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Summary of the Findings of NEA WPNCS Subgroup 16 on the OE2 Benchmarks for PWR UO₂ Decay Heat

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**OECD Nuclear Energy Agency
STEERING COMMITTEE FOR NUCLEAR ENERGY**

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for PWR UO₂ Decay Heat**

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Foreword

Under the guidance of the Nuclear Energy Agency (NEA) Nuclear Science Committee (NSC), the Working Party on Nuclear Criticality Safety (WPNCS) deals with technical and scientific issues relevant to criticality safety.

This report summarises the findings obtained by Subgroup (SG) 16 of the WPNCS, which ran for two years from January 2024 to December 2025. SG-16 was dedicated to defining and running two decay heat benchmarks, to comparing calculated and measured values, and to comparing calculated values between themselves.

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List of abbreviations and acronyms

ASNR	Nuclear Safety and Radiation Protection Authority (France)
BASE	Federal Office for the Safety of Nuclear Waste Management (Germany)
BGZ	Berlin Society for International Co-operation (Germany)
BOL	Beginning of life
BWR	Boiling water reactor
CEA	French Alternative Energies and Atomic Energy Commission (France)
CIEMAT	Centre for Energy, Environmental and Technological Research (Spain)
CRIEPI	Central Research Institute of Electric Power Industry (Japan)
EDF	Électricité de France
ENDF	Evaluated nuclear data file
EOL	End of life
GRS	German Institute for Nuclear Safety
IFIC	Institute for Corpuscular Physics (Spain)
KIT	Karlsruhe Institute of Technology (Germany)
LANL	Los Alamos National Laboratory (United States)
JSI	Jožef Stefan Institute (Slovenia)
MOX	Mixed oxide
NAGRA	National Co-operative for the Disposal of Radioactive Waste (Switzerland)
NNL	National Nuclear Laboratory (United Kingdom)
NSC	Nuclear Science Committee (NEA)
ORNL	Oak Ridge National Laboratory (United States)
PSI	Paul Scherrer Institute (Switzerland)
PWR	Pressurised water reactor
RR	Reaction rate
SCK-CEN	Belgian Nuclear Research Centre
SG	Subgroup
SKB	Swedish Nuclear Fuel and Waste Management Company
SNF	Spent nuclear fuel
NEA	Nuclear Energy Agency
UNF	Used nuclear fuel
VTT	Technical Research Centre of Finland
WPNCs	Working Party on Nuclear Criticality Safety (NEA)
WTI	Scientific-technological information (Germany)

Executive summary

The estimation of the decay heat is of prime importance for the safe and efficient handling, transport, storage, reprocessing and long-term disposal of spent nuclear fuel (SNF, also called used nuclear fuel, or UNF). In 2024, participants in the Nuclear Energy Agency's Working Party on Nuclear Criticality Safety (WPNCS) published a state-of-the-art document summarising the current knowledge in the estimation of the SNF decay heat (Rochman et al., 2024), prompting a follow-up study dedicated to a realistic case in order to review the methods discussed in SG-12. Subgroup 16 (SG-16) was consequently designed to define and run two decay heat benchmarks (a two-dimensional pincell and assembly) (Rochman, 2024). These benchmarks were defined based on the 0E2 17×17 PWR UO₂ assembly, irradiated at Sweden's Ringhals-3 reactor. The initial ²³⁵U enrichment is 3.1% and the reached burn-up at end of life is 41.6 MWd/kg. Six calorimetric measurements for the assembly decay heat were performed at the Central Interim Storage Facility for Spent Nuclear Fuel (Clab), with cooling times between 16 and 22 years.

Eighteen participating institutions performed the required calculations, leading to 43 calculations for the assembly benchmark, and 38 for the pincell benchmark. Different combinations of simulation codes and libraries were used, with nonetheless a high number using the Monte Carlo transport code SERPENT2 and the nuclear data library evaluated nuclear data file (ENDF)/B-VII.1. Together with the calculated decay heat at the measurement periods, participants were also required to provide additional quantities (about 160 in total), such as the neutron multiplication factor for an infinite medium k_{∞} , actinides and fission products concentrations for different burn-up values and cooling times. Finally, the individual decay heat rate values for the main contributors were also requested. Apart from the decay heat rate values, requested quantities were not measured and were only compared between themselves.

