Deliverable 8.6:
Performance of sophisticated and best-practice industry codes based on SKB-50 data and data produced in subtasks 2.2 and 2.3

Work Package 8

Spent Fuel Characterisation and Evolution until Disposal (SFC)

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N°847593.

http://www.ejp-eurad.eu/

Document information

Project Acronym	**EURAD**
Project Title	**European Joint Programme on Radioactive Waste Management**
Project Type	**European Joint Programme (EJP)**
EC grant agreement No.	**847593**
Project starting / end date	**1st June 2019 – 30 May 2024**
Work Package No.	**8**
Work Package Title	**Spent Fuel Characterisation and Evolution Until Disposal**
Work Package Acronym	**SFC**
Deliverable No.	**8.6**
Deliverable Title	**Performance of sophisticated and best-practice industry codes based on SKB-50 data and data produced in subtasks 2.2 and 2.3**
Lead Beneficiary	**Uppsala University**
Contractual Delivery Date	**31/05/2024**
Actual Delivery Date	**03/07/2024**
Type	
Dissemination level	**PU**
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To be cited as:

Seidl M., Alvarez-Velarde F., Dagan R., Kierkegaard J., Kromar M., Mosconi M., Plukiene R., Rochman D., Romojaro P., Schillebeeckx P., Shama A., Sjöstrand H., Solans V., Vallet V., Verwerft M., (2024): Title. Final version as of 28.06.2024 of deliverable D8.6 of the HORIZON 2020 project EURAD. EC Grant agreement no: 847593.

Disclaimer

Acknowledgement

This document is a deliverable of the European Joint Programme on Radioactive Waste Management (EURAD). EURAD has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 847593.

Status of deliverable		
	By	Date
Delivered	M. Seidl	27.05.2024
Verified	H. Sjöstrand	30.05.2024
Reviewed	P. Schillebeeckx	27.06.2024
Approved (PMO)	P. Carbol	30.06.2024
Submitted to EC	Andra (Coordinator)	03.07.2024

Executive Summary

Characterisation of spent nuclear fuel is required for a safe, ecological, and economical handling, transport, storage and disposal. The main observables of interest are the neutron and gamma-ray emission properties, decay heat, reactivity, long-term radiotoxicity and the inventory of fissile nuclides and mobile long-lived radionuclides. In most industrial circumstances these characteristics can only be reliably estimated by theoretical calculations using validated depletion codes. One of the main objectives of WP8 of EURAD was to assess the performance of these codes of different levels of sophistication by a comparison with experimental data. New experimental data from post-irradiation experiments, non-destructive assay and calorimetry produced within EURAD were taken into account in addition to experimental data available in the SFCOMPO database and reported in the open literature. The main conclusions are summarised in the following. The effect of nuclear data to calculate nuclide concentrations and related observables is as important as fuel related input data. This particularly concerns fission yields and neutron capture on heavy actinides. The quality of calculations, in particular for observables with a non-linear dependence on burnup and a burnup with spatial dependence, can be improved by providing detailed fuel and irradiation history parameters from a 3D core simulator. Significant differences are observed in calculated observables and their uncertainties using nuclear data from different evaluated nuclear data libraries. Therefore, to improve the sophistication of depletion codes the main recommendations are: creation of a dedicated reference data book for depletion code validation and a project for the establishment of recommended, evaluated nuclear data for backend purposes. Use of 3D core simulator data to provide detailed fuel irradiation histories. Further development of detection systems based on total neutron and gamma-ray emission measurements to verify depletion calculations. Since spent fuel observables many decades into the future can only be predicted by theoretical calculations these recommendations will further reduce uncertainties, enhance the safety case and allow for more economical solutions of final disposal.

Keywords

Blind test, Burnup, Decay heat, Depletion calculations, Gamma-ray emission, Neutron emission, Nuclide inventory, Spent nuclear fuel

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Glossary

BU	Burnup
BWR	Boiling water reactor
Clab	Central interim storage facility for spent nuclear fuel
CMSYS	Core management system
CT	Cooling time
DDEP	Decay data evaluation project
DDSI	Differential die-away self-interrogation
EFPD	Effective full power day
ERU	Enriched reprocessed uranium
EURAD	European joint programme on radioactive waste management
HLPC	High-performance liquid chromatography
ICP-MS	Inductively coupled plasma mass spectrometry
IE	Initial enrichment
LWR	Light water reactor
MOX	Mixed oxide fuel
ND	Nuclear Data
NDA	Non-destructive assay
PIE	Post irradiation examination
PSI	Paul Scherrer Institute
PWR	Pressurised water reactor
REGAL	Rod-extremity and gadolinia analysis
SFC	Spent fuel characterisation and evolution until disposal
SFCOMPO	Spent fuel isotopic composition
SKB	Swedish nuclear fuel and waste management company
SNF	Spent nuclear fuel

1 Introduction

Characterisation of spent nuclear fuel (SNF) is required for a safe, ecological, and economical handling, transport, storage and disposal. The main observables of interest are the neutron and gamma-ray emission properties, decay heat, reactivity, long-term radiotoxicity and the inventory of fissile nuclides and mobile long-lived radionuclides. Most of them are difficult to measure, in particular under industrial conditions, and depend on a complex inventory of nuclides. Different observables have different rankings of relevant nuclides, and the ranking is a function of the irradiation and decay time. The lists of the most relevant nuclides for criticality safety, decay heat and neutron and gamma-ray emission have been determined in e.g. [1], [2], [3]. Due to the contributions of nuclides with different characteristics, the observables of interest at long cooling times cannot be derived by an extrapolation from estimations at shorter cooling times. Hence, a reliable characterisation of the SNF and an estimation of its characteristics over the next thousands of years can only be determined by theoretical calculations using validated codes.

For decay heat empirical approaches have been developed in the past ([4], [5], [6], [7]), providing, however, in many cases rather conservative estimates. Traditionally for criticality safety analysis the average assembly burnup has been used as a leading parameter [8], with the burnup mostly defined as the cumulative energy release per unit mass of the initial heavy metal (heavy metal refers in the case of UOX fuel to the initial mass of uranium). With increasing requirements to improve margins the focus has shifted to an accurate determination of its nuclide vector which is not only a function of burnup but also depends on the history of the neutron spectrum and the axial and radial profile of power generation among other parameters. To determine the nuclide inventory at the end of irradiation, depletion codes are used which couple the Boltzmann equation for neutron transport with the Bateman equation describing the build-up and decay of nuclides. Once the nuclide inventory after irradiation is determined its evolution can be calculated by following the decay chains again using the Bateman equation. Using this type of calculations avoids too conservative loading schemes, the production of over-engineered casks and canisters for storage and disposal and reduces the volume of underground galleries for geological disposal. However, it requires depletion codes, which are validated by high-quality experimental data to determine safety margins and procedures for safe handling, storage and disposal.

In this EURAD deliverable, the performance of depletion codes was verified using experimental data available in the SFCOMPO database and reported in the open literature together with additional data that were produced within WP8 and specified in EURAD deliverable 8.5. A quantity used to validate the calculations is the ratio between the calculated and experimental estimate of an observable, which will be denoted by C/E. In the report, all uncertainties are standard uncertainties quoted at a 68 % confidence level and are given in standard compact notation. As much as possible the terminology of the International Vocabulary of Metrology is used [9].

