

Supplemental Online Material

Validation of decay heat calculation results of ORIGEN2.2 and CASMO5 for light water reactor fuel

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This Supplemental Online Material consists of 19 pages, including twelve figures and five tables.

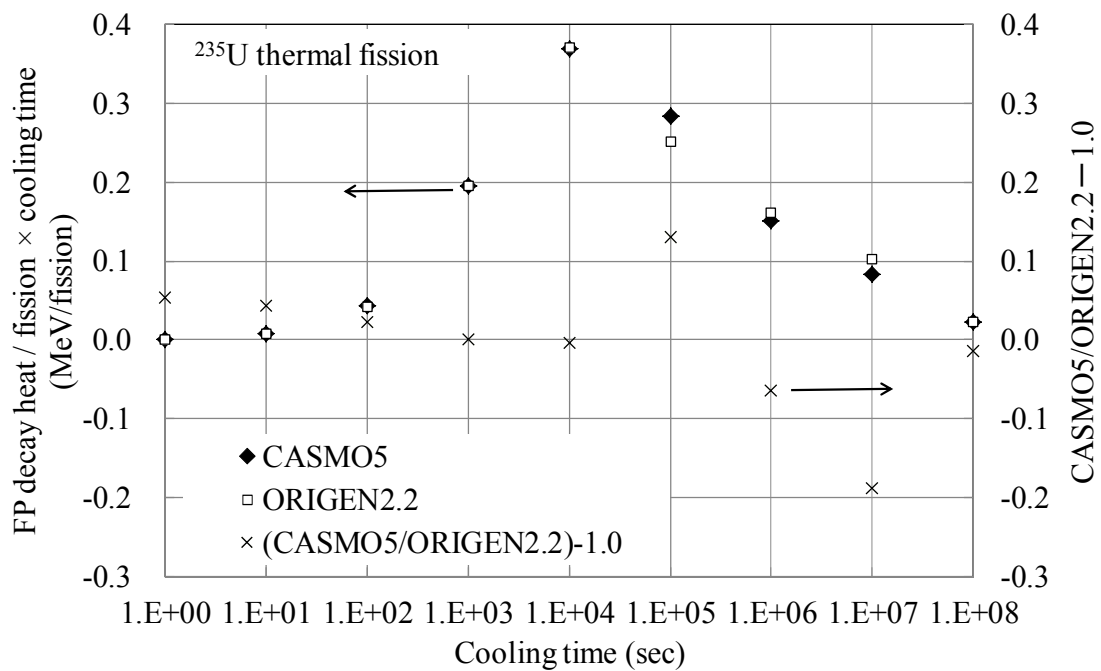


Figure S1 Decay heat per fission after the irradiation time of 10^4 sec for ^{235}U thermal fission for CASMO5 and ORIGEN2.2 calculations (the left vertical axis) and their comparison CASMO/ORIGEN2.2-1.0 (the right vertical axis) are shown. The left vertical axis shows the product of decay heat (MeV/sec/fission) and cooling time (sec) for the convenience in showing in a linear vertical axis.

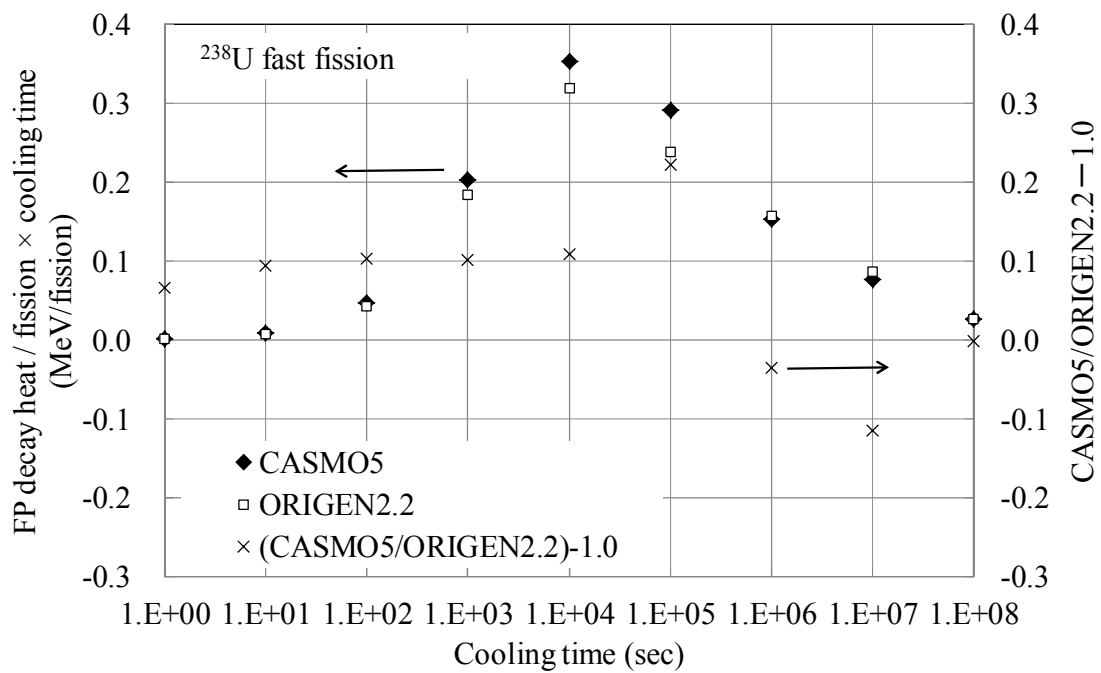


Figure S2 Decay heat per fission after the irradiation time of 10^4 sec for ^{238}U fast fission for CASMO5 and ORIGEN2.2 calculations (the left vertical axis) and their comparison CASMO/ORIGEN2.2-1.0 (the right vertical axis) are shown. The left vertical axis shows the product of decay heat (MeV/sec/fission) and cooling time (sec) for the convenience in showing in a linear vertical axis.