The main conclusions are that the pincell benchmark leads to a systematic overestimation of the calculated decay heat, with an average bias of +2.6% (or 14 W, and a standard deviation of 0.9%), whereas the assembly benchmark allows a more satisfactory estimation of the measured decay heat, with an average bias of -1.1% (or 6 W) and a standard deviation of the calculated values of 1.2%. In the case of the pincell benchmark, the overestimation is due to a H/U concentration ratio (related to the moderation factor), which does not correspond to the measured assembly. Other calculated quantities have shown various ranges of dispersion. In the case of assembly k_{∞} at the beginning of irradiation, the spread (one standard deviation) is close to 370 pcm, similar to the value obtained in SG-10 (Carmouze et al., 2023). For the ¹⁴⁸Nd concentration at the end of irradiation, a spread of 1% is obtained, very close to (Carmouze et al., 2023), too.

1. Introduction

This report summarises the findings obtained by Subgroup (SG) 16 of the NEA Working Party on Nuclear Criticality Safety (WPNCS), which ran for two years from January 2024 to December 2025. SG-16 was dedicated to defining and running two decay heat benchmarks, to comparing calculated and measured values, as well as comparing calculated values between themselves. Additional conclusions of SG-16 are detailed in an extended publication (Rochman, forthcoming), and short descriptions of the main findings are presented in the following.

Decay heat is one of the main characteristics to be assessed for a safe and economical handling of spent nuclear fuel (SNF) assemblies. Motivations and measurement and calculation methods were extensively presented in (Rochman et al., 2024), as a deliverable of the previous Subgroup on decay heat (SG-12). One of the remaining questions after the completion of SG-12 was related to the ability to calculate decay heat for a typical pressurised water reactor (PWR) UO₂ assembly. The assessment for other types of fuel or reactor is also of high importance; nonetheless a representative case, the 0E2 assembly, was selected at first. This assembly represented several advantages: fuel and design data were in the public domain, as well as its simplified irradiation history. Additionally, various calorimetric measurements were performed for this assembly (at the Clab facility, Sweden) and published in public reports. Finally, decay heat calculations for this assembly were previously performed and published, indicating the high quality of the measurements, as well as the availability of all necessary information to perform simulations.

The 0E2 assembly was irradiated at the Ringhals 3 reactor for a total of four consecutive cycles, from 1984 to 1988. The final burn-up for the assembly was 41.6 MWd/kg (kg of initial uranium) and the initial ²³⁵U enrichment was 3.1%. The original description for the assembly, its irradiation history and measurements were published by the Swedish Nuclear Fuel and Waste Management Company (SKB) and Oak Ridge National Laboratory (ORNL) (original references can be found in (Rochman, 2024)). In total, six decay heat measurements were reported for cooling periods between 16 and 22 years. Based on the available information, two benchmarks were created, as defined in (Rochman, 2024): one for a pincell and one for an assembly. Both cases are two-dimensional models. The pincell benchmark is obtained from one of the 17×17 fuel rods, and there were no modifications of its dimensions to obtain a modified pincell representative of the assembly. It was therefore expected that the calculated decay heat from the pincell benchmark would differ from the assembly benchmark. The advantage of the pincell benchmark was its simplicity and short simulation time.

A number of different quantities were requested from the participants: the six decay heat rate values at the measurement times, the contributions from a specific number of nuclides (the most relevant fission products and actinides, covering more than 99% of the total decay heat for the specified cooling times), the k_{∞} , and the number densities for a set of nuclides, at the beginning and end of each reactor cycle. In order to help disentangle differences in decay heat values, fission rates were also requested at the end of each cycle. Information about codes, nuclear data libraries and possible selected options were also requested. All specifications were detailed in (Rochman, 2024) and extensively checked by the participants. Rochman (2024) remained the unique description of the benchmarks for the entire SG-16, without modifications.

2. Submitted results and analysis

In total, 38 results were submitted for the pincell model, and 43 for the assembly model. The list of used codes and nuclear data libraries is presented in Table 1. It can be observed that a variety of codes and libraires, both deterministic and Monte Carlo codes, were used as well as recent libraries and relatively historical ones. One of the characteristics of the participants' selection is the high number of cases for the Monte Carlo code SERPENT, as well as for the evaluated nuclear data file ENDF/B-VII.1 library.