2 Depletion codes

2.1 Principles

Various approaches exist to determine the SNF observables of interest. They differ in their level of sophistication. In the following they are referred to as level 1 to 3. In level 1 the fuel assembly is represented as a 1D model. In most cases simplified formulas are implemented, e.g. those available in standards for decay heat calculations. In level 2 the fuel assembly is represented as a 2D model, usually using dedicated neutronics codes. In this representation, a detailed 3D assembly design and irradiation characteristics are approximated, i.e. averaged, into 2D models. In level 3 the fuel assembly is represented as a 3D model. Such a representation allows to account for detailed design and irradiation parameters. Core simulators of nuclear reactors are capable of providing detailed 3D irradiation data (e.g., history of moderator density and power distribution). The assembly models are usually available

with detailed mechanical and nuclear designs (e.g., axial enrichments and spacers) enabling a 3D approach.

Formulas implemented in level 1 codes are available in standards applicable for decay heat calculations (ANS-5.1 [4], DIN-25463 [5],[6] or JAERI [7].). In principle, it is possible to approximate some of the observables such as decay heat and total neutron and gamma-ray emission rates as a function of burnup, enrichment and other parameters (e.g. burnable neutron absorber concentration, neutron energy spectrum). Examples of such approaches are machine learning strategies [10]. However, whether this kind of approach is capable to predict beyond the time horizon given by the training data needs further research.

Level 2 codes are the most widespread and include CASMO [11] , the TRITON/NEWT and POLARIS modules in the SCALE6 [12], [13] code system and DARWIN. Level 2 codes typically assume a fuel assembly within an infinite lattice of identical assemblies (thus implementing reflective boundary conditions) and usually a flat axial power profile. The fuel assembly is represented as a 2D model, usually using dedicated 2D neutronics codes. In this representation, the detailed 3D assembly design and irradiation characteristics are approximated, i.e., averaged, into 2D models. The codes track the nuclide evolutions during the assembly irradiation and its subsequent decay.

Codes capable of level 3 are usually integrated into core simulators like CASCADE-3D [14], SIMULATE [15] or are part of (or add-ons to) codes which can simulate a 3D core power distribution as a function of burnup like Serpent2 [16], [17] or MCNP [18]. The fuel assemblies are represented as a 3D model. At this level of sophistication, it is possible to account for detailed design and irradiation parameters and the axial and radial influence of a fuel assembly's neighbours during irradiation. This includes the radial neutron gradients as well as spectrum shifts from different burnup and fuel compositions (e.g. enrichment, UOX or MOX) in a fuel assembly's neighbourhood. Core simulators of nuclear reactors are capable of providing detailed 3D irradiation data (e.g., history of moderator density and power distribution).

Codes like Serpent2 or MCNP can also be used as level 2 codes if an infinite lattice of identical assemblies is used for the geometry, for example. Serpent2 and MCNP6 have internal depletion capabilities. Versions of MCNP and other neutron transport solvers have been linked to the Bateman solver externally. For example, ALEPH2 [19] and EVOLCODE2 [20] follow this strategy. In some instances, an approach is used which can be described as level 1.5. Fuel assembly properties are treated point-like by averaging 2D or 3D results from level 2 or 3 calculations. Compared to a level 1 approach the relevant equations for neutron transport and nuclide build-up and decay are based on a 1D approximation of more precise 2D or 3D models. An example of such an approach is ORIGEN-ARP [21]. Fuel assembly properties are 1D and the user can select either from a set of pre-calculated macroscopic cross sections for representative PWR or BWR fuel assemblies or perform TRITON/NEWT calculations and convert 2D or 3D results to 1D.

All mentioned codes need information about the irradiation history. This information can be extracted from online core monitoring tools like BEACON [22], GARDEL [23] or POWERTRAX [24], which are based on level 3 depletion codes. They are calibrated periodically to measured core power maps during reactor operation. For example, KWU KONVOI reactors are equipped with an aeroball measurement system [25]. This system consists of small steel balls containing an indicator nuclide, which are pneumatically transported into the reactor core where they are activated in unoccupied guide tube positions. After a few minutes they are transported out of the core onto a measurement table to determine their activation, which determines the axial power distribution at 28 radial positions during each measurement. Subsequently the core wide power distribution is reconstructed with the help of a level 3 code. Finally, the macroscopic cross sections in the core model are adapted to reproduce with a maximum likelihood the measured power distribution [26]. In this way the core power distribution is followed in a level 3 code as a function of time yielding a fuel assembly's power history. From this information the stated average fuel assembly burnup is determined as well as other information like fuel rod of fuel pellet burnup through pin-power reconstruction methods.

For use in level 2 codes, the average fuel assembly burnup is extracted after each cycle from core monitoring results. The full irradiation history is then reconstructed in a simplified form by prescribing the fuel assembly average power versus time history (often assuming a constant average power during each cycle unless more detailed information is provided).

In more sophisticated use of level 2 codes the 3D node-wise burnup distribution is extracted from core monitoring data and the above-described procedure is repeated for each axial node separately (mimicking a level 3 approach). Thus, it is possible to capture the detailed axial changes in the irradiation parameters (e.g., axial power values) and the fuel neutronics and mechanical aspects as well (e.g. axial enrichments and spacers).

In some special cases, for example when a fuel rod is undergoing a post irradiation examination (PIE), the power history for a single rod can also be extracted from core monitoring data by means of pin-power-reconstruction methods. Usually, the uncertainty of the reconstructed irradiation history increases with increasing spatial detail.

2.2 Code inputs: nuclear and fuel data

Results of depletion calculations strongly depend on the quality of the input data. Two types of input are needed: nuclear data (ND) and fuel-related data, i.e. fuel properties and operational history. In addition, due to the complexity of the problem and the lack of detailed engineering characteristics and irradiation conditions, model assumptions have to be made.

The first step towards the determination of the nuclide inventory is to solve the time-dependent (with regard to burnup) neutron transport problem during a fuel assembly's operation in the reactor core. For this purpose, the evolution of specific nuclides [27], [28] is followed (as part of the solution of the coupled neutron transport and Bateman equation [29]) to determine the core's criticality condition, flux levels, among other parameters. This vector is relevant for the reactor operation and monitoring. However, this vector is not necessarily equal to the vector needed for the determination of the SNF characteristics after discharge.

In a second step, the irradiation history is recalculated for the full list of the relevant nuclides for SNF characterisation. This step can account for detailed spatial representation as well (e.g. fuel assembly average or for an axial fuel assembly node or fuel rod), for example using the SNF code [30] of Studsvik's CMS code package. It separates the material regions relevant for the neutronic transport solution from the region detail desired to determine the spent fuel characteristics. Inadvertently, an averaged neutron flux over the regions of interest is used to reduce computational requirements.