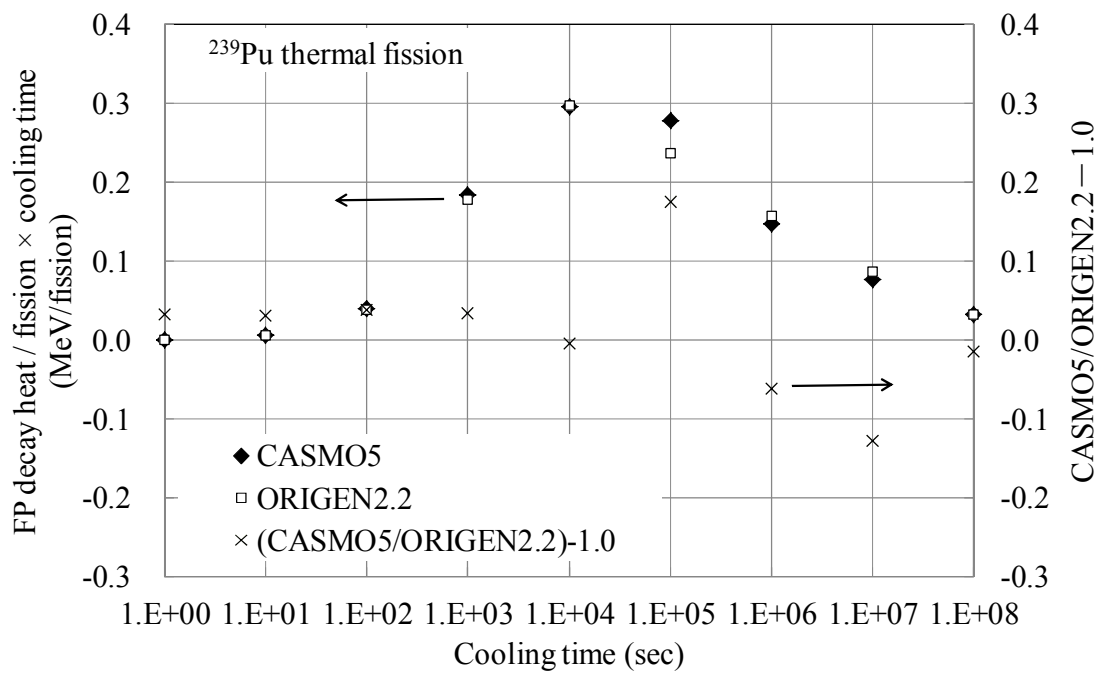


Figure S3 Decay heat per fission after the irradiation time of 10^4 sec for ^{239}Pu thermal fission for CASMO5 and ORIGEN2.2 calculations (the left vertical axis) and their comparison CASMO/ORIGEN2.2-1.0 (the right vertical axis) are shown. The left vertical axis shows the product of decay heat (MeV/sec/fission) and cooling time (sec) for the convenience in showing in a linear vertical axis.

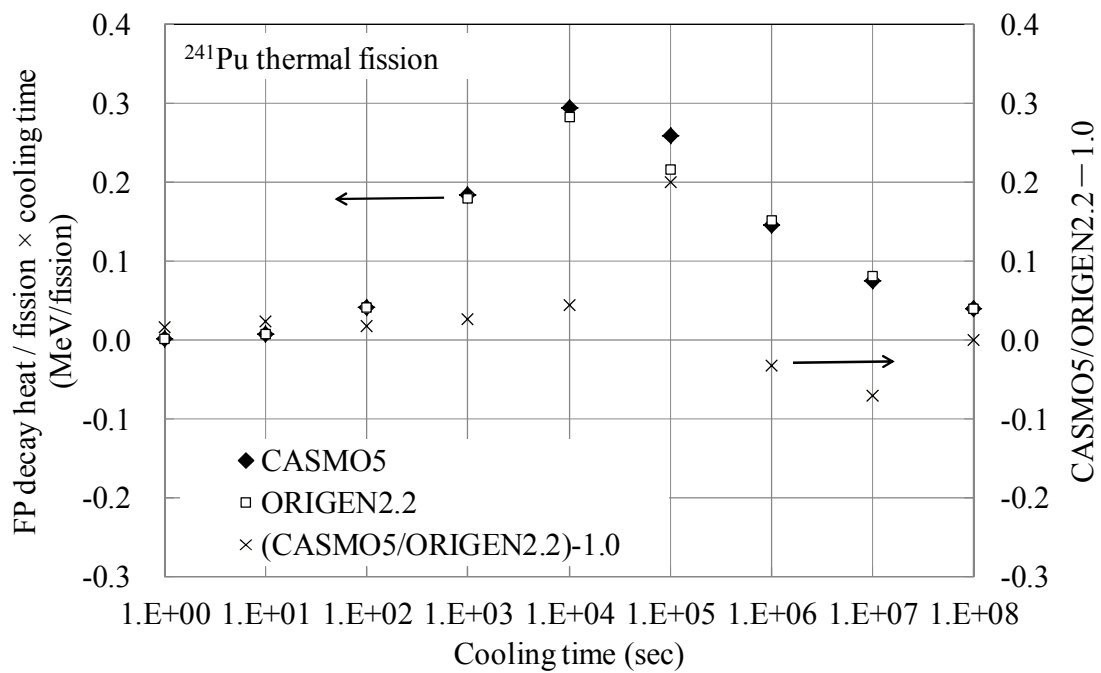


Figure S4 Decay heat per fission after the irradiation time of 10^4 sec for ^{241}Pu thermal fission for CASMO5 and ORIGEN2.2 calculations (the left vertical axis) and their comparison CASMO/ORIGEN2.2-1.0 (the right vertical axis) are shown. The left vertical axis shows the product of decay heat (MeV/sec/fission) and cooling time (sec) for the convenience in showing in a linear vertical axis.