Table 1. Type and number of neutron transport codes and nuclear data libraries, associated with the model case

Code	Pincell	Assembly	Library	Pincell	Assembly
SERPENT	16	14	ENDF/B-VII.0	1	1
MVP	4	4	ENDF/B-VII.1	15	19
MCNP(X)	3	9	ENDF/B-VIII.0	5	4
TRITON	3	3	ENDF/B-VIII.1	2	1
ORIGEN	0	4	JEFF-3.1.1	4	3
POLARIS	1	1	JEFF-3.2	2	3
DARWIN	1	1	JEFF-3.3	2	3
HELIOS2	1	2	JENDL-4.0	3	3
VESTA	1	1	JENDL-5.0	3	3
CASMO5	1	3	JEF-2.2	1	0
SNF-1.7	0	1	Other	0	3
DRAGON	7	0			

Consequently, the simple analysis of the submitted results would be biased towards this code and library, being not representative of actual calculations performed within possible institutional constraints. A method was then developed to provide averages and standard deviations solely based on results coming from unique codes, nuclear data libraries and modellers (or users). The number of combinations is relatively large (a few thousand) but can be estimated with a simple Monte Carlo search. This was performed and (Rochman, forthcoming) contains results based on this approach and based on simple statistics from the submitted values. Examples are provided in (Rochman, forthcoming), and an example is given in Table 2.

Table 2. Example of calculated quantities in the case of the pincell and assembly benchmarks. Values with a \pm sign are average $\pm 1\sigma$, whereas values within solid brackets ([]) are 95%/95% tolerance limits

Quantity	k_{∞}^{BOL} (-)	$^{238}\text{U}^{\text{BOL}}$ RR (%)	$^{235}\text{U}^{\text{BOL}}$ RR (%)	$^{148}\text{Nd}^{\text{EOL}}$ (g/tHM)
Pincell model				
All	[1.26094 – 1.28439]	[5.7 – 6.7]	[93.2 – 94.3]	[450.5 – 472.9]
All	1.27266 \pm 0.00482	6.2 \pm 0.2	93.8 \pm 0.2	461.7 \pm 4.6
ULC	1.27236 \pm 0.00456	6.4 \pm 0.3	93.8 \pm 0.3	462.3 \pm 4.2
U	1.27277 \pm 0.00597	6.3 \pm 0.3	93.7 \pm 0.3	462.5 \pm 4.8
L	1.27476 \pm 0.00700	6.3 \pm 0.3	93.7 \pm 0.3	462.2 \pm 4.2
C	1.27119 \pm 0.00418	6.3 \pm 0.3	93.7 \pm 0.3	462.6 \pm 4.4
Assembly model				
All	[1.27645 – 1.29497]	[5.0 – 6.3]	[93.7 – 94.9]	[451.7 – 473.0]
All	1.28571 \pm 0.00381	5.7 \pm 0.3	94.3 \pm 0.3	462.3 \pm 4.5
ULC	1.28538 \pm 0.00371	5.7 \pm 0.2	94.3 \pm 0.2	462.6 \pm 4.6
U	1.28539 \pm 0.00411	5.7 \pm 0.2	94.3 \pm 0.2	463.5 \pm 4.3
L	1.28591 \pm 0.00305	5.6 \pm 0.2	94.3 \pm 0.2	461.8 \pm 4.8
C	1.28488 \pm 0.00482	5.8 \pm 0.3	94.2 \pm 0.3	462.7 \pm 3.9

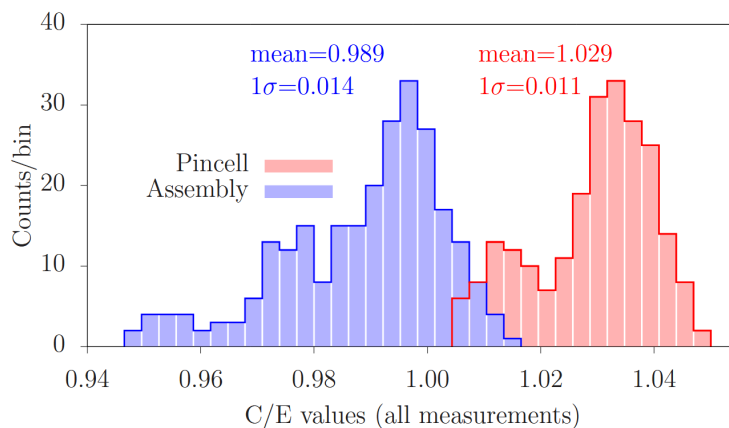
Note: Figures in bold are indicated reference values. RR refers to reaction rates.