Other strategies solve the neutron transport and the Bateman equation simultaneously for all nuclides for which ND is available and for all regions relevant for both neutron transport and SNF characterisation. In this case the storage requirements of the neutronic solution grows quickly as more detail is desired. For example, in the ORIGEN module [30] from SCALE, Serpent or in ALEPH2 more than 1000 nuclides are followed and it depends on user input how many material regions per fuel assembly are considered relevant. For example, for decay heat calculations, often only a single average fuel material region for the fuel is used. The spatial resolution is typically strongly reduced in these cases unless a high-performance computer is available.

In data records, the state of a fuel assembly for determination of observables like decay heat is often given by at least:

- its fuel type (e.g. UOX, ERU or MOX),
- its initial heavy metal mass (or mass of the initial fuel),
- its initial enrichment of ^{235}U or fissionable Pu isotopes and
- its final burnup (and sometimes the burnup per cycle and the shutdown cooling periods).

The average fuel burnup is an integral parameter. From what has been said above about the factors influencing the nuclide concentrations it is not obvious that the above information alone is sufficient to

accurately determine the observables of interest. The evolution of the nuclide vector is a non-linear process and the creation and destruction of nuclides during irradiation depend on more than a single factor like the integral of power generated.

In more sophisticated approaches to determine the nuclide vector at discharge, the irradiation history is simulated by a 3D reactor physics code (level 3 code). Instead of storing the above-mentioned information for each single fuel assembly, the full reactor model is stored with all details necessary to obtain a high-quality neutron transport solution:

- 3D pin layout of fuel assemblies (cladding and fuel geometry and materials),
- top, bottom and side of active core zone reflector properties,
- fuel assembly spacer and mixing grid geometries and material properties,
- reactor power, control rod and burnable poison histories,
- fuel assembly core loading histories.

In some cases, the 3D reactor model is also adapted to measured core power maps to further increase consistency [26].

All codes use nuclear data, which are usually based on evaluated nuclear data files like ENDF/B (Evaluated Nuclear Data File) [32] or JEFF (Joint Evaluated Fission and Fusion Nuclear Data Library) [33]. The information in these files cannot be used directly for computation, requiring further processing into usable formats and structure using tools such as NJOY [34]. In this process, several user dependent factors accumulate in differently processed nuclear data, eventually leading to differences in calculated SNF characteristics. For example, the differences at this step include the group structure of the cross sections, the set of temperatures used for interpolation, or the choice of the set of infinite dilution cross sections (among other differences) which influence the simulation results.

3 Performance testing

3.1 Data

3.1.1 Nuclide inventory

At present, a performance assessment of depletion codes strongly relies on nuclide inventory data that result from destructive chemical and radiochemical analysis of spent fuel rod segments, i.e. results from PIE. The SFCOMPO database [35] contains specifications of PIE programmes, including the fuel assembly design and operational data that are required to perform the depletion calculations. Other data, not part of the SFCOMPO database, are available in the literature, e.g. data from the ARIANE [36], MALIBU [37], REBUS [38] and LWR - PROTEUS Phase II programs [39]. Most of the high-quality data are for PWR UO_2 fuel. PIE data for MOX samples are rather scarce, e.g. SFCOMPO includes 750 fuel samples of which only 11 are marked as MOX fuel. Within WP8 additional data for UO_2 segment samples extracted from assemblies irradiated in both BWR and PWR reactors were made available.

Results of radiochemical analyses of eight samples taken from a GE14 10x10 BWR assembly together with the design properties and irradiation history were provided by ENUSA to the EURAD WP8 partners. Part of this information is available in [40]**.** The assembly was produced by ENUSA and irradiated in the BWR Forsmark 3 (Sweden). The samples were taken at different axial positions from the same rod, with a peak BU of 54 MWd/kg and average BU of 41 MWd/kg. The characterisation measurements were carried out by the Studsvik Laboratory in Sweden. They included a gamma-ray spectroscopic rod scan and Inductively Coupled Plasma Mass Spectrometry (ICP-MS), including isotope dilution analysis, to determine the burnup and inventory of 60 nuclides covering 21 elements. The ICP-MS measurements were performed after separation by high performance liquid chromatography (HPLC). The HPLC is performed to separate elements to avoid isobaric interferences in the ICP-MS measurements. These data were used within EURAD WP8 to verify the performance of CASMO5 [41].

A UOX fuel sample with an initial enrichment of 3.8 wt% ^{235}U, previously irradiated in the PWR Gösgen (Switzerland) was used for radiochemical analysis. The fuel segment consists of UO_2 fuel pellet and Zircalloy-4 cladding, which was irradiated to an average rod burnup of 50.4 MWd/kg. To determine the inventory of actinides and fission and activation products, cladding and fuel samples were prepared from the sample. For the analysis of the irradiated Zircaloy-4 cladding material, a specimen was cut from the plenum section of the segment, not being in contact with the fuel stack. In addition, fuel fragments as well as the cladding material, previously in contact with the fuel, were retrieved from the irradiated pellet. Details of the performed radiochemical separations as well as the determined inventories are reported in EURAD deliverable 8.5 and in the PhD Thesis of T. König [42].

3.1.2 Neutron emission

An innovative Non Destructive Assay (NDA) method was developed within WP8 to determine the neutron emission rate of a spent fuel segment sample, avoiding any reference to a representative spent nuclear fuel sample to calibrate the detection system. The method and experimental and analysis procedures are described in [43], [44]. The method was applied to determine the neutron production rate of a segment sample taken from a rod that was irradiated in the Tihange 1 reactor. The study of this rod is part of the Rod-Extremity and Gadolinia AnaLysis (REGAL) program coordinated by the SCK CEN [45]. The assembly from which the rod was taken, was an AFA 2G assembly type manufactured by AREVA. It consists of a 15×15 array of fuel rods with 21 guide tubes for insertion of control rods or instrumentation. The segment sample for the neutron measurements was taken from the zone with a flat burnup profile. An adjacent sample was taken to determine the nuclide inventory by radiochemical analysis. The inventory of ^{137}Cs, ^{148}Nd and ^{244}Cm and the axial variation of the ^{137}Cs inventory derived from a gamma-ray spectroscopic scan were provided to the EURAD partners. The difference in burnup between the two samples, derived from the gamma-ray scan, was less than 0.2%. The sample used for the neutron measurements was characterised for its net fuel weight. Measurements to determine the neutron production rate of the spent fuel segment were performed at the Laboratory for High and Medium level Activity (LHMA) facility of the SCK CEN in Belgium. The neutron production rate of this REGAL sample due to spontaneous fission derived from the measurements is S_{sf} = 680 (15) $s^{-1}g^{-1}$. The value derived from the direct neutron measurements is within uncertainties in agreement with the one derived from the nuclide inventory of the adjacent sample, which is S_{sf} = 699 (28) $s^{-1}g^{-1}$. Note that the uncertainty of the direct neutron measurement is more than a factor 2 smaller. Hence, this NDA method is a valuable radiometric method to complement radiochemical analysis techniques for depletion code validation. Results of these measurements were used within EURAD WP8 to study the performance of depletion codes.

