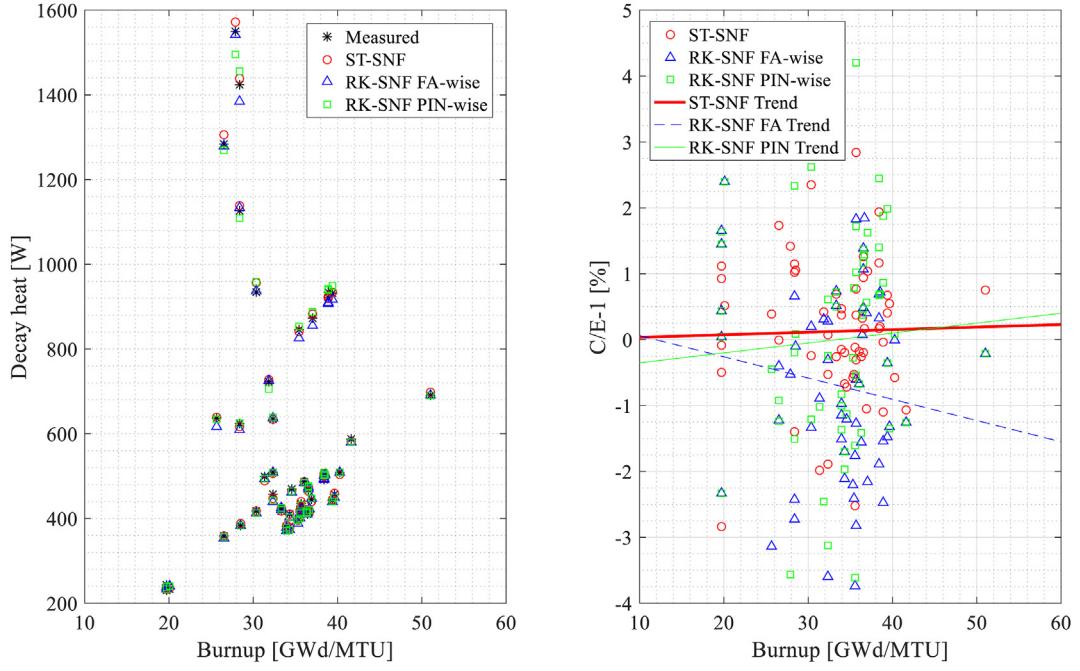


Fig. 5. Decay heat and relative errors as a function of discharged burnup.

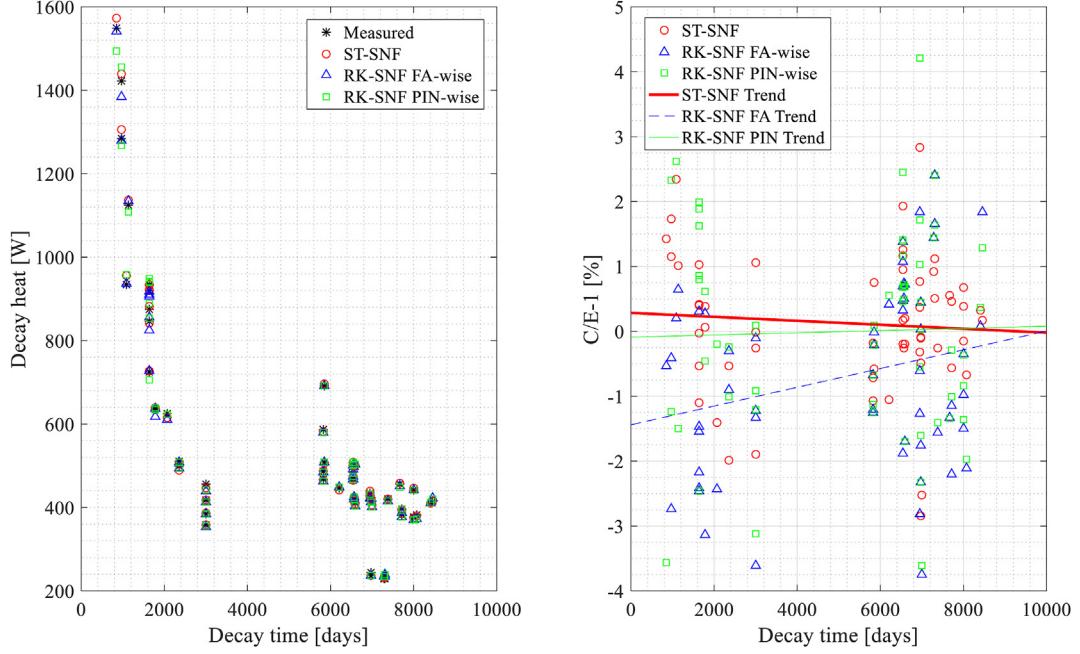


Fig. 6. Decay heat and relative errors as a function of decay time.

the FAs from the reactors. The irradiation history information, fuel rod and assembly specifications, fuel temperature, moderator density/temperature, and boron concentration were obtained from a previous study [14].

4.2. Validations

The analysis of 58 FA decay heat measurements is presented in Table 5. The values of decay heat difference ($C-E$) and relative errors are shown in this table. Moreover, the table contains the results calculated by the STREAM-SNF code and the newly implemented

SNF analysis capability in RAST-K. FA and pin-wise calculation are different in terms of the interpolation scale. The summation of pin-wise decay heat results is used for consistent comparisons with the FA calculation. Overall, the STREAM-SNF calculation has an average relative error of $0.13 \pm 1.07\%$. The newly implemented code RAST-K SNF has an average ($C/E - 1$) of $-0.69 \pm 1.43\%$ from the FA calculation and $0.00 \pm 1.59\%$ from the pin-wise calculation. The error scales of RAST-K SNF are similar to those of STREAM-SNF. In addition, calculated decay heat results of 58 FA samples are presented in Appendix (Table A. 1 and Table A. 2).

The decay heat relative errors are represented in Fig. 4, 5 and 6

Table 7

Decay heat results of Ringhals Unit 2.