In this table, simple averages and standard deviations are given in the “All” row, whereas results based on unique users, libraries and codes are presented in the row named “ULC”. Similarly, the three following rows (named U, L and C) present the results with either a unique user (U), unique library (L), or unique codes (C). It can be seen for instance that differences are generally small, but this is not systematically observed, as in the case of k_{∞} at the beginning of life (BOL). Additional details will be provided in a supporting publication (Rochman, upcoming).

2.1. Results for decay heat

The different values for the calculated decay heat at the six cooling times were compared to measurements. Figure 1 presents the histograms for all C/E (calculated over experimental) values for both the pincell (in red) and assembly (in blue) benchmarks. Averages and standard deviations are also indicated. The first observation is that for the pincell benchmark, the C/E values are systematically higher than C/E=1, due to a different moderation factor, not corresponding to the actual 0E2 assembly.

Figure 1. Distributions of the decay heat C/E values for the six measurements (directly from the submitted values)

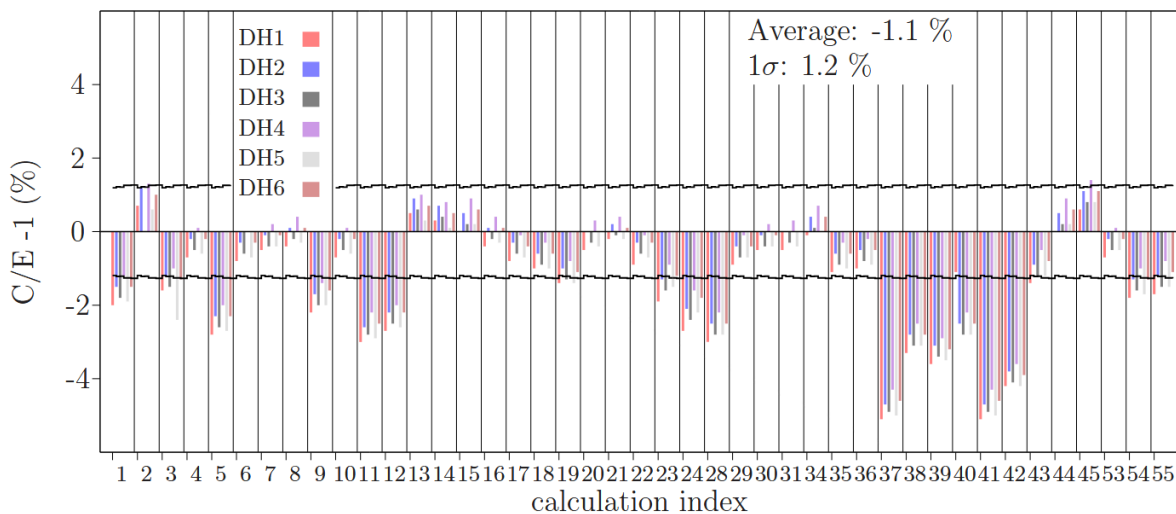


For the assembly model, there is on average a slight underestimation, but the agreement with the measured values is more satisfactory. It can be observed that both distributions are not Gaussian, implying that one standard deviation does not cover 68% of probability. Additional statistical quantities can be found in (Rochman, forthcoming), including tolerance limits.

For the assembly benchmark, individual cases are presented in Figure 2. For each submitted case, six C/E values were obtained, corresponding to the six measurement times. Therefore each “calculation index” corresponds to the submitted results (equal to 43 for the assembly benchmark) and the detailed table (providing corresponding codes, nuclear data libraries and institutes) can be found in (Rochman, forthcoming). It can be seen that there is a consistency between the C/E values for each participant: the six C/E values are generally very close to each other, emphasising that no cooling-time dependent bias is observed. Additionally, groups of results can be seen, for instance from index 37 to 42, corresponding to the same institute and same code. In this case, the observed variations are due to the change of the nuclear data library.

Finally, in the case of the assembly benchmark, the bias and standard deviation for the C/E-1 value resulted in $(-1.1 \pm 1.4) \%$ if the full results are analysed, and $(-1.1 \pm 1.2) \%$ if the unique appearances of users, codes and nuclear data libraries (ULC values) is considered. Both sets of values are very similar and given the reported experimental uncertainties (varying from 1.2 to 1.3%), the overlap can be considered satisfactory, indicating a modest bias.