3.1.3 Decay Heat

A blind benchmark exercise was conducted within EURAD WP8. It involved results of calorimetric measurements on PWR and BWR spent fuel assemblies. By the time the project finished 32 decay heat measurements were available together with results of gamma ray and neutron emission data. The measurements were performed by SKB at the Clab storage facility in Sweden. They are part of the so-called SKB-50 campaign [46], which consists of 25 PWR and 25 BWR SNF with UOX fuel. They are a continuation of a measurement series made before 2006, which has been described in [47]. The data were distributed to the EURAD partners as part of EURAD deliverable 8.5.

The main purpose of the blind benchmark exercise was:

- to compare code-to-code performance without knowledge of the measurements and evaluate the impact of the modelling assumptions implemented by the users,
- to compare measurement and numerical calculations and evaluate the codes' predictive power of the SNF decay heat,
- to assess how a reliable decay heat determination can be made for a large set of SNF destined for disposal.

The main fuel assembly parameters are given in *Table 1* in Appendix A. For each fuel assembly: the fuel type, initial enrichment, heavy metal mass, cycle-wise powers, and final burnup were given. The power history was described as an assembly average power per cycle and cycle length together with shutdown time between cycles. No pin layout or other radial descriptions of the fuel assemblies were given. Therefore, the pin-wise enrichment had to be assumed identical for all fuel pins and no consideration of burnable absorbers was made. In addition, control rod insertion times and information regarding axial moderator and coolant densities were not made available.

Typical radial layouts of the SKB-50 fuel assembly types had been published already in [48], [49] and more information is available in reports for the Swedish safety authorities [50]**.** In order to standardise the blind benchmark and to reduce model differences between participants, an extended dataset was created and distributed. This allowed participants to base the calculations on a consistent set of 2D fuel assembly data and to limit differences in the models' geometry and material composition.

Although the data provided by SKB appears very limited much information is contained implicitly in the burnup values at the end of each cycle that were given. These values come from the plant's online core monitoring systems as described in the introduction and imply a very detailed tracking of the power and control rod history. Hence, the provided average values of energy release and burnup for each fuel assembly are coming from detailed determined state points. In this sense the blind benchmark was also a test for how well average fuel assembly properties like decay heat can be determined with a good knowledge of average assembly burnup and without additional information regarding 2D or 3D conditions. For the PWR cases the estimated uncertainty of the stated burnup was about 2% and for the BWR cases 4%.

In *Figure 1* to *Figure 4* in Appendix A; the distributions of initial enrichment, burnup, cooling times, and burnup versus cooling times are shown.

In *Table 2* to *Table 3* in Appendix A; examples of a PWR and BWR standardised xml dataset are shown which were generated for each SNF from the data provided by SKB, compiling additional information from the above mentioned reports [48], [49], [50].

In the blind-benchmark, 10 institutions participated:

- P01: using DARWIN2 code [51] with nuclear data based on JEFF3.1.1 [52]
- P02: using EVOLCODE [20] with nuclear data based on JEFF-3.3 [33]
- P03: using TRITION/NEWT sequence of the SCALE 6.2.3 code system [13], [53] with 238 energy groups cross-section library based on ENDF/B-VII.1 [32]
- P04: using Serpent 2 [16] with nuclear data based on ENDF/B-VII.1
- P05: using MCNP6 [54] combined with CINDER [55] and with nuclear data based on ENDF/B-VII.1
- P06: using both the Polaris and TRITON/NEWT sequence of the SCALE 6.3 code system with 56 and 238 energy group cross-section library, respectively, based on ENDF/B-VII.1. Both codes utilise ORIGEN for the depletion and decay calculations.
- P07: using the TRITION/NEWT sequence of SCALE 6.2.3 with 238 energy groups cross-section library based on ENDF/B-VII.1
- P08: using CASMO5 [11] with 542 energy group cross sections based on ENDF/B-VII.1
- P09: using Serpent 2 code [16] with nuclear data based on JEFF-3.3
- P10: using Origen-ARP [21] with spectrum average cross section data, based on Westinghouse 17x17 assemblies and the ENDF/B-V library.

The blind benchmark was conducted in the following steps:

- all participants received the standardised fuel assembly descriptions as described above (original SKB-50 data plus standardised xml description) and were expected to provide the decay heat in units of Watt per ton of initial heavy metal mass for each fuel assembly.

- results were compared among participants without revealing the measurement results. This phase provided opportunities for introspection and removal of potential misunderstanding and mistakes in the inputs.
- participants were allowed to provide revised results.
- final results were submitted, then the measured decay heat values were declared and comparison with measurements were made.

The decay heat measurement data was evaluated independently by JRC and SKB and the results are reported in EURAD Deliverable 8.5. Final evaluation results between JRC and SKB were in agreement. Details of the evaluation of the raw measurement data performed within EURAD will be described in a forthcoming publication [56]. The work of SKB will be part of an EPRI report that is in preparation.

3.2 Results

3.2.1 Nuclide inventory

One of the main goals of the present research was to assess the performance of depletion codes to predict the concentration of nuclides that are needed to calculate the main observables of interest. To reach this goal, the results discussed in section 3.1.1 were taken into account, together with the C/E values from references [48], [57], [58], [59]. In these references, C/E inventory data for a variety of PWR and BWR samples are given, including UOX fuel, MOX fuel and a large range of sample burnup.

Nuclear data is generally the largest contributor to uncertainties on nuclide concentrations (cross-sections and fission yields; the impact of thermal scattering data was shown to be negligible [60]). Detailed results are published in [41], [61], [62], [63], [1], [64], [65], [66]. The only noticeable exceptions are ^{239}Pu, for which the moderator temperature can be almost as important as nuclear data in the case of PWR samples, and ^{235}U, ^{239}Pu and ^{241}Am for which the void fraction is also an important source of uncertainties for BWR samples. Neutron induced capture cross-sections are the major sources of uncertainties to predict the inventory of actinides. The inventory of fission products is mainly influenced by fission yields (with some exceptions, such as ^{134}Cs and ^{154}Eu).

Large variations of calculated uncertainties can be obtained using covariance data recommended in different evaluated data libraries, sometimes up to a factor of 10, especially for specific fission products. Fission products are generally sensitive to the fission yields, and less to thermal capture cross-sections (with some exceptions, such as some Cs, Nd, Gd and Eu isotopes). The lack of use of a consistent set of nuclear data is one reason. For example, part of the covariances of independent and cumulative fission yields require alignment. Further, there are discrepancies between nuclear data libraries which need to be resolved.

For actinides, the spread of uncertainties is smaller than for fission products, except for ^{237}Np and some neutron-rich curium isotopes. In the case of Cm, strong differences of uncertainties are observed in nuclear data libraries for nuclides in the chain of the Cm built-up (as for instance ^{242}Pu). For ^{237}Np, the main component of uncertainty change is the type of considered sample: UOX or MOX. It was observed that for MOX samples, the calculated uncertainty of the ^{237}Np concentration is much higher than for the UOX sample, due to the difference in production routes.

The effect of thermal scattering data, more especially H in H_2O is minimal on nuclide concentrations and decay heat. Details can be found in [60].

Nuclide uncertainties can differ if one considers a single assembly model, or a full core model (e.g. on ^{148}Nd [63]). These variations are likely linked to the calculation method and normalisation, which are intrinsically different between single assembly and full core models.