Assembly ID	Burnup [GWd/MTU]	Enrichment [w/o ²³⁵ U]	Decay time [days]	C/E – 1 (%)			Measurement $2\sigma^*$
				STREAM-SNF		RAST-K SNF	
				FA	PIN	FA	
C01	36.7	3.095	8468	0.17	1.84	1.28	2.80
C12	36.4	3.095	8403	0.32	0.07	0.36	2.82
C20 ^{a,c}	35.7	3.095	6950	2.84	1.84	4.21	2.80
C20	35.7	3.095	6951	0.37	-0.60	1.71	2.77
C20	35.7	3.095	6952	-0.31	-1.27	1.02	2.76
C20 ^b	35.7	3.095	6959	0.77	-2.82	-0.55	2.74
D27	39.7	3.252	7669	0.55	-1.32	-1.34	2.68
D38	39.4	3.252	8005	0.67	-0.36	-0.36	2.72
E38	34	3.199	7999	-0.16	-1.50	-1.36	2.94
E38	34	3.199	8000	0.38	-0.98	-0.83	2.95
E40	34.3	3.199	8075	-0.68	-2.11	-1.97	2.92
F14	34	3.197	7722	0.47	-1.15	-1.00	2.92
F21	36.3	3.197	7376	-0.25	-1.56	-1.41	2.78
F25	35.3	3.197	7725	-0.57	-2.21	-0.28	2.87
F32	51	3.197	5860	0.75	-0.21	-0.21	2.27
G11 ^{b,c}	35.5	3.188	6990	-2.52	-3.75	-3.60	2.80
G23	35.6	3.206	6984	-0.11	-1.75	-1.61	2.79
I09	40.2	3.203	5849	-0.57	-0.01	0.09	2.56
I24	34.3	3.203	6601	-0.19	-1.69	-1.70	2.82
I25	36.9	3.203	6198	-1.05	0.41	0.56	2.71

*Measurement uncertainty calculated by Eq. (10).

^a is over the 2-sigma in case of STREAM calculation.^b is over the 2-sigma in case of developed code system with FA-wise calculation.^c is over the 2-sigma in case of developed code system with PIN-wise calculation.**Table 8**

Decay heat results of Ringhals Unit 3.

Assembly ID	Burnup [GWd/MTU]	Enrichment [w/o U-235]	Decay time [days]	C/E – 1 (%)			Measurement 2σ
				STREAM-SNF		RAST-K SNF	
				FA-wise	PIN-wise	FA	
0E2	41.6	3.103	5823	-1.06	-1.25	-1.26	-2.41
0E6	36	3.103	5829	-0.18	-0.67	-0.67	-2.61
1C2	33.3	3.101	6559	-0.25	0.51	0.50	-2.80
1E5	34.6	3.103	5818	-0.71	-1.21	-1.13	-2.65
2A5	20.1	2.100	7297	0.51	2.40	2.40	-3.83
2C2	36.6	3.101	6550	-0.19	0.48	0.46	-2.66
3C1	36.6	3.101	6545	0.95	1.07	1.16	-2.65
3C9	36.6	3.101	6552	1.26	1.38	1.37	-2.65
4C4	33.3	3.101	6572	0.69	0.73	0.72	-2.78
5A3	19.7	2.100	6972	-0.49	0.04	0.03	-3.79
5A3	19.7	2.100	6975	-0.09	0.44	0.44	-3.80
5A3	19.7	2.100	6977	-2.85	-2.33	-2.33	-3.74
5A3	19.7	2.100	7291	0.92	1.45	1.45	-3.86
5A3	19.7	2.100	7304	1.12	1.65	1.65	-3.87
0C9*	38.4	3.101	6551	1.93	0.33	2.45	-2.60
1C5*	38.5	3.101	6593	0.20	0.72	0.70	-2.58
3C5*	38.4	3.101	6543	1.17	-1.89	1.41	-2.57
4C7*	38.4	3.101	6549	0.17	0.69	0.67	-2.58

*PYREX pins are in FA (Fig. 3a).

against initial enrichment, discharged burnup, and decay time, separately. These graphs demonstrate that the relative errors are within $\pm 4.3\%$, and it has weak relationship with the parameters. Table 6 presents the error trend analysis results, and the linear trend graphs are represented in Fig. 4. The trend is calculated by the linear least square method [21]. STREAM (ST) and RAST-K v2.0 (RK) pin-wise calculation have a closer trend compared with the RK FA calculation results. As shown in Table 6, the R^2 values of all parameters are far from 1. Therefore, the relationship between the parameters and the relative errors is weak.

4.2.1. Swedish PWR

This section presents the detailed results of Swedish PWRs, Ringhals-2 and Ringhals-3 assemblies, in Table 7 and Table 8, respectively. The decay time is the time between the assembly discharged from the reactor and decay heat measurement. The uncertainty of measurements is obtained from Ref. [14], and the sigma values in Tables 7 and 8 are calculated using Eq. (10)

$$\sigma [\%] = \left((E[W] \pm u^M[W]) / E[W] - 1 \right) * 100 [\%] \quad (10)$$

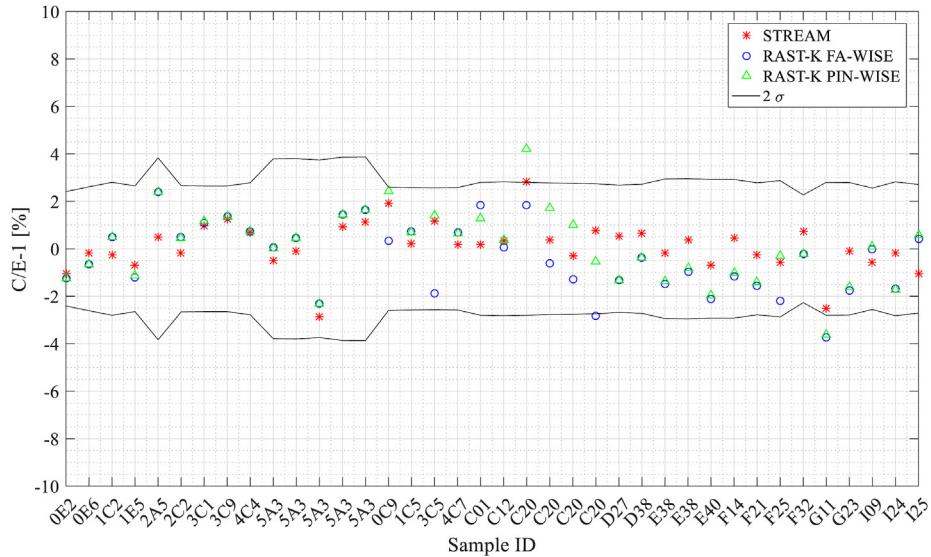


Fig. 7. RAST-K SNF decay heat results for Swedish PWRs.