Figure 2. Relative differences between measured and calculated decay heat for the assembly benchmark



Note: Experimental uncertainties are indicated in solid horizontal black lines. Indexes correspond to specific calculations performed by different institutes and modellers.

2.2. Results for other quantities

As mentioned, many calculated quantities were requested for the benchmark comparisons. They include reaction rates, nuclide concentrations, neutron multiplication factors, decay heat contributors, all of them for different irradiation and cooling times. Details of these values and differences are given in (Rochman, upcoming), and a summary is provided in Table 3. This table indicates quantities at the end of life (EOL) for both benchmarks, except for the decay heat, where global C/E-1 are provided for the six measurements.

Concerning the neutron multiplication factor k_{∞} , the spreads can be considered large at EOL and can originate from many factors (e.g. different nuclear data libraries, different nuclide concentrations). The comparison was also performed at the BOL, where a spread of 370 pcm was observed, in agreement with the results from (Carmouze et al., 2023). In the case of ^{148}Nd , a spread of 1% among calculated values was obtained, also in agreement with (Carmouze et al., 2023). While many parameters of the simulations were imposed in the benchmark definitions, differences in number densities, k_{∞} , as well as reaction rates are not negligible. This information can be considered when performing uncertainty assessment for depletion and decay calculation, as well as criticality calculations of spent fuel: variations of concentrations for actinides and fission products can certainly affect radioactive and criticality values. It was nevertheless noticed during the subgroup discussions that, when performing burn-up calculations under strict quality-assurance conditions, the spread of values presented in Table 3 would be significantly smaller.

Table 3. Summary table of the calculated uncertainties (Δ corresponds to 1σ) for both benchmarks

	Pincell	Assembly		Pincell	Assembly
Decay heat	(+2.6 ± 0.9) %	(-1.1 ± 1.2) %	Δk_{∞}	± 551 pcm	± 1225 pcm
RR $\Delta^{235}\text{U}$	± 1.9 %	± 1.8 %	RR $\Delta^{238}\text{U}$	± 3.1 %	± 1.1 %
RR $\Delta^{239}\text{Pu}$	± 0.4 %	± 0.7 %	RR $\Delta^{241}\text{Pu}$	± 1.3 %	± 1.2 %
$\Delta^{234}\text{U}$	± 2.6 %	± 2.0 %	$\Delta^{235}\text{U}$	± 2.1 %	± 1.9 %
$\Delta^{236}\text{U}$	± 1.0 %	± 0.7 %	$\Delta^{238}\text{U}$	± 0.08 %	± 0.08 %
$\Delta^{238}\text{Pu}$	± 3.7 %	± 3.9 %	$\Delta^{239}\text{Pu}$	± 1.0 %	± 1.8 %
$\Delta^{240}\text{Pu}$	± 1.8 %	± 2.5 %	$\Delta^{241}\text{Pu}$	± 1.8 %	± 1.3 %
$\Delta^{242}\text{Pu}$	± 2.9 %	± 1.6 %	$\Delta^{241}\text{Am}$	± 9.7 %	± 12 %
$\Delta^{242m}\text{Am}$	± 23 %	± 20 %	$\Delta^{243}\text{Am}$	± 4.8 %	± 6.4 %
$\Delta^{242}\text{Cm}$	± 7.0 %	± 8.1 %	$\Delta^{243}\text{Cm}$	± 12 %	± 14 %
$\Delta^{244}\text{Cm}$	± 6.5 %	± 5.2 %	$\Delta^{90}\text{Sr}$	± 1.0 %	± 0.9 %
$\Delta^{134}\text{Cs}$	± 4.8 %	± 5.3 %	$\Delta^{137}\text{Cs}$	± 1.2 %	± 0.9 %
$\Delta^{148}\text{Nd}$	± 0.9 %	± 1.0 %	$\Delta^{154}\text{Eu}$	± 6.1 %	± 3.1 %

Note: For the decay heat, the C/E - $1 \pm 1\sigma$ over the six measurements is given. RR means fission reaction rates. For all quantities except the decay heat, values are given at EOL. If not specified, uncertainties concern nuclide concentrations.

Note that in the case of ^{241}Am , a nuclide relevant for interim storage, its concentration strongly increases with cooling times as long as ^{241}Pu significantly decays by beta emission. The spread indicated in Table 3 significantly reduces with cooling time to reach values close to the one for ^{241}Pu .