3.2.2 Neutron emission

Results of the neutron measurements discussed in section 3.1.2 were used to study the performance of depletion codes, i.e. ALEPH2, SCALE6 and Serpent2, for the prediction of the neutron output of spent

fuel. For SCALE6 the TRITON/KENO-V.a module coupled to ORIGEN was used. All calculations were normalised to the same ^{148}Nd inventory. The study included a code-to-code and code-to-experiment comparison using different nuclear data libraries [44].

The study included a comparison of the average assembly burnup provided by the codes when normalising the calculations to the same ^{148}Nd inventory. The burnup derived from the different code/libraries combinations varied between 53.33 MWd/kg and 55.07 MWd/kg. This suggests that a normalisation of calculated data to the delivered power can vary by 3.3% depending on the code and nuclear data library that is used. The observed variation can only partly be explained by differences in nuclear data influencing the ^{148}Nd inventory. The calculated burnup also depends on assumptions made about the energy production due to neutron induced fission and some capture reactions. This study also indicates that the ^{147}Nd(n,γ) cross section in the main evaluated data libraries should be reviewed and supports a reduction of the ^{147}Nd(n,γ) cross section as proposed in [68], [69].

To compare the theoretical and experimental production rate the uncertainty of the neutron production rate has to be combined with the uncertainty of the experimental inventory of ^{148}Nd, which is at present 2%. This results in a combined uncertainty of 2.7%. The value calculated with Serpent2 based on a reduced ^{147}Nd(n,γ) cross section is within the combined uncertainty of 2.7% fully consistent with the experimental value.

The neutron production rate associated to spontaneous fission results for 97.7% and 1.6% from ^{244}Cm(sf) and ^{246}Cm(sf), respectively. Hence, the uncertainty of the calculated production rate is strongly determined by the uncertainty of the ^{244}Cm inventory. Results in [70], [71], [72] and [73] show that presently this uncertainty is about 10% and mainly due to the uncertainty of the ^{242}Pu(n,γ) and ^{243}Am(n,γ) cross sections. The good agreement between calculated and experimental neutron production rate suggests that the calculated uncertainty of about 10% is overestimated and the uncertainty of the ^{242}Pu(n,γ) cross section can be reduced. Due to the complexity of the ^{244}Cm production process errors in the different capture reaction cross section involved in the calculations can be compensated. Therefore, a re-evaluation of the ^{242}Pu(n,γ) and ^{243}Am(n,γ) reaction cross sections is recommended.

3.2.3 Decay Heat

Within EURAD WP8 extensive studies were carried out to assess the uncertainty of the decay heat predicted by depletion calculation due the nuclear data, fuel related input data and model assumptions. The results of these studies are reported in [61], [62], [63], [1], [70], [74], [75], [76], [77], [78], [79], [80]. These studies indicate that uncertainties due to nuclear data, manufacturing tolerances and irradiation history are at least 2.5% for cooling times above 10 years and can reach 6-7% for shorter cooling times. In general, nuclear data uncertainties together with the uncertainty of the burnup are the largest contributors.

Other specific findings from these studies can be summarised as follows:

- In [75], differences of measured and calculated decay heat and their uncertainties for 4 PWRs and 4 BWRs have been studied. The uncertainty due to nuclear data and fuel design and operation parameters was between 2 and 3%. The authors' estimated fuel design and operation uncertainties were roughly double the size of those estimated for nuclear data. Differences between calculations and measurements data from Clab were generally within the 2σ band. However, for older measurements at GE-Morris facilities differences up to 4σ are observed, despite having already large experimental uncertainties.
- In [78] a sensitivity study was carried out to study the influence of several factors such as enrichment, fuel temperature or moderator temperature on PWR decay heat. Assuming expert guesses on uncertainty for these quantities the effects on decay heat are smaller than 1%.
- In [77] and [79] changes of simulation code and changes in boundary conditions are studied regarding their effect on PWR decay heat. Effects of 2% and 3% respectively have been identified.

- In [61], [62] for 2 PWR UOX cases the effect of nuclear data uncertainty on nuclide composition and decay heat have been studied. Nuclear data was concluded to be a major contribution to calculated uncertainties, especially when considering different data libraries. Temperature and other operation parameter uncertainties are expert guesses since no direct measurements are available for the active core zone. Hence the relation between nuclear data uncertainties and operation uncertainties is tentative. Combined uncertainties were estimated to be smaller than 4%.
- In [41][1] a BWR sample was analysed comparing measured and calculated nuclide concentrations. Consistent decay heat uncertainties were determined. The conclusion was similar to the two above mentioned PWR samples, resulting in combined uncertainties of smaller than about 4%.
- In [76] another BWR sample was studied and with regard to decay heat it was concluded: "… in about 2 years after irradiation the uncertainties caused by burnup grow up to around 2% and remain there for a few hundred years."
- In [70] about 9200 assembly-cycles for Swiss reactor cores were studied and the uncertainties due to nuclear data on the decay heat was estimated smaller than 7% (1σ).

Also, part of this project has been a comparison of the cumulative fission yield and the recoverable energy in different libraries for ^{90}Sr and ^{137}Cs (for fission of ^{235}U) at thermal energy. From this comparison a systematic difference of about 2% is expected. Such a difference might not be reflected in average C/E values due to compensating effects.

A comparison of the average C/E using the same library but different versions of CASMO5 have shown a difference of about 2% for both PWR and BWR (a later CASMO5 version partially addressed this issue with an improved ^{137}Cs buildup chain). The results derived by different users using the same code and library indicate that differences due to a user effect, reflecting also model assumptions, are of the same order of magnitude than differences due to nuclear data.

Evidently, the performance of depletion codes to predict the decay heat is best assessed through a comparison with results from calorimetric measurements. Results obtained from the Clab calorimeter published in SKB's R-05-62 report were already used to validate codes. An overview of C/E data published in the literature is given in *Table 5* of Appendix B. Within EURAD WP8 similar studies were carried out to verify the performance of ALEPH2, Serpent2, CASMO5, SNF and the POLARIS and TRITON/NEWT modules of SCALE. The results of these studies are included in *Table 5*. In [66] in the impact of different nuclear data libraries and code versions of CASMO and SNF is shown together with the predictive power of four decay heat standards. The average C/E values using the latest DIN standard is relatively close to unity, while the three other standards provide a rather conservative overestimation (ANS-5.1 [4], US NRC RG-3.54 2018 [81], ISO 10645/2022 [82] and DIN 25463-1:2014 [5]). For the depletion codes the average C/E for PWR ranges from 0.972 to 1.019, and for BWR it ranges from 0.971 to 1.014. The range for the PWRs (4.8%) is slightly larger than the BWRs (4.4%). This contrasts with the standard deviation, which for almost all cases is about a factor 2 larger for BWR. The increase in standard deviation is probably due to the larger variation of the moderator density and its spatial dependence, resulting in more complex neutron transport calculations, and to the lower decay power which have a larger experimental relative uncertainty. The average C/E in *Table 5* suggests that the calculated SNF decay heat is within expected uncertainty of the calculation of about 3% fully consistent with the experimental one. However, the data in *Table 5* reveal that differences due to different users, code versions and nuclear data libraries are of a similar magnitude.