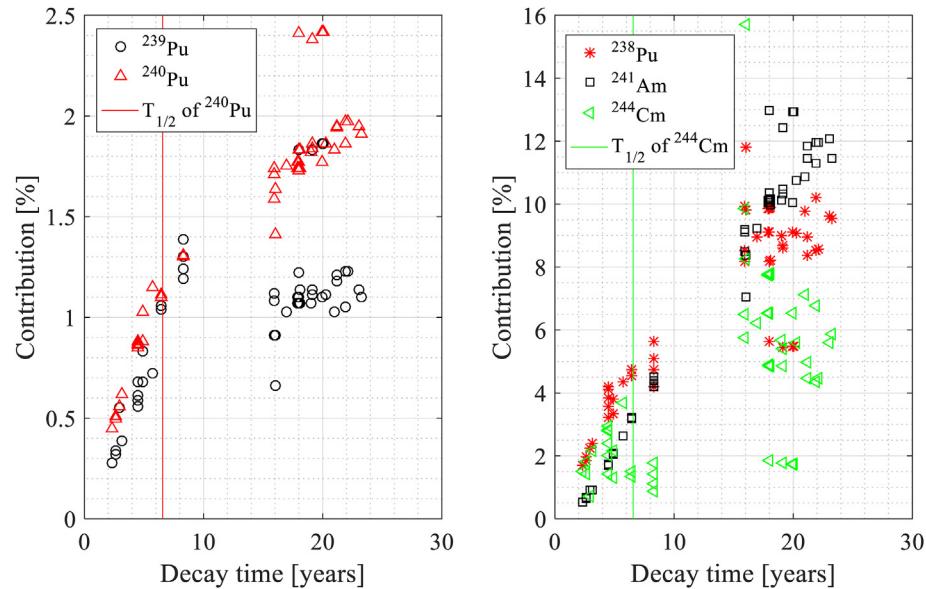


Fig. 8. Contribution of actinide isotope to decay heat.

Table 9
Comparison results of Turkey Point Unit 3.

Assembly ID	Burnup [GWd/MTU]	Enrichment [w/o U-235]	Decay time [days]	C/E – 1 (%)		
				STREAM-SNF	RAST-K SNF	
					FA-wise	PIN-wise
B-43	25.6	2.557	1782	0.39	-3.13	-0.45
D-15	28.4	2.557	957	1.16	-2.73	2.33
D-15	28.4	2.557	1139	1.02	0.65	-1.50
D-15	28.4	2.557	2072	-1.41	-2.43	-0.20
D-22	26.5	2.557	958	1.74	-0.41	-1.24
D-34	27.9	2.557	859	1.42	-0.53	-3.56

where σ is the uncertainty of measurements in percent unit, E is the experimental data presented in Ref. [14], and u^M is the measurement uncertainty in Watts. For the Ringhals-2 assemblies in Table 7

and Ringhals-3 assemblies in Fig. 8, the maximum relative error of STREAM-SNF occurs for assembly C20 at less than 3%. In the newly implemented RAST-K SNF analysis method, the maximum relative

Table 10

Comparison results of Point Beach Unit 2.

Assembly ID	Burnup [GWd/MTU]	Enrichment [w/o U-235]	Decay time [days]	C/E – 1 (%)		
				STREAM-SNF		RAST-K SNF
				FA-wise	PIN-wise	FA-wise
C-52	31.9	3.397	1635	0.41	0.31	-2.46
C-56	38.9	3.397	1634	-0.03	-1.54	1.88
C-64	39.4	3.397	1633	0.40	-1.47	1.99
C-66	35.4	3.397	1630	-0.53	-2.41	0.79
C-67	38.9	3.397	1629	-1.09	-2.47	0.87
C-68	37.1	3.397	1630	1.03	-2.16	1.62

Table 11

Comparison results of San Onofre Unit 1.

Assembly ID	Burnup [GWd/MTU]	Enrichment [w/o U-235]	Decay time [days]	C/E – 1 (%)		
				STREAM-SNF		RAST-K SNF
				FA-wise	PIN-wise	FA-wise
C-01	26.5	3.865	3011	-0.01	-1.22	-0.92
C-16	28.5	3.865	3012	1.06	-0.10	0.09
C-19	30.4	3.865	3011	-0.25	-1.33	-1.20
C-20	32.4	3.865	3011	-1.89	-3.60	-3.12
D-01	31.4	4.005	2358	-1.98	-0.89	-1.01
D-46	32.3	4.005	2360	-0.53	-0.31	-0.24
E-18	32.4	4.005	1794	0.07	0.27	0.62
F-04	30.4	3.996	1078	2.35	0.21	2.62

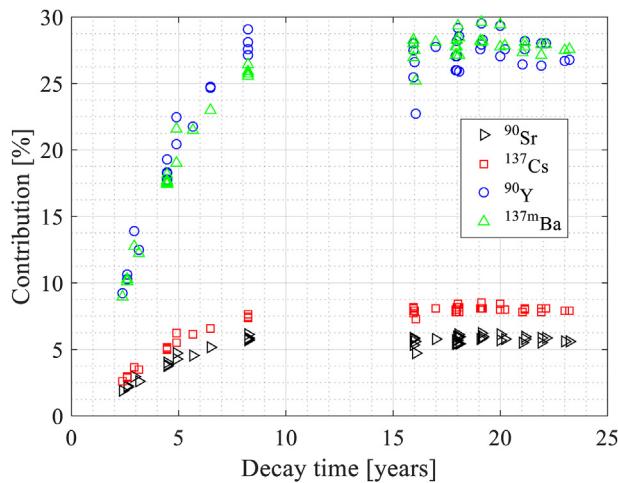
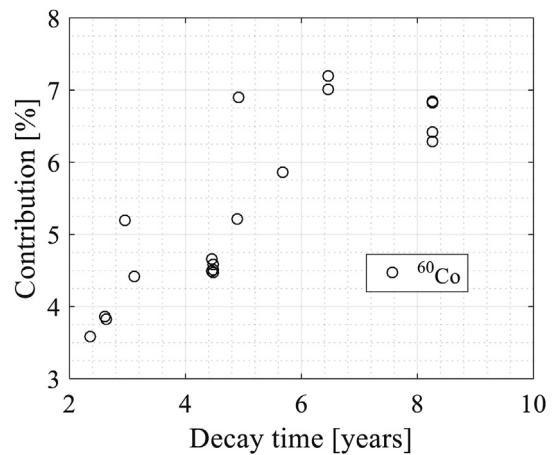


Fig. 9. Contribution of fission product to decay heat.