Comparison of the calculated decay heat between CASMO5 and ORIGEN2.2 for practical irradiation conditions of typical light water reactor fuel assemblies

The calculation conditions of practical irradiation time of typical PWR and BWR fuel assemblies were set as shown in **Table S1**. The irradiation condition of each cycle was 13-month operation with a constant specific power irradiation and 60-day outage. The decay heat of one-, two- and three-cycle-burn fuel assemblies for the PWR fuel and one-, two-, three-, four- and five-cycle-burn fuel assemblies for the BWR fuel was calculated. The cooling time was set to be from 1 sec to 10^8 sec (1157 days). No structure material was considered. In the ORIGEN2.2 calculations, the library PWR41J40 (PWR 17×17 fuel assembly, ^{235}U enrichment 4.1 wt%) [3] for the PWR fuel assembly and BS340J40 (BWR 9×9 fuel assembly, ^{235}U enrichment 4.1 wt%, in-channel void fraction 40%) [3] for the BWR fuel assembly were used. In the CASMO calculations, the two-dimensional assembly model was devised based on the published information. The in-channel void fraction was set to 40% for the BWR fuel assembly.

The calculated results of ORIGEN2.2 for the FP and actinide nuclides and total decay heat in (W/tU) were shown in **Table S2** for the PWR fuel assembly and **Table S3** for the BWR fuel assembly. The tables also show the ratios of the calculated results of CASMO5 to those of ORIGEN2.2. The results indicates that the calculated decay heat of CASMO5 gives FP decay heat larger by 4% at the maximum than that of ORIGEN2.2 at cooling time of 1 sec. The overestimation decreases with the cooling time and almost disappears at the cooling time of 10^4 sec.

The tables show the comparison of decay heat of actinide nuclides. There are trends depending on the fuel assembly type, cooling time and numbers of irradiation cycles. This reflects the differences in the libraries of CASMO5 and ORIGEN2.2. The trend in the ratios of CASMO5 to ORIGEN2.2 for actinide nuclide decay heat at the cooling time 10^8 sec (1157 days) is also seen in the analysis of the assembly decay heat measurements for the U.S. PWR and BWR fuel assemblies at the cooling time around 1000 days.

Table S1 Calculation conditions of finite irradiation of typical PWR and BWR fuel assemblies

Reactor type	Fuel assembly type	Enrichment (wt% ^{235}U) ^a	Specific power (MW/tU)	Operation cycle (395 day operation+60 day outage)
PWR	17×17	4.1	36.83	1, 2, 3
BWR	9×9-9 ^b	3.8	26.00	1, 2, 3, 4, 5

^a Assembly average value. ^b a 9×9 assembly with nine fuel rods replaced by a water channel.

Table S2 Calculated decay heat (W/tU) of ORIGEN2.2 for the PWR fuel assembly and comparison with that of CASMO5

Cooling time (sec)			1	1.E+01	1.E+02	1.E+03	1.E+04	1.E+05	1.E+06	1.E+07	1.E+08
(day)			1.157E-05	0.00011574	0.001157	0.01157	0.1157	1.157	11.57	115.7	1157
ORIGEN2.2	1 cy burn	FP	2.05E+06	1.58E+06	1.04E+06	6.34E+05	3.06E+05	1.47E+05	7.03E+04	1.84E+04	1.28E+03
		Actinide	8.82E+04	8.80E+04	8.60E+04	7.03E+04	4.15E+04	3.04E+04	1.76E+03	8.48E+01	3.24E+01
		Total	2.14E+06	1.67E+06	1.13E+06	7.05E+05	3.47E+05	1.78E+05	7.21E+04	1.85E+04	1.31E+03
	2 cy burn	FP	2.01E+06	1.55E+06	1.02E+06	6.25E+05	3.04E+05	1.52E+05	7.45E+04	2.23E+04	2.39E+03
		Actinide	1.03E+05	1.03E+05	1.01E+05	8.27E+04	4.96E+04	3.65E+04	3.08E+03	7.28E+02	1.36E+02
		Total	2.11E+06	1.65E+06	1.13E+06	7.08E+05	3.54E+05	1.89E+05	7.76E+04	2.30E+04	2.53E+03
	3 cy burn	FP	1.99E+06	1.53E+06	1.01E+06	6.19E+05	3.03E+05	1.57E+05	7.77E+04	2.51E+04	3.48E+03
		Actinide	1.20E+05	1.20E+05	1.18E+05	9.71E+04	5.93E+04	4.40E+04	5.30E+03	2.02E+03	3.97E+02
		Total	2.11E+06	1.65E+06	1.13E+06	7.16E+05	3.62E+05	2.01E+05	8.30E+04	2.72E+04	3.88E+03
CASMO5 / ORIGEN2.2	1 cy burn	FP	1.04	1.03	1.02	1.01	1.00	0.99	0.99	0.99	1.01
		Actinide	1.03	1.03	1.03	1.04	1.05	1.05	1.04	0.97	0.99
		Total	1.04	1.03	1.02	1.01	1.01	1.00	0.99	0.99	1.01
	2 cy burn	FP	1.03	1.03	1.02	1.01	1.00	0.98	0.99	0.99	1.00
		Actinide	1.03	1.03	1.03	1.03	1.05	1.04	1.01	0.97	0.98
		Total	1.03	1.03	1.02	1.01	1.00	1.00	0.99	0.99	1.00
	3 cy burn	FP	1.03	1.02	1.02	1.01	0.99	0.98	0.99	0.99	1.00
		Actinide	1.02	1.02	1.02	1.03	1.05	1.04	0.99	0.97	0.98
		Total	1.03	1.02	1.02	1.01	1.00	0.99	0.99	0.99	1.00

Note: The unit of decay heat is W/tU and “aE+b” means “a×10^b.”