For the blind decay heat benchmark, measured decay heat for 29 of the 50 fuel assemblies (19 PWR and 10 BWR) were available at the end of this project. *Figure 5* of Appendix B shows all the results of the final submitted calculations and the measurement results. The corresponding C/E results are shown in *Figure 6* of Appendix B. Values at 0 indicate that either a measurement was not available for this fuel assembly or participant did not provide results for this case. All participants made predictions for all the PWR cases. Only some participants made predictions for the BWR cases.

The following first observations from the measurement-calculations comparison can be made.

- For the PWR cases calculations the maximum difference is less than 5%. For the BWR cases differences are within 10%.
- The ranking of calculations between participants is roughly constant, e.g. participants who make the lowest prediction for the first case, for example, are also in the lowest segment in later cases.
- The first results of P02 for the BWR cases differed significantly from the results of the others, with an overestimation of about 10%. After a first comparison of the data, the root cause was identified as the void fraction assumption.
- In PWR case no. 16 a wrong power history for the assembly was provided.
- Participant P05 revised results before final submission because of a misunderstanding regarding result normalisation.
- Participant P09 revised results before final submission because of user related input mistakes removed.
- In most cases the calculated values are within the expected calculated uncertainty of about 2.5% consistent with the experimental values. *Figure* 7 in Appendix B shows the PWR and BWR C/E histograms. For PWR the mean and standard deviation is 1.003 and 2.2%, respectively, and for BWR they are 0.985 and 4.4%, respectively. These values are based on the final values provided by P02, P05 and P09 and do not include case 16.

In the remaining analysis the following data points were excluded as outliers: initial submission of P05 and P09, P02 results for BWR cases, results for PWR case 16. However, the identification of these results as outliers provided valuable input for recommendations.

Participants P01 to P09 followed a level 2 code approach. Participant P10 used a level 1.5 approach. Since the input data was standardised, differences between results are user related due to different choices of input parameters, not defined by the standardised fuel assembly description, differently translated into the code input, different method options provided by the codes or a different choice and preparation of cross section data libraries.

Participants P03, P06 and P07 used modules from the SCALE6 code package and the spread of results covers already a large part of the spread of the whole group, see *Figure 9* in Appendix B. Participant P06 implemented some different user-related assumptions from the benchmark specifications based on a user's interpretation of fuel design data of previously measured SNF at Clab. This includes different enrichment maps, accounting for spacers in the fuel design, accounting for the presence of Gd-rods in the BWRs, among other differences. This contributes to the observed differences between the results obtained by different SCALE users.

Sometimes corrections factors are used as multipliers for calculation results with the motivation to improve predictive capabilities (for the scope of fuel assemblies represented by the measurements). Correction factor determination can be done, for example, by using the first measurement (or the average of a subset of measurements) as an anchor to obtain an exact C/E value of 1. All later calculations are then also multiplied by this same factor. In this way for the PWR cases the mean and standard deviation is changed to 1.002 and 1.6%, for the BWR cases it is 1.018 and 4.1% (see *Figure 8* in Appendix B). The very modest improvement of C/E values indicates that random factors probably dominate the differences between calculations and measurements.

The performance of user P10 for PWR cases does not noticeably differ from the results of remaining participants. This indicates that the used default libraries (Westinghouse 17x17) are representative for the SKB-50 PWR cases.

The usefulness of averaging results of all participants to improve overall performance has been contemplated. Empirically the averaged blind test results for the PWR and BWR cases are much better predictors for the measured decay heat compared to individual predictors. Averaging results cannot remove systematic differences between measurements and calculations but can remove random influences affecting each participant's formulation of the computational model.

4 Conclusions

4.1 Code performance assessment

4.1.1 Overall code performance

One of the main objectives of Task 2 of EURAD WP8 was to study the performance of depletion codes used for the characterisation of spent fuel. Therefore, the aim was to analyse which code level is sufficient for spent fuel characterisation and under which circumstances it should be employed. There are circumstances which may give level 1 codes sufficient predictive power and other circumstances which can only be addressed with level 3 codes. Unfortunately, no participant had access to 3D fuel assembly burnup data or a 3D irradiation history from a core simulator for the SKB-50 data. Therefore, only indirect conclusions can be drawn. Additionally, fuel assembly averaged quantities like decay heat and measurement data in the currently observable time frame of cooling times and at moderate burnup may not be the most sensitive to detect 3D effects.

Spent nuclear fuel observables are related to the nuclide compositions at the end of irradiation, and their decay scheme. Considering that the decay data for the nuclides of relevance for decay heat are mostly well known, a correct estimation of the nuclide concentration leads to an accurate estimation of the observables.

Given the uncertainty of experimental data (e.g. decay heat measurements and irradiation history) and the uncertainty from nuclear data it was difficult to decide if a level 1.5, 2 or 3 code yields higher quality results. This relates primarily to the selected conditions of most fuel assemblies at discharge and the implicit dependence of irradiation history data on a level 3 approach from online core simulator data. Outcome of the blind benchmark exercise indicate that collapsed irradiation history information from a level 3 code (i.e. time averaged void or moderator density, axially averaged burnup) for specific assemblies can give level 2 or even 1.5 codes sufficient predictive power.

A comparison between experimental and calculated decay heat data reveals that best estimate calculations for the spent fuel decay heat are of added value compared to conservative approaches. Nonetheless, best estimate calculations are not always used in the industrial context, due to time and effort constraints. In this case, conservative approaches, based on standard methods (i.e. ANSI or ISO methods), are used. It inherently leads to less efficient and under-optimised systems (e.g. cask loading), possibly artificially increasing various costs, eventually paid by consumers. The advantage of best estimate calculations needs to be emphasised from an economical point of view, but also from a scientific and technological safety aspect: both decay heat and criticality originate from the same nuclide inventory, and the use of standard methods for decay heat does not allow to link them. This is an unnecessary decoupling between these two aspects of spent fuel characterisation, leading to a loss of information and possibly inconsistencies.

4.1.2 PWR versus BWR performance

The performance of CASMO5 was verified at the Paul Scherrer Institute (PSI) using PIE data from UOX and MOX samples taken from fuel rods that were irradiated in PWR and BWR. The results of these studies reveal that modelling the irradiation conditions of an assembly in a BWR is more complicated than for PWR due to the heterogeneous irradiation conditions. This is also one of the conclusions of the blind benchmark exercise using the SKB-50 decay heat data from the Clab calorimeter. All codes used in the blind benchmark exercise had undergone generic licensing (e.g. [36], [83], [84], [85]) and the final inputs were generated by experienced users. Nevertheless, calculation results for PWRs differed by about 5% and for BWR by up to 10% among participants. The reason that BWR results are further apart than PWR results is due to less well-known fuel assembly design and irradiation parameters in the BWR case. This includes the void fraction, the temperatures of the fuel assembly bypass and water channels, control rod history regarding the irradiation parameters. It also includes the actual enrichment maps regarding the fuel assembly design parameters. Numerous parameters absent in the benchmark

specification were assumed, either in the distributed specification or additionally by the users themselves.