Fig. 10. Contribution of activation nuclide ^{60}Co .

error is observed for assembly G11 by FA calculation at less than 4%. The RAST-K SNF pin-wise calculation shows a maximum relative error of over 4% for assembly C20.

Fig. 7 shows the relative errors of 38 decay heat validation cases together with the uncertainty of measurements. Except two cases, results of the RAST-K SNF assembly calculation are within the 2-sigma error band.

4.2.2. US PWR

This section demonstrates the calculation-experiment comparison results of the assemblies from the three US PWRs: Turkey Point 3 (15 by 15 FA), Point Beach 2, and San Onofre 1 (14 by 14 FA). The difference between Point Beach 2 and San Onofre 1 is active height (365.8 cm for Point Beach 2 and 304.8 cm for San Onofre 1). The decay heat measurement of Turkey Point 3 assemblies was performed at Florida Power and Light Company using the boil-off

calorimeter at the HEDL facility [14]. As noted previously, the spacer grids of Turkey Point 3 and Point Beach 2 contain stainless steel with cobalt, which produces a non-negligible amount of decay heat when activated [14,23]. In our US PWR models, these spacer grids are smeared into the coolant to account for the activation. For the Turkey Point 3 assemblies, the mean relative error is $0.72 \pm 1.04\%$ for STREAM-SNF, $-1.43 \pm 1.40\%$ for RAST-K assembly calculation, and $-0.77 \pm 1.76\%$ for RAST-K pin-wise calculation. Although, the mean relative error for the RAST-K assembly calculation is the highest, all relative errors are within $\pm 3\%$, as in Table 9.

The decay heat of Point Beach 2 assemblies was measured at the GE-Morris Operation facility. The details of comparison results are described in Table 10, and the relative errors are within $\pm 3\%$. San Onofre 1 fuel rods have stainless steel cladding, whose activation is considered for accurate decay heat prediction. Table 11 presents the comparison results of San Onofre 1 assemblies, and the relative errors are within $\pm 4\%$. The average relative error is $-0.15 \pm 1.00\%$ for

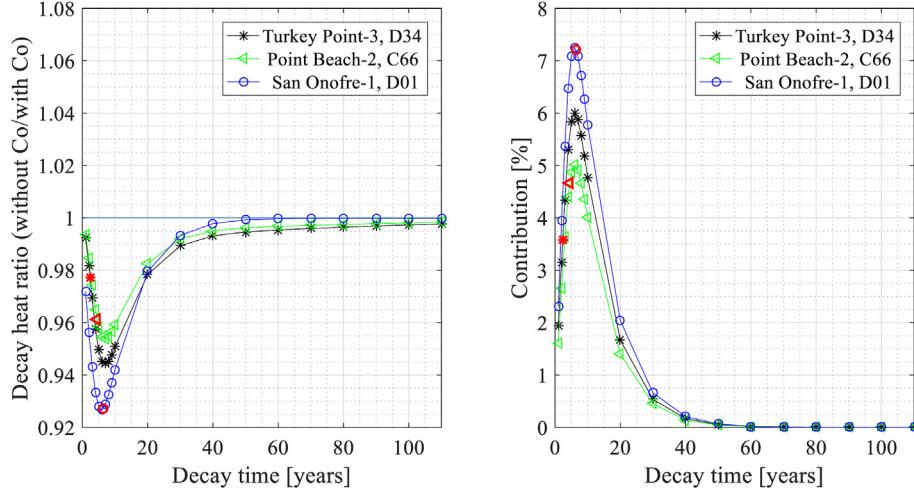


Fig. 11. Decay heat ratio with contribution of ^{60}Co .

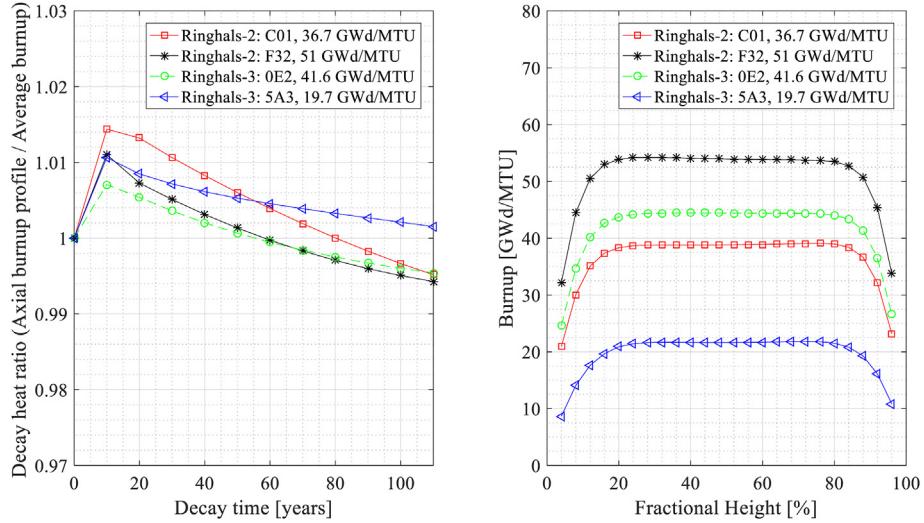


Fig. 12. Effect of axial burnup profile on decay heat.

STREAM, -0.87 ± 1.04 for RAST-K assembly calculation, and -0.40 ± 1.06 for RAST-K pin-wise calculation.