Table S3 Calculated decay heat (W/tU) of ORIGEN2.2 for the BWR fuel assembly and comparison with that of CASMO5

Cooling time (sec)		1.E+00	1.E+01	1.E+02	1.E+03	1.E+04	1.E+05	1.E+06	1.E+07	1.E+08	
(day)		1.157E-05	0.0001157	0.001157	0.01157	0.1157	1.157	11.57	115.7	1157	
ORIGEN2.2	1cy burn	FP	1.46E+06	1.13E+06	7.41E+05	4.52E+05	2.18E+05	1.04E+05	4.98E+04	1.30E+04	8.66E+02
		Actinide	5.65E+04	5.63E+04	5.51E+04	4.50E+04	2.65E+04	1.94E+04	1.07E+03	3.36E+01	1.72E+01
		Total	1.52E+06	1.18E+06	7.97E+05	4.97E+05	2.44E+05	1.23E+05	5.09E+04	1.30E+04	8.83E+02
	2 cy burn	FP	1.43E+06	1.11E+06	7.31E+05	4.46E+05	2.17E+05	1.07E+05	5.25E+04	1.55E+04	1.56E+03
		Actinide	6.36E+04	6.35E+04	6.21E+04	5.09E+04	3.03E+04	2.23E+04	1.65E+03	3.02E+02	6.04E+01
		Total	1.50E+06	1.17E+06	7.93E+05	4.97E+05	2.47E+05	1.29E+05	5.41E+04	1.58E+04	1.62E+03
	3 cy burn	FP	1.41E+06	1.09E+06	7.23E+05	4.41E+05	2.16E+05	1.09E+05	5.42E+04	1.72E+04	2.21E+03
		Actinide	7.26E+04	7.24E+04	7.08E+04	5.84E+04	3.53E+04	2.62E+04	2.79E+03	9.49E+02	1.53E+02
		Total	1.49E+06	1.17E+06	7.94E+05	5.00E+05	2.51E+05	1.35E+05	5.70E+04	1.81E+04	2.36E+03
	4 cy burn	FP	1.40E+06	1.08E+06	7.17E+05	4.38E+05	2.15E+05	1.11E+05	5.58E+04	1.86E+04	2.86E+03
		Actinide	8.39E+04	8.37E+04	8.19E+04	6.78E+04	4.17E+04	3.11E+04	4.34E+03	1.86E+03	3.32E+02
		Total	1.49E+06	1.17E+06	7.99E+05	5.06E+05	2.57E+05	1.42E+05	6.01E+04	2.05E+04	3.19E+03
	5 cy burn	FP	1.40E+06	1.08E+06	7.13E+05	4.36E+05	2.15E+05	1.14E+05	5.75E+04	2.00E+04	3.50E+03
		Actinide	9.49E+04	9.47E+04	9.27E+04	7.71E+04	4.79E+04	3.59E+04	5.98E+03	2.91E+03	6.51E+02
		Total	1.49E+06	1.17E+06	8.06E+05	5.13E+05	2.63E+05	1.50E+05	6.35E+04	2.29E+04	4.15E+03
CASMO5 / ORIGEN2.2	1cy burn	FP	1.04	1.03	1.02	1.01	1.00	0.99	0.99	0.99	1.01
		Actinide	1.01	1.01	1.01	1.01	1.03	1.03	1.02	0.97	0.97
		Total	1.04	1.03	1.02	1.01	1.00	1.00	0.99	0.99	1.01
	2 cy burn	FP	1.04	1.03	1.02	1.01	1.00	0.99	0.99	0.99	1.01
		Actinide	1.01	1.01	1.01	1.02	1.03	1.03	1.00	0.94	0.97
		Total	1.04	1.03	1.02	1.01	1.00	0.99	0.99	0.99	1.01
	3 cy burn	FP	1.03	1.03	1.02	1.01	1.00	0.98	0.99	0.99	1.01
		Actinide	1.01	1.01	1.02	1.02	1.03	1.03	0.97	0.92	0.97
		Total	1.03	1.03	1.02	1.01	1.00	0.99	0.99	0.99	1.00
	4 cy burn	FP	1.03	1.02	1.02	1.01	1.00	0.98	0.99	0.99	1.00
		Actinide	1.01	1.01	1.01	1.01	1.03	1.02	0.95	0.91	0.96
		Total	1.02	1.02	1.02	1.01	1.00	0.99	0.99	0.98	1.00
	5 cy burn	FP	1.02	1.02	1.02	1.01	0.99	0.97	0.99	0.98	0.99
		Actinide	1.00	1.00	1.00	1.01	1.03	1.01	0.92	0.89	0.93
		Total	1.02	1.02	1.02	1.01	1.00	0.98	0.98	0.97	0.98

Note: The unit of decay heat is W/tU and “aE+b” means “a×10^b.”