Very few fuel assemblies in the SKB-50 dataset had particularly small or high average burnups. Hence it can be expected that the PWR assemblies had a relatively small axial and radial burnup gradient. Moreover, PWRs are typically operating with minimal control rod insertion. Therefore, this set was well suited to average both in space (axially, radially) and time the relevant operating conditions. Averaging in the PWR cases was also more feasible considering the neutronic homogeneity of the assemblies, e.g. their radial and axial enrichments. Still due to user interpretation, different nuclear data libraries and different numerical methodologies the calculations and the C/E results differed by up to 5% (2σ). Thus, it should be concluded that currently this is a realistic estimate for all possible uncertainties affecting PWR decay heat estimates.

The good performance of ORIGEN-ARP (a level 1.5 code) used in the benchmark for the PWR cases should not be interpreted that level 3 codes are unnecessary in these cases. First, it was already emphasised that high quality operating history data is provided from level 3 codes integrated into online core simulators. Second, there can also be PWR cases for which a level 1 or 2 code description is insufficient. For example, if fuel is irradiated only one cycle and then is destined for final storage (for example if a plant is permanently shut down) the axial and radial burnup gradient can be large, burnable neutron absorbers may not fully be depleted and a flat 1D or 2D description may not be sufficient. Also, in some special cases PWR fuel assemblies may operate with long-term control rod insertion or be used longer term for core barrel (the boundary between downward and upward flow in a PWR) shielding purposes. In other examples the fissile material enrichment is axially not uniform also in PWR cases. Therefore, the provision of 3D irradiation information will be beneficial to avoid unnecessary guessing about correct fuel conditions. Alternatively, the suitability of the 2D approach in the PWR cases could be assessed on a case-by-case basis, depending on the pre-described potential variations and the required level of accuracy on the calculated parameters.

BWR results differed by up to 10%. It is expected that given more detailed irradiation information the performance can be improved potentially to the PWR level. For BWR assemblies a level 3 code approach may show its advantages compared to level 2. But it requires more detailed information about operation conditions. However, such analysis awaits the availability of such detailed irradiation information, to fully assess the gain in applying 3D models for the BWR cases compared to the current 2D ones.

4.2 Normalisation

One of the main quantities in the depletion calculations is the total neutron fluence, which acts as a normalisation factor. The procedure to derive the total neutron fluence or normalise the data, mostly depends on the type of the applications. In case of PIE data, the normalisation is mainly done by adjusting to the inventory of a specific nuclide such as ^{148}Nd or a combination of such nuclides, known as burnup indicators. Normalisation of the depletion calculations by the inventory of a burnup indicator is not possible in case an assembly has to be characterised in a routine, industrial operation. For such applications, the normalisation is mostly based on the average assembly burnup given by the operator and derived from calculations with a 3D core simulator.

Normalisation of transport and depletion calculations strongly affect nuclide concentrations. This globally affects all calculated nuclide concentrations, as well as derived quantities (e.g. decay heat). Consequently, all calculated quantities are correlated to this normalisation and potentially include a common systematic error, and a common uncertainty. This aspect needs to be studied in more detail, as often the experimental uncertainty on Nd concentrations is notably small, and uncertainties on calculated sample burnup are not always considered. For the last quantity, the validation of codes providing the burnup values, i.e. core simulators, needs to be considered as well.

During irradiation in the core, the production of nuclides is for most of them not a strict linear process as function of neutron fluence. Therefore, systematic errors due to a normalisation to an average assembly

burnup in 2D calculations (level 2) will only be avoided for observables that are directly proportional to the burnup. This is in first approximation true for the ^{137}Cs inventory. However, the dependence of the inventory of ^{134}Cs and ^{154}Eu and higher actinides, e.g. ^{244}Cm, on burnup is strongly non-linear.

4.3 Fuel related input data for depletion calculations

The discussion in the previous sections reveals that the quality of the calculated results improves by including more information about the irradiation conditions. Obtaining reliable data for fuel irradiation histories is more difficult than obtaining data for fuel assembly designs which are specified in detail (provided the information is shared with backend organisations). Cooperation with utilities is necessary to access the information from online core simulators which can provide time averaged data for moderator density, void content, control rod history and soluble neutron absorbers. If necessary, also node-wise information can be provided. Although some publications have concluded that nuclear data uncertainty is one of the main contributors to overall uncertainty, the contribution from irradiation history is of similar order of magnitude and has also been analysed in earlier publications, e.g. [86]. However, this assessment depends on expert guesses of the irradiation history uncertainties. Ideally, they should be experimentally verified.

The bulk of experimental data used for code validation comes from commercial fuel. Reactors operating for electricity production are not equipped with the degree of core surveillance one would require for dedicated research reactor experiments. Hence, it is difficult to distinguish between systematic effects from nuclear data and effects which are due to imperfect knowledge of irradiation and fuel initial conditions since both contributions are expected to be of the same order of magnitude. The observed differences between measurements and calculations may even give too optimistic impression due to compensating effects.

The blind benchmark has shown that an important effect is the choice of user-provided parameters for creating the computational model. Already level 2 codes offer a wide range of possible choices, for example:

(1) Microscopic cross section library version and options for preparation of macroscopic cross sections from evaluated data files
(2) Number of energy groups
(3) Number of nuclides to follow during irradiation and assumed impurities of fuel
(4) Boundary conditions at the fuel assembly's periphery
(5) Number of material and burnup zones per fuel rod and fuel assembly
(6) Number of burnup steps per cycle
(7) Methodology to solve the neutron transport equation (e.g. stochastic or deterministic)
(8) Use of time averaged quantities for burnup, soluble neutron absorbers, control rod and power history, and moderator and void content.

Most level 3 codes which are in use in core simulators undergo licensing from the safety regulatory authorities and must demonstrate reliable agreement with measured core power maps. Therefore, even if the above-mentioned points are user dependent, the validation and licensing efforts usually lead to a choice of parameters which empirically describe the core power histories with the best possible detail. The blind benchmark and many other sample descriptions implicitly benefit from this procedure because the provided burnups and cycle averaged power histories were provided from such a core simulator.

4.4 Consequences for safety

For some nuclides differences between their measured and calculated nuclide inventory on the scale of a pellet can be relatively large [48], [67], [87] compared to differences that are acceptable for applications such as criticality safety. On the other hand, there are effects which reduce the impact of such differences on safety relevant quantities of a full fuel assembly and for time scales relevant for geological storage. Most of the observables of interest are an aggregate property of a fuel assembly with contributions from a set of nuclides, which might result in compensating effects. For example, from a

safety perspective the decay heat of a full fuel assembly is the leading parameter for the overall cask thermal limits. Errors in nuclide concentrations in single fuel pellets or fuel rods will partly average out. In addition, fuel assemblies with higher burnup usually have a flatter radial and axial burnup profile, because they are intentionally placed inside the core with a strategy to minimise burnup gradients during their lifetime. Therefore, burnup differences have been homogenised, which improves the accuracy of the calculated data. It is also noteworthy that the subset of irradiation data used for code validation are not representing the full possible set of histories. Most reactors are operated near equilibrium cycles with a near repetition of loading patterns and therefore similar irradiation histories. Thereby the consequences of the non-linear dependence of nuclide concentrations on irradiation history is diminished.