4.3. Contribution of isotope to the decay heat

The contribution of isotope to the decay heat is described in Figs. 8 and 9 with 58 decay heat measurements on 48 FAs. Five actinide isotopes are presented in Fig. 8: ^{239}Pu ($T_{1/2} = 2.411 \times 10^4$ years), ^{240}Pu ($T_{1/2} = 6561$ years), ^{238}Pu ($T_{1/2} = 87.7$ years), ^{241}Am ($T_{1/2} = 432.6$ years) and ^{244}Cm ($T_{1/2} = 18.11$ years) [15]. These isotopes show an increasing trend with respect to the decay time (= cooling time). Contribution of the isotopes shown on the right-side graph is much larger than that of the isotopes described on the left-side graph. In case of ^{240}Pu and ^{244}Cm , the slope of contribution decreases after the isotope half-life is reached. Four fission products are described in Fig. 9: ^{90}Sr ($T_{1/2} = 28.79$ years), ^{137}Cs ($T_{1/2} = 30.08$ years), ^{90}Y ($T_{1/2} = 2.67$ days), and $^{137\text{m}}\text{Ba}$ ($T_{1/2} = 2.552$ min). Those isotopes have constant contribution in total decay heat after 10 years which is the decreasing point of the actinide isotope contribution slope; in other words, decay is dominant after 10 years. Fig. 10 demonstrates the contribution of cobalt in 20 decay heat

samples of US PWRs. The activation nuclide, ^{60}Co , is generated by ^{59}Co as a neutron capture reaction [15] and shows an increasing trend as the decay time increases. The effects of cobalt on US FA samples are described in Fig. 11. The decay heat ratio (without cobalt to with cobalt) and contribution of ^{60}Co are described as a function of decay time. Three samples are employed for analysis: D34 of Turkey Point-3, C66 of Point Beach-2, and D01 of San Onofre-1. Before the cooling time of 40 years, the effect of ^{60}Co is not negligible. Considering the range of cooling time of US PWR samples (2.35 years–8.25 years) could give as large as a 7% error. The red points are the decay time of measurements in Fig. 11, and it is recognized that the San Onofre case is located at the maximum point of the difference between the cases without cobalt and with cobalt. After 40 years, the effect of ^{60}Co ($T_{1/2} = 5.26$ years) decreases because the contribution of cobalt-60 decreases.

4.4. Effect of axial burnup profile to decay heat

The axial burnup profile at discharge is given in the case of Ringhals-2 and Ringhals-3 [7,13]. Four cases are selected to consider the average burnup of FA samples: C01 and F32 of Ringhals-2 and

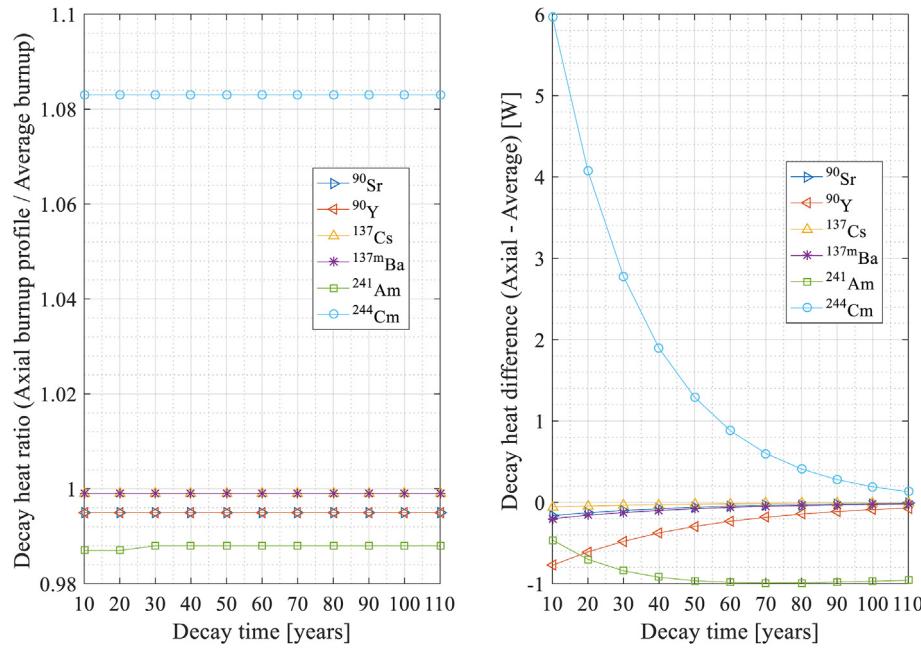


Fig. 13. Effect of actinide and fission products according to the axial burnup profile.

Table 12
Power history correction factor effect.

Assembly ID	Reactor name	Measurement laboratory	Measured decay heat [W]	Decay time [years]	RAST-K (C/E-1 [%])	
					Without PCF*	With PCF
B-43	Turkey Point 3	HEDL	637	4.88	-6.23	-3.13
D-15			1423	2.622	-10.02	-2.73
D-15			1126	3.121	-5.99	0.65
D-15			625	5.677	-5.12	-2.43
D-22			1284	2.62	-6.37	-0.41
D-34			1550	2.353	-8.84	-0.53
C-52	Point Beach 2	Point Beach 2	724	4.479	-6.16	0.31
C-56			921	4.477	-8.94	-1.54
C-64			931	4.474	-8.69	-1.47
C-66			846	4.466	-10.19	-2.41
C-67			934	4.463	-9.89	-2.47
C-68			874	4.466	-8.82	-2.16
C-01	San Onofre 1	San Onofre	359	8.249	-2.20	-1.22
C-16			384	8.252	-1.33	-0.10
C-19			418	8.249	-2.71	-1.33
C-20			456	8.249	-4.54	-3.60
D-01			499	6.46	-15.93	-0.89
D-46			510	6.466	-2.68	-0.31
E-18			635	4.915	-4.37	0.27
F-04			934	2.953	0.21	0.21

*PCF is defined in Eq. (6).