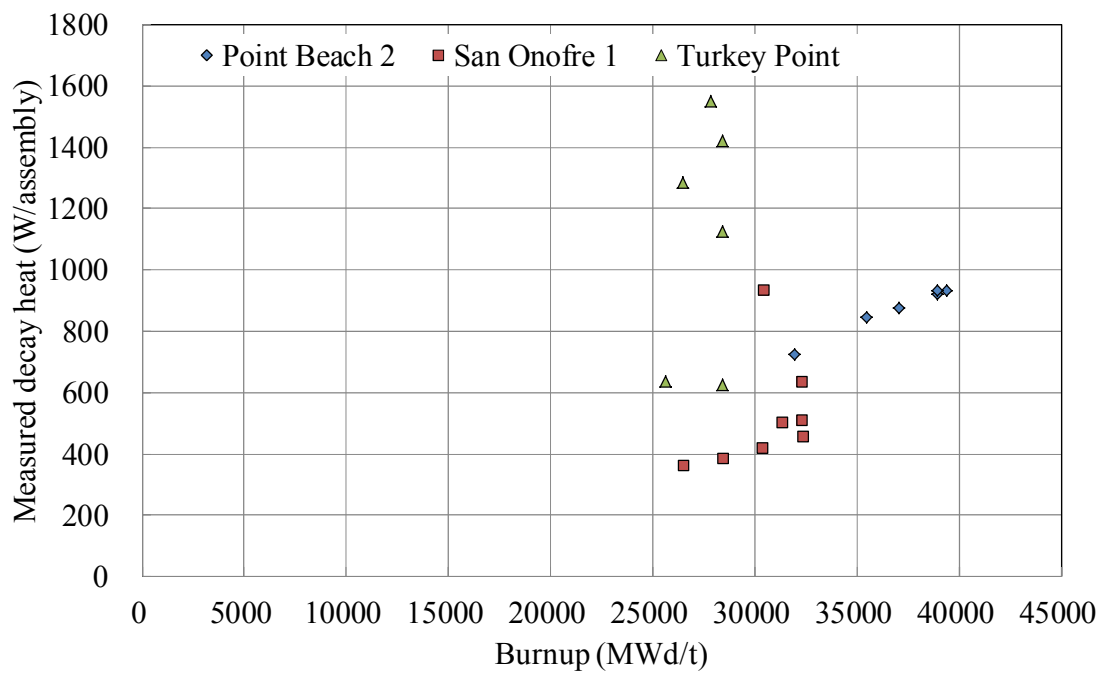


Figure S5 Measured decay heat of irradiated U. S. PWR fuel assemblies as a function of assembly average burnups [13].

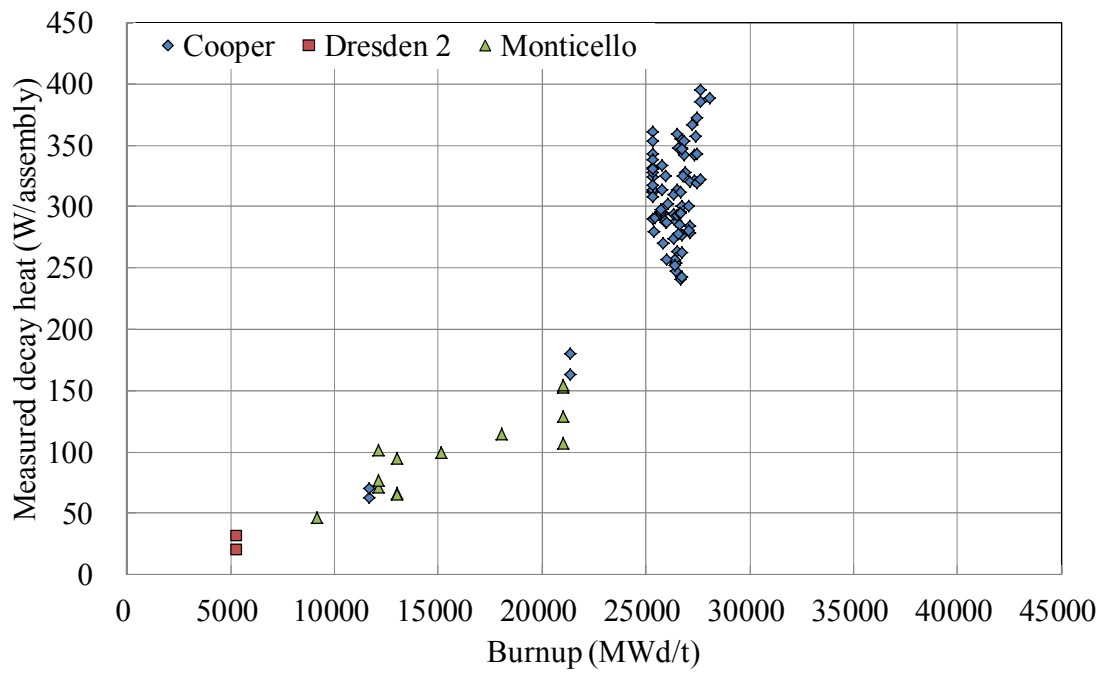


Figure S6 Measured decay heat of irradiated U. S. BWR fuel assemblies as a function of assembly average burnups [13].

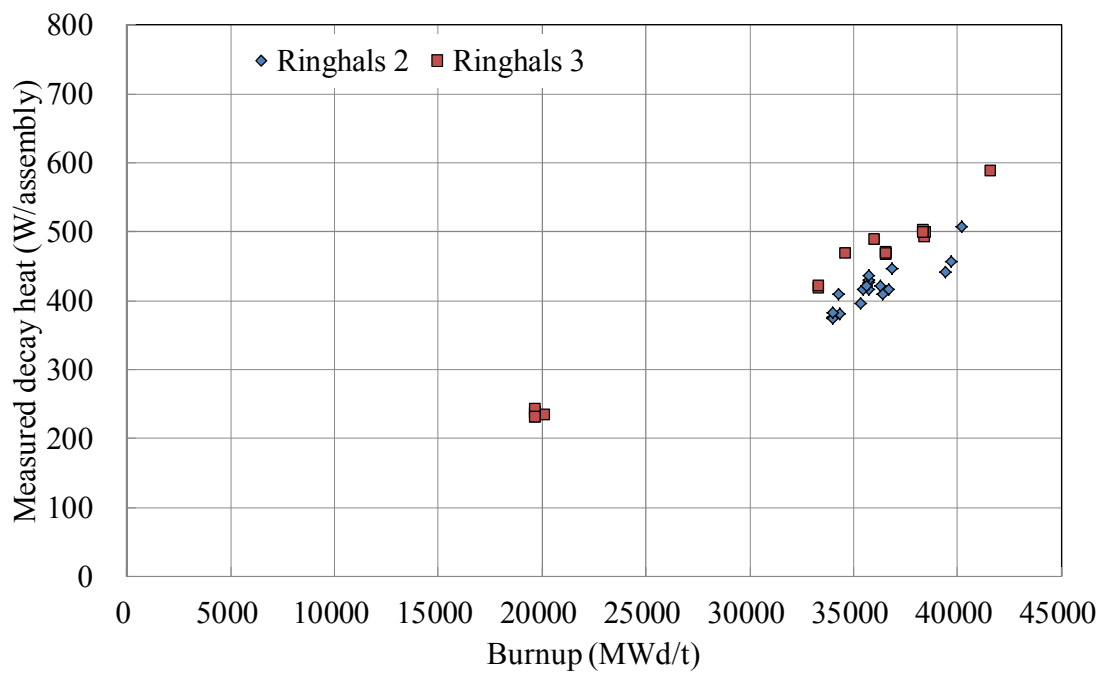


Figure S7 Measured decay heat of irradiated Swedish PWR fuel assemblies as a function of assembly average burnups [13].