3. General remarks

Details of the individual participant results analysed during the subgroup activity can be found in a supplemental publication (Rochman, forthcoming).

Decay heat: Concerning the pincell benchmark, it has led to an overestimation of the calculated decay heat compared to the measurements, with an average bias C/E -1 of $(+2.6 \pm 0.9)\%$. In terms of C-E, this bias corresponds to $+14 \pm 5$ W. This comes from a different moderator ratio, leading to a larger production of actinides compared to the assembly benchmark. For the assembly benchmark, more accurate calculated decay heat values were obtained, with an average bias C/E -1 of $(-1.1 \pm 1.2)\%$. In terms of C-E, this bias corresponds to -6 ± 7 W. The assembly benchmark is therefore recommended to obtain better agreement with the measured decay heat. Given the reported experimental uncertainties (close to 1.2%), the agreement between measured and calculated decay heat values can be judged satisfactory. Different implications can arise, depending on national constraints, for the safety and economics of installations where spent fuel decay heat is a relevant quantity.

Nuclide compositions, k_{∞} and reaction rates: Different values are obtained between both the pincell and the assembly benchmarks, but more relevant is the spread of calculated quantities among the participants. It was found that the dispersions are not negligible, reflecting various effects, including nuclear data, codes and users. Calculations such as those performed in criticality safety can also be affected by such spreads of values.

4. Conclusion

Two two-dimensional decay heat benchmarks were created in the context of the NEA WPNCs SG-16, based on the 0E2 PWR UO₂ Westinghouse 17×17 assembly, irradiated at the Ringhals-3 reactor in Sweden. One simplified benchmark consists of a pincell model, whereas the other benchmark represents an assembly, both being two-dimension models. The initial ²³⁵U enrichment was 3.1%, and the assembly irradiated for four cycles, up to 41.6 MWd/kg. Calorimetric decay heat measurements at the Clab facility were realised for this assembly for cooling times between 16 and 22 years. Six values are used in these benchmarks.

A total of 38 pincell and 43 assembly calculations were performed by 21 participants, providing the following quantities: decay heat at the time of measurements, the neutron multiplication factor for an infinite medium, reaction rates, nuclide concentrations and decay heat contributors. Such benchmark calculations were performed while the measurement values were already available, but the calculation results were submitted by each participant without knowledge of the results of others.

A large variety of codes, libraries and modelling approaches were used, covering deterministic and Monte Carlo neutron transport (and depletion) codes. The Monte Carlo code SERPENT was used many times and the nuclear data library ENDF/B-VII.1 was also over-represented. To compensate for this effect, averages and standard deviations based on a single code/library/participant representation are also provided with the values directly obtained from the unprocessed set of results. Details of the analysis are presented in (Rochman, forthcoming).

In the case of the pincell benchmark, it was found that the decay heat values are systematically overestimated by all participants, with C/E-1 ± 1σ of (+2.6 ± 0.9)%. This was expected as the moderation ratio is overestimated in the pincell benchmark. For the assembly model, the average bias is smaller, with (-1.1 ± 1.2)%.

In addition, uncertainties are also provided for other unmeasured quantities, such as the neutron multiplication factor k_{∞} at the beginning of irradiation and for each cycle, nuclide concentrations at the end of irradiation, and fission reaction rates. The uncertainties correspond to the spread (1σ) of the results compared to the average calculated quantities. These quantities are also of interest for criticality safety calculations.

5. Future developments

With respect to performing additional decay heat benchmarks, two possibilities were considered during the SG-16 discussions. The first concerns a future blind benchmark, like the one performed and presented in (Jansson et al., 2022). If new calorimetric measurements are performed at Clab, estimating decay heat values (without knowing in advance the measured ones) helps create a realistic situation with a limited amount of information. Such possibility could be realised in 2026 or 2027, depending on the availability of new calorimetric data.

A second possibility concerns repeating the work performed in SG-16, but for a different fuel type, such as a UO₂ boiling water reactor (BWR) assembly, or a mixed oxide (MOX) PWR assembly. An alternative would be to consider a UO₂ PWR assembly with higher initial enrichment, or higher burn-up at the end of life. In principle, the availability of decay heat measurements will be helpful, but one can envisage defining a new benchmark and performing calculations if measurements are not available.

Efforts were focused on the estimation of decay heat for spent nuclear fuel in the case of typical UO₂ PWR assemblies, and there are still validation gaps for different fuel types, higher initial enrichments and higher burn-up.

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