OE2 and 5A3 of Ringhals-3. Fig. 12 shows the decay heat ratio of the axial burnup profile case to average burnup case as a function of decay time. The calculation is performed with a decay time range of 0–110 years with a time step interval of 10 years. The axial nodes of 24 are used as represented in Fig. 12. The difference between the axial burnup profile case and average burnup case is smaller than 1% error in case of F32, OE2, and 5A3. In case of C01, after about 35 years of decay time, the difference between the axial burnup profile and average case is under 1% error. Fig. 13 shows the decay heat ratio of actinide and fission products in OE2 as a function of decay time. ^{244}Cm and ^{241}Am have a considerable effect compared with the other four isotopes. The absolute difference between the axial burnup profile case and the average burnup case decreases as the decay time increases. According to the increase in decay time, the variation in amount of ^{244}Cm ($T_{1/2} = 18.11$ years) is much larger

than that of ^{241}Am ($T_{1/2} = 432.6$ years) because the half-life of ^{244}Cm is much smaller than that of ^{241}Am .

In this sensitivity study, the power conditions are set with discharged burnup as a constant parameter because the references only contain the axial burnup profile at the discharged point [7,13]. In case of the average burnup of FA, reference [13] produced the detail conditions in each end of cycle (EOC) operation. To consider the details of the load condition following operation, the average burnup is used for decay heat calculation.

4.5. Effect of PCF

PCF is important to consider the decay effect because of the different power levels used in the STREAM 2D branch calculations and RAST-K 3D calculations. Table 12 shows the effect of PCF in the

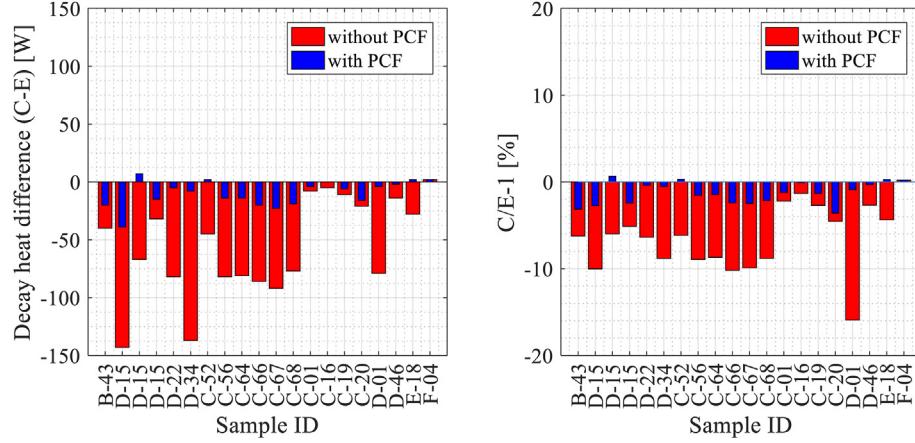


Fig. 14. Effect of PCF on decay heat difference and relative errors.

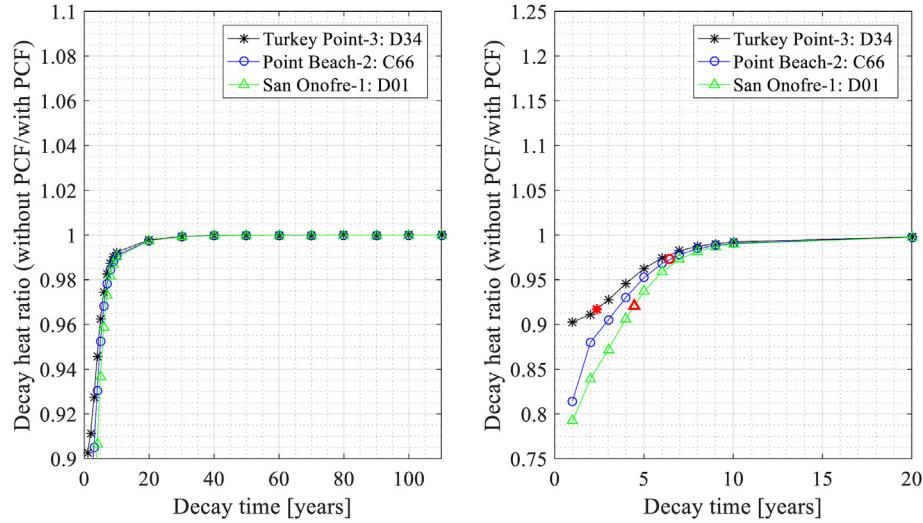


Fig. 15. Decay heat ratio as a function of decay time.

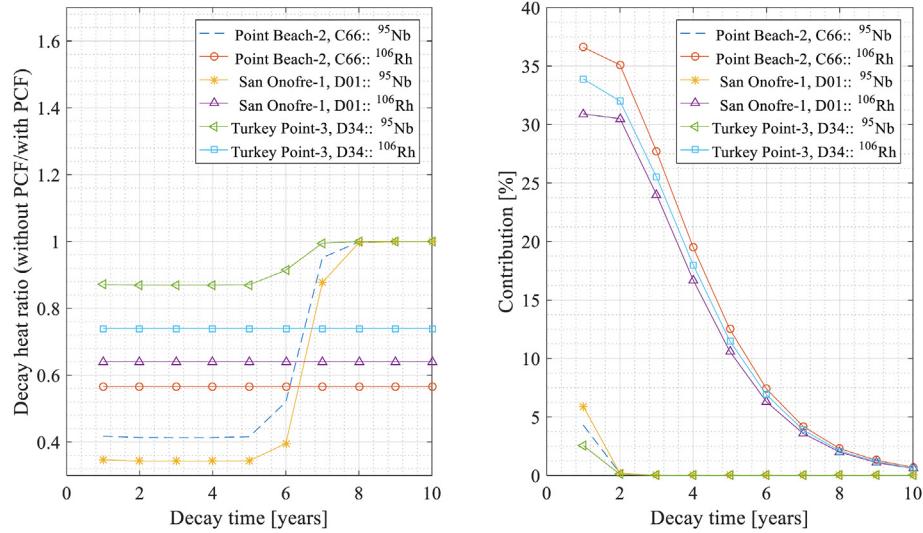


Fig. 16. Decay heat ratio and contribution of selected isotopes.