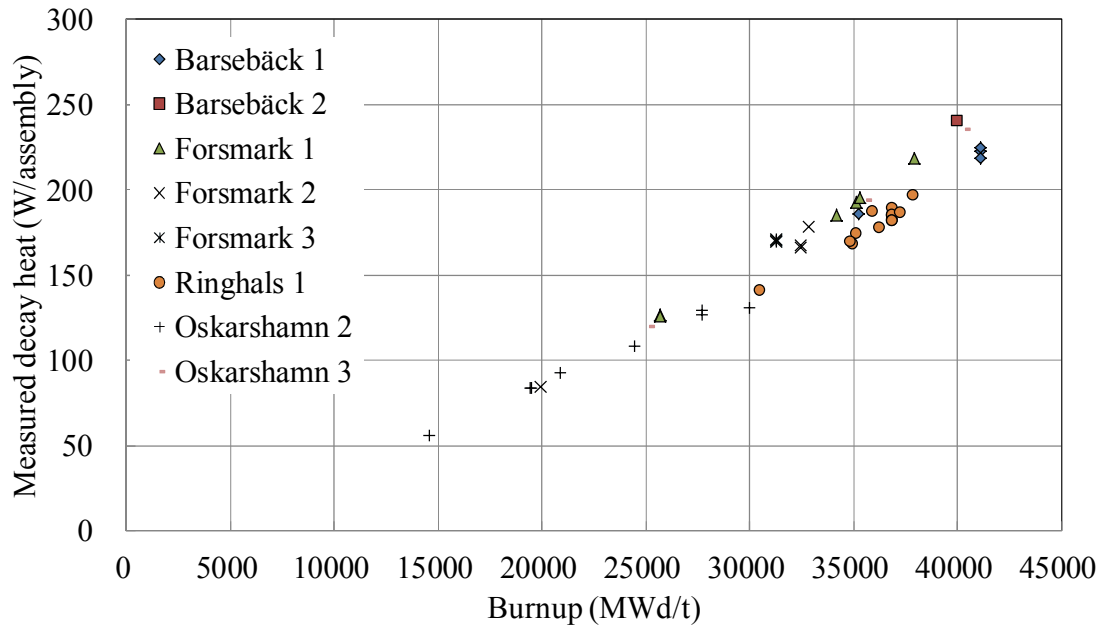


Figure S8 Measured decay heat of irradiated Swedish BWR fuel assemblies as a function of assembly average burnups [13].

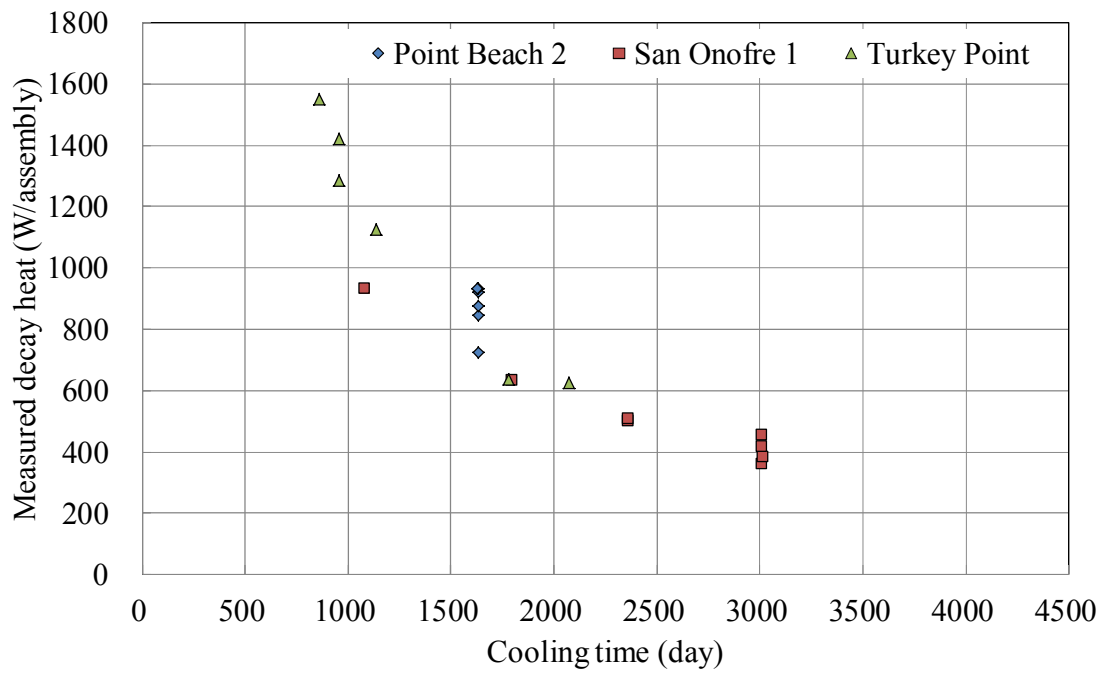


Figure S9 Measured decay heat of irradiated U. S. PWR fuel assemblies as a function of cooling time [13].