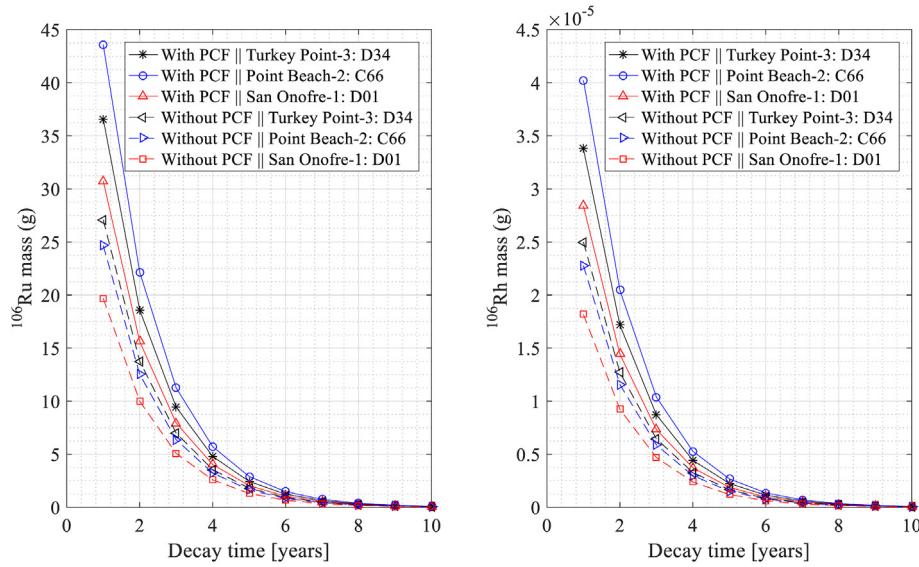
Fig. 17. Mass of ^{106}Ru and ^{106}Rh as a function of decay time.

Table 13
Comparison results of simulation time for analysis of SNF.

Reactor	ST SNF		RK SNF FA-wise		RK SNF PIN-wise	
	Mean* ¹	STD* ²	Mean	STD	Mean	STD
Ringhals Unit 2	1204.9	308.3	31.0	5.1	313.7	26.4
Ringhals Unit 3	982.3	132.2	25.7	1.5	187.4	8.6
Turkey Point Unit 3	641.6	75.4	30.0	7.7	210.9	8.9
Point Beach Unit 2	1826.7	8.4	25.5	0.2	168.4	10.7
San Onofre Unit 1	1218.0	56.8	26.6	3.1	179.2	13.2
Overall	1136.0	348.9	27.9	24.4	225.9	62.1

*1 and *2, see the footprint of Table 5.

20 measurements of US PWR assemblies. A comparison is made with the assembly calculation results. The average relative errors are $-1.26 \pm 1.23\%$ and $-6.44 \pm 3.73\%$, with and without the PCF, respectively. The maximum relative error of the calculation without PCF is $+15.93\%$, and this value is 4.425 times larger than the maximum relative error of calculation with the effect of PCF. Fig. 14 presents the effect of PCF on the decay heat difference (C-E) and relative errors. A maximum difference of 150 W between the

calculated and measured decay heat is observed for assembly D-15 without the PCF. This difference is 100 W larger compared to when the PCF is used.

Three US FA samples are employed for sensitivity study of PCF, as shown in Fig. 15: D34 of Turkey Point-3, C66 of Point Beach-2, and D01 of San Onofre-1. The effect of the power correction factor is high until 10 years of decay time. The red points on the right-side graph of Fig. 15 show the measured points of the realistic benchmark problem. The errors occurred by main two isotopes: ^{95}Nb ($T_{1/2} = 35$ years) and ^{106}Rh ($T_{1/2} = 29.8$ s) [24]. Fig. 16 represents the decay heat ratio (without PCF to with PCF) and the contribution of these two isotopes as a function of decay time. Although the decay heat ratio of ^{106}Rh is the same, the total decay heat ratio (i.e. decay heat difference between without PCF and with PCF) decreases as the contribution of ^{106}Rh reduces. The mass of ^{106}Ru reduces as a function of decay heat because the amount of ^{106}Ru is decreased and the half-life of ^{106}Rh is much smaller than that of ^{106}Ru . Furthermore, the production rate (^{106}Ru to ^{106}Rh , $T_{1/2} = 1.02286$ years) is smaller than the decay rate (^{106}Rh to ^{106}Pd , $T_{1/2} = 29.8$ s). Fig. 17 illustrates the behavior of mass amount according to different decay times.

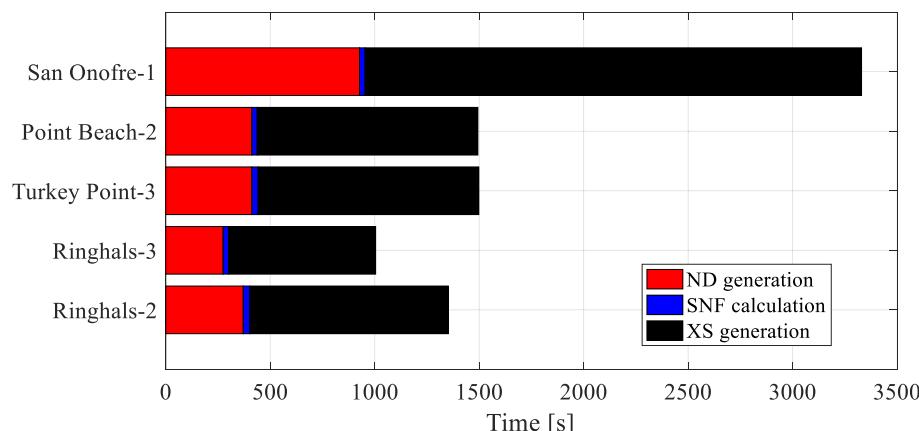


Fig. 18. Simulation time.

4.6. Simulation time

The newly implemented code system can reduce the computational time of the source term calculation. Table 13 contains the computation time comparison for STREAM-SNF and RAST-K SNF. The average of the RAST-K SNF assembly calculation is 40.7 times faster than that of the STREAM-SNF calculation. This is because typically the STREAM-SNF needs to perform depletion calculation using the power history information from the core simulation codes such as RAST-K as in Fig. 1. The average of RAST-K SNF pin-wise calculation is 5 times faster than that of STREAM-SNF and 8 times slower than that of the RAST-K SNF assembly calculation. The difference between the RAST-K SNF assembly and pin-wise calculation is caused by the reading of files. The pin-wise number density file for interpolation is about 9 gigabytes per assembly and is 225 times larger than the assembly-wise number density file. An assembly number density file is only 40 megabytes. The number density files are written in the ASCII format and contain 29 burnup steps, with 1640 isotope information, including flux, pin position, number density, isotope name, and history branch calculation type.