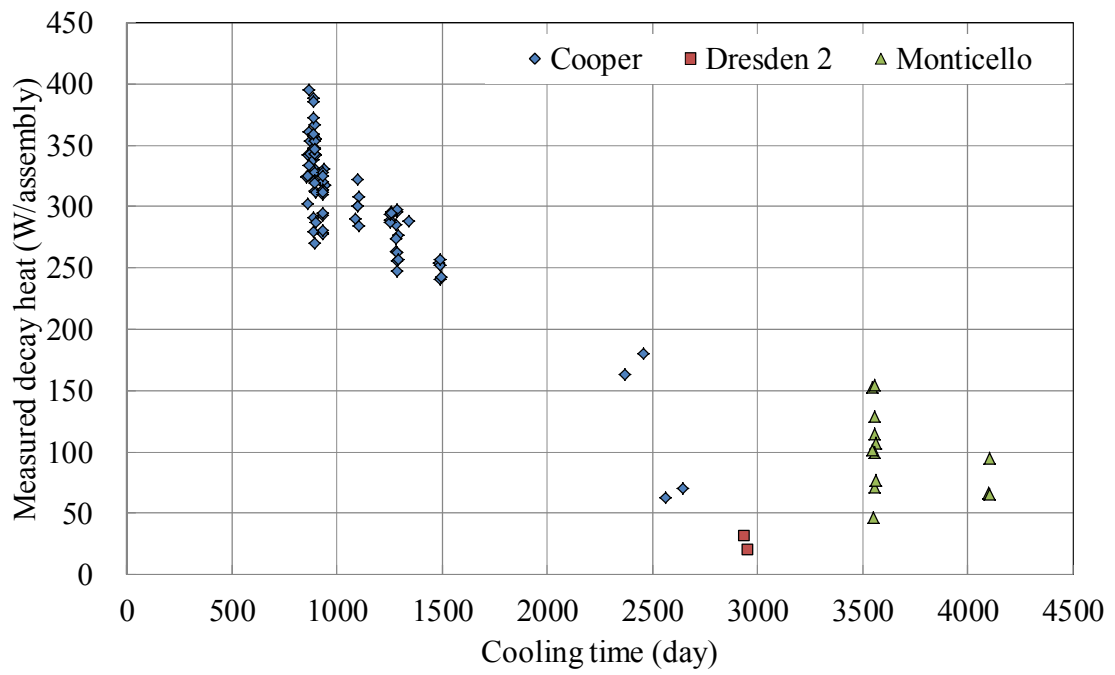


Figure S10 Measured decay heat of irradiated U. S. BWR fuel assemblies as a function of cooling time [13].

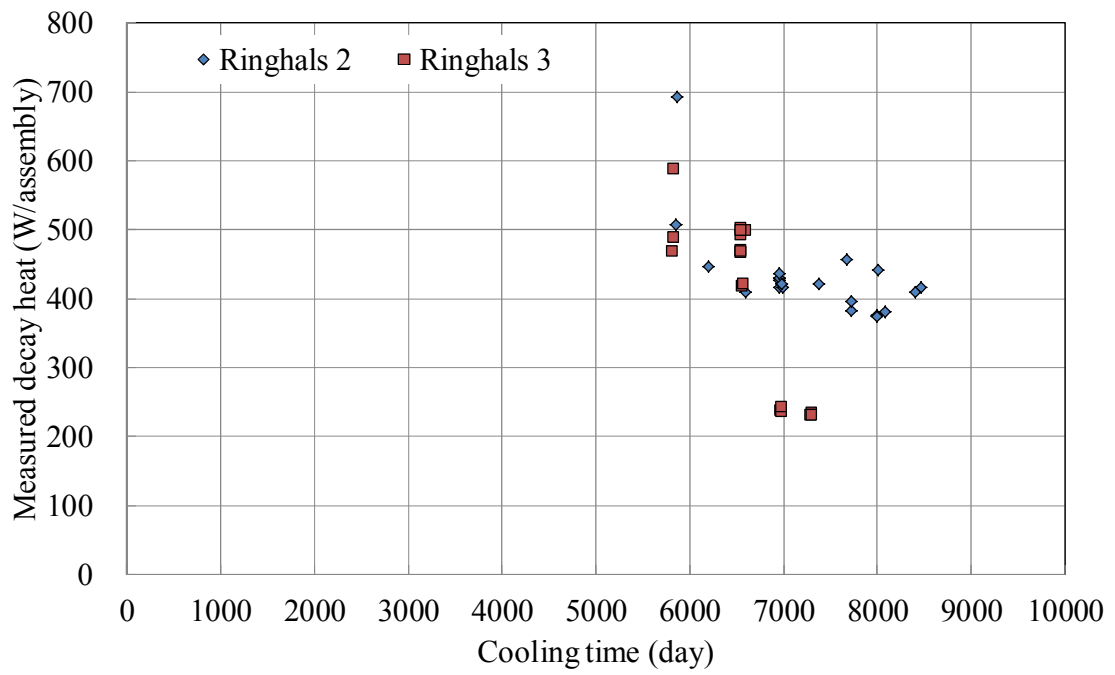


Figure S11 Measured decay heat of irradiated Swedish PWR fuel assemblies as a function of cooling time [13].