Fig. 18 illustrates the computational time of the entire RAST-K SNF calculation of the benchmark problem. Because STREAM-SNF uses the direct method with on-the-fly method for generation of the cross-section (i.e., STREAM-SNF does not use the two-step method), the whole calculation time of RAST-K SNF including XS and ND generation time is about 2000 s longer than that of STREAM-SNF. In Fig. 18, ND generation denotes the computational time of branch history calculation, and XS generation is the branch calculation. The SNF calculation is the computational time of Lagrange non-linear interpolation and the power correction factor. When analyzing SNFs of the commercial reactor, the source term calculation is performed after two-step core simulation. Therefore, a certain amount of XS generation time is required in both the calculation tools. For the case of a commercial reactor with 121 FAs and 24 axial nodes per FA (i.e., 2904 calculation nodes per cycle), STREAM-SNF needs 916 h (i.e., about 38 days) to deplete all the nodes in core. One node calculation with 3D core operating condition requires 1136 s (i.e., mean value of overall STREAM-SNF calculation as shown in Table 13). The implemented SNF analysis tool takes 23 h (i.e., about one day) for analysis of the SNF, including ND generation time. The SNF analysis time is 27.9 s and the ND generation time is 600 s. Because ND generation and XS generation correspond to the initial computational cost, RAST-K SNF can achieve the maximum benefit in repetitional calculation, for instance

core design, analysis of commercial reactor SNF, and re-calculation to fix the input error.

5. Conclusions

An SNF analysis method for spent nuclear fuel decay heat calculation was newly implemented in the STREAM/RAST-K two-step code system. The implementation is based on Lagrange non-linear interpolation and the use of power history correction factors. A total of 58 realistic benchmarks of decay heat measurements performed on 38 assemblies discharged from PWRs operated in Sweden and United States are used in the validation. Furthermore, the validated SNF decay heat calculation of STREAM is employed for verification. The verification shows that the RAST-K SNF implementation is of comparable accuracy to STREAM-SNF. The RAST-K SNF average ($C/E - 1$) is $-0.69 \pm 1.43\%$, and most of the decay heat calculation results are within the measurement uncertainty. This study demonstrates that the implemented code system can be used to analyze discharged FAs in back-end nuclear fuel cycle management.

We plan to analyze the decay heats of SNF assemblies discharged from South Korean PWRs. Furthermore, we intend to introduce binary files in the generation of number density data to reduce the size and to achieve higher efficiency calculations. These two plans are within the scope of future work.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix

Calculated decay heat results of 58 FAs are presented in Table A. 1 and Table A. 2. Table A. 1 and Table A. 2 contains the decay heat results of Swedish FAs and US FAs as a unit watt (W), respectively.

Table A. 1
Decay heat results of Swedish FAs

Reactor name	FA ID	Burnup [GWd/MTU]	Measured decay Heat [W]	Calculated decay heat [W]		
				STREAM-SNF [W]		RAST-K SNF
				FA-wise [W]	Pin-wise [W]	
Ringhals-3	0E2	41.6	588	582	581	581
	0E6	36	488	487	485	485
	1C2	33.3	418	417	420	420
	1E5	34.6	469	465	463	463
	2A5	20.1	234	235	239	239
	2C2	36.6	467	466	469	469
	3C1	36.6	470	475	475	476
	3C9	36.6	468	474	475	475
	4C4	33.3	422	425	425	425
	5A3	19.7	238	237	238	238
	5A3	19.7	237	236	238	238
	5A3	19.7	243	236	238	238
	5A3	19.7	231	233	234	234
	5A3	19.7	230	233	234	234
	0C9	38.4	491	501	493	503

Table A. 1 (continued)

Reactor name	FA ID	Burnup [GWd/MTU]	Measured decay Heat [W]	Calculated decay heat [W]		
				STREAM-SNF [W]	RAST-K SNF	
					FA-wise [W]	Pin-wise [W]
Ringhals-2	1C5	38.5	499	500	503	503
	3C5	38.4	501	507	492	508
	4C7	38.4	499	500	502	502
	C01	36.7	416	416	423	421
	C12	36.4	410	412	411	412
	C20	35.7	416	428	423	433
	C20	35.7	426	428	423	433
	C20	35.7	429	428	423	433
	D27	39.7	456	459	450	450
	D38	39.4	442	445	441	441
	E38	34	376	376	371	371
	E38	34	374	376	371	371
	E40	34.3	381	379	373	374
	F14	34	382	384	377	378
	F21	36.3	421	420	414	415
	F25	35.3	397	394	388	396
	F32	51	692	697	691	691
	G11	35.5	416	406	401	401
	G23	35.6	421	420	413	414
	I09	40.2	508	505	508	508
	I24	34.3	410	409	403	403
	I25	36.9	446	441	448	448

Table A. 2

Decay heat results of US FAs

Reactor name	FA ID	Burnup [GWd/MTU]	Measured decay Heat [W]	Calculated decay heat [W]		
				STREAM-SNF [W]	RAST-K SNF	
					FA-wise [W]	Pin-wise [W]
Turkey Point-3	B-43	25.6	637	639	617	634
	D-15	28.4	1423	1439	1384	1456
	D-15	28.4	1126	1137	1133	1109
	D-15	28.4	625	616	610	624
	D-22	26.5	1284	1306	1279	1268
	D-34	27.9	1550	1572	1542	1495
Point Beach-2	C-52	31.9	724	727	726	706
	C-56	38.9	921	921	907	938
	C-64	39.4	931	935	917	950
	C-66	35.4	846	842	826	853
	C-67	38.9	934	924	911	942
	C-68	37.1	874	883	855	888
San Onofre-1	C-01	26.5	359	359	355	356
	C-16	28.5	384	388	384	384
	C-19	30.4	418	417	412	413
	C-20	32.4	456	447	440	442
	D-01	31.4	499	489	495	494
	D-46	32.3	510	507	508	509
	E-18	32.4	635	635	637	639
	F-04	30.4	934	956	936	958

Appendix A. Supplementary data

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.net.2020.06.028>.

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