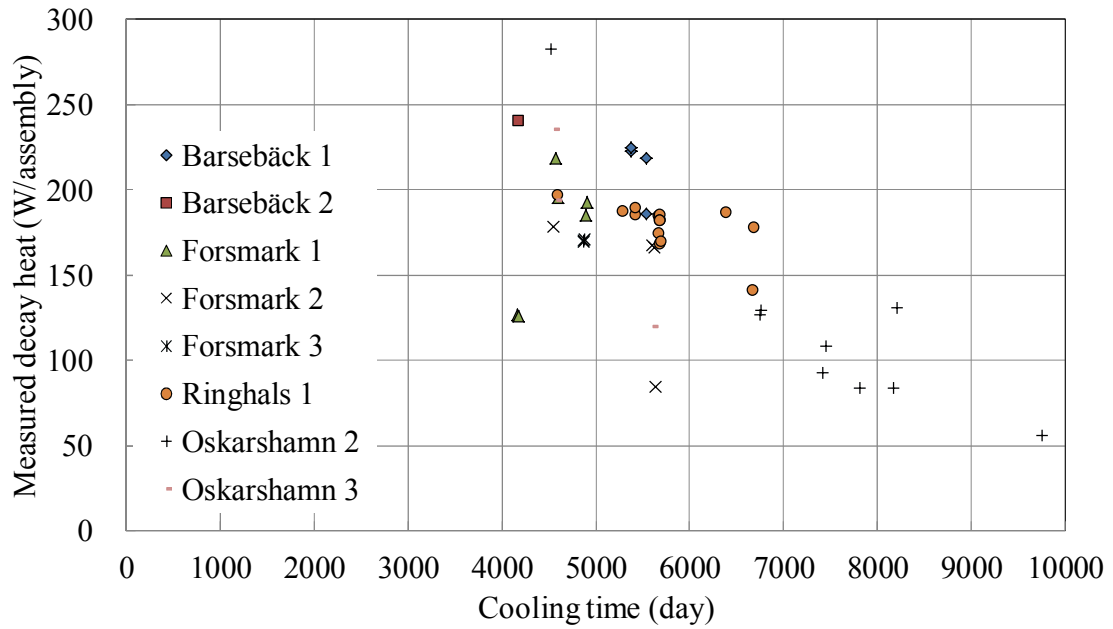


Figure S12 Measured decay heat of irradiated Swedish BWR fuel assemblies as a function of cooling time [13].

Table S4 Sensitivity of calculated decay heat (W/tU) to fuel assembly burnup for the U.S. PWR and BWR fuel assemblies and in-channel moderator density for the BWR fuel assemblies.

Reactor type	Reactor	Fuel assembly type	Assembly ID	Enrichment (wt%)	Nominal burnup (MWd/t)	Cooling time (day)	Nominal decay heat (W/tU)			
							(Ratio of modified to nominal decay heat) ^a			
							< Ratio of modified to nominal decay heat > ^b			
							FP	Actinide	Activation	Total
PWR (U.S.A)	Point Beach	14×14	C-52	3.397	31914	1635	1561.6 (1.06)	211.5 (1.13)	58.5 (1.06)	1831.7 (1.07)
	San Onofre	14×14	C-01	3.865	26540	3011	761.2 (1.05)	142.9 (1.10)	84.2 (1.06)	988.3 (1.06)
	Turkey Point	15×15	B-43	2.559	25595	1782	1169.3 (1.06)	168.9 (1.12)	45.9 (1.05)	1384.1 (1.07)
	Turkey Point	15×15	D-34	2.557	27863	859	3252.3 (1.05)	240.6 (1.10)	70.4 (1.04)	3563.4 (1.05)
BWR (U.S.A)	Cooper	7×7	CZ102	1.090	11667	2565	332.2 (1.05) <1.00>	72.3 (1.07) <0.97>	1.0 (1.04)	405.5 (1.05) <1.00>
	Cooper	7×7	CZ147	2.500	26709	1294	1306.4 (1.06) <1.00>	178.2 (1.11) <0.96>	2.3 (1.03)	1486.8 (1.07) <0.99>
	Dresden	7×7	DN212	2.130	5280	2938	156.2 (1.05) <1.00>	12.3 (1.08) <0.97>	0.2 (1.06)	168.7 (1.05) <1.00>
	Monticello	7×7	MT116	2.25	18039	3559	454.4 (1.05) <1.00>	93.5 (1.08) <0.97>	0.8 (1.03)	548.6 (1.05) <1.00>

^a: Ratio of the calculated decay heat with fuel assembly burnup increased by 5% to that with the nominal value.

^b: Ratio of the calculated decay heat with in-channel moderator density increased by 10% to that with the nominal value.

Table S5 Sensitivity of calculated decay heat (W/tU) to fuel assembly burnup for the Swedish PWR and BWR fuel assemblies and in-channel moderator density for the BWR fuel assemblies.

Reactor type	Reactor	Fuel assembly type	Assembly ID	Enrichment (wt%)	Nominal burnup (MWd/t)	Cooling time (day)	Nominal decay heat (W/tU)			
							(Ratio of modified to nominal decay heat) ^a			
							< Ratio of modified to nominal decay heat > ^b			
FP	Actinide	Activation	Total							
PWR (Sweden)	Ringhals 2	15×15	C01	3.095	36688	8468	596.6 (1.04)	354.6 (1.10)	4.5 (1.05)	955.7 (1.06)
	Ringhals 3	17×17	0C9	3.101	38442	8468	728.6 (1.04)	382.2 (1.11)	11.3 (1.06)	1122.0 (1.07)
	Ringhals 3	17×17	2A5	2.100	20.107	7297	366.4 (1.05)	163.1 (1.07)	5.7 (1.05)	535.2 (1.05)
BWR (Sweden)	Barsebäck 1	8×8-1	9329	2.920	41127	5371	839.7 (1.04) <1.00>	387.8 (1.13) <0.97>	7.3 (1.05)	1234.8 (1.07) <0.99>
	Forsmark 1	8×8-1	3838	2.086	25669	4170	520.7 (1.05) <1.00>	243.5 (1.10) <0.97>	5.1 (1.05)	769.3 (1.06) <0.99>
	Forsmark 2	SVEA 64	11494	2.920	32431	5618	675.3 (1.04) <1.00>	228.2 (1.11) <0.97>	5.5 (1.05)	909.0 (1.06) <0.99>
	Ringhals 1	8×8-1	1177	2.642	36242	6690	654.7 (1.04) <1.00>	328.7 (1.11) <0.97>	3.7 (1.05)	987.1 (1.07) <0.99>
	Oskarshamn 2	8×8-1	1377	2.201	14546	9750	237.3 (1.05) <1.00>	81.6 (1.06) <0.97>	0.6 (1.05)	319.5 (1.05) <1.00>

^a: Ratio of the calculated decay heat with fuel assembly burnup increased by 5% to that with the nominal value.

^b: Ratio of the calculated decay heat with in-channel moderator density increased by 10% to that with the nominal value.