Yet, secondary properties like peak cladding temperatures during storage can still be sensitive to local fuel conditions. In some cases, high burnup assemblies are placed at the core periphery for a prolonged time to reduce neutron leakage and can have significant radial burnup gradients at end-of-life. In case of long cooling times, nuclides with relatively short half-life and a strong dependency on the power history are no longer relevant. However, higher actinides are sensitive to irradiation history and dominate properties after that shorter-lived fission products have decayed. Hence a broad scope of fuel conditions used for code validation is important.

4.5 Nuclear data

The effect of nuclear data to calculate nuclide concentrations and related observables is as important as fuel related input data, i.e. fuel design and operational parameters, e.g. burnup. This particularly concerns fission yields (e.g. ^{90}Sr, ^{137}Cs, ^{148}Nd) and neutron capture in heavy actinides. For example, the uncertainty of the calculated ^{244}Cm inventory and related neutron emission is at present about 10%, due to the uncertainty of the ^{242}Pu(n,γ) cross section. An assessment of the status of cross section evaluations of the ^{238,240,241,242}Pu isotopes in [88] reveals that the evaluation procedures to estimate these cross sections for the latest versions of the main evaluated libraries did not include all experimental data reported in the literature. Hence, the status of these cross sections in the data libraries can be improved. This will reduce the uncertainty of the calculated ^{244}Cm inventory and improve the performance of depletion codes to predict the neutron emission rate. This is important if the neutron emission rate is used as a burnup monitor.

A documented evaluation of the recoverable energy, including uncertainties and possibly covariance information, to calculate the burnup is needed for the four main nuclides: ^{235}U, ^{238}U, ^{239}Pu and ^{241}Pu. Depletion and core simulation codes should document which energy is considered, i.e. which components are included and which not. This is particularly valid for industrial codes which often use nuclear data that are not accessible for the routine, industrial user. Recommended procedures to calculate the total recoverable energy will reduce potential systematic errors due to the normalisation of depletion calculations based on the burnup. To reduce errors in the normalisation of PIE data using ^{148}Nd as burnup indicator the ^{147}Nd(n,γ) cross section should be re-evaluated.

The use of different nuclear data libraries and code versions might produce notable differences in the nuclide inventory and derived observables. In addition, recommended nuclear data in libraries such as JEFF and ENDF/B should be made consistent with Decay Data Evaluation Project (DDEP) and results of other high quality evaluations, e.g. the evaluation of prompt neutron emission multiplicity distributions for spontaneous fission [89].

Therefore, there is a clear need to improve the quality of nuclear data, including their covariances, of interest for depletion calculations. Although for most of the observables of interest only a limited number of nuclides are important, nuclear data projects such as NUDAME and SANDA did not contain nuclear data activities dedicated to depletion calculation. This calls for a dedicated project to produce a recommended nuclear data library for depletion calculation.

4.6 Data for code validation

Most of the PIE data from the open literature are compiled in the SFCOMPO database. Some additional measured nuclide concentrations are not publicly available. These data are used to validate transport and depletion calculation schemes. The data, i.e. experimental nuclide inventories and design and irradiation histories, are obviously of varying quality, which might affect results of code validation. To improve the use of PIE data for code validation the quality of the data has to be improved. In addition, it would be useful to provide for the most trusted PIE data associated benchmarks for specific application (criticality safety, short-term & long-term cooling, transport, storage, fuel type, burnup values, etc). Efforts within the SFCOMPO Technical Review Group (TRG) aim toward improvement of the quality of PIE data, their re-evaluation, and potentially deriving benchmark specifications [90].

Currently, only one calorimeter is used worldwide, i.e. the calorimeter installed at the Clab facility in Sweden. Earlier measurements at the GE-Morris and the HEDL facilities have their own deficiencies such as their large experimental uncertainties, limiting their usefulness in code validation compared to the Clab measurements. However, in case the data of the Clab calorimeter suffers from a hidden error, all validation exercises based on these data will suffer from a systematic error. Additionally, the fuel assemblies measured with this calorimeter are not representative for cases from different countries, due to different enrichments, designs or fuel types. Hence, it is not straightforward to use the Swedish Clab data for validation of spent fuel calculations in other countries.

Overall, the creation of a reference data book for code validation should be pursued after a careful quality control and critical evaluation of the experimental data. It should contain a consistent set of observables (decay heat, gamma and neutron emission data) and PIE results. The value of the data could be enhanced by providing detailed fuel and irradiation history from a 3D core simulator. Also, the breadth of fuel assembly states concerning burnup, decay time, enrichment and reactor type should be increased.

4.7 Quality control methods

To identify quality issues and to detect errors from the model-modeller interaction the blind benchmark has been a useful exercise. This approach is similar to the diversity requirement in nuclear system design where equipment from independent suppliers is required for certain safety functions.

Many organisations have quality control and quality assurance policies to eliminate trivial mistakes and release results with a high degree of confidence in their correctness. However, rarely results are derived by independent means within the same organisation. The blind benchmark conducted within EURAD WP8 and its predecessor published in [91] enhanced confidence in results by helping participants to recognise code input mistakes, to recognise one mistake in the provided irradiation history data, and to independently confirm results. Overall, the quality of input data and results were improved. Moreover, the measured data used for the code validation was evaluated independently by two organisations that minimised further sources of errors.

The blind benchmark showed that a participant-to-participant comparison of results alone cannot exclude errors in case of wrong description of fuel assembly input data, like the irradiation history. For large-scale operations like characterisation and packaging of spent fuel assemblies destined for disposal in a deep geological repository, it is not possible to perform time-consuming decay heat measurements done for every fuel assembly.

However, results of the EURAD deliverable D8.4 reveal that measurements that can be routinely performed under industrial conditions, like total neutron and gamma-ray emission measurements, can be used as a quality control to validate the input data and the results of depletion calculations. Results of neutron and gamma-ray measurements from the SKB-50 PWR assemblies were analysed [92], [93]. The neutron data resulted from measurements with the Differential Die-Away Self-Interrogation (DDSI) prototype instrument [94] . Although a promising technique for analysing the DDSI data was developed the quality of the data derived from the measurements with a DDSI prototype instrument at Clab requires

further improvement to validate the proposed analysis procedure. Ultimately, only the total neutron emission data were used. It was also shown that the decay heat for PWR fuel assemblies with cooling time < 70y can be correlated to the total neutron emission and gamma-ray data to estimate the decay heat with a deviation to the direct calorimetric measurements of 2-4% [95].

In another study within WP8 of EURAD, data taken at the NPP of Doel were used to study the potential of a FORK-type detector [96] to validate the input data and the results of depletion calculations. The FORK detector is a detection system that is used for routine safeguards inspection under industrial conditions. The study, which is reported in EURAD deliverable D8.4, demonstrates that the neutron response of such a detector can be calculated by combining depletion calculations predicting the primary neutron production in the fuel with a neutron transport to account for both the neutron multiplication in the fuel and the intrinsic neutron detection response. It was demonstrated that by combining the total number of detected neutrons with the calculated detector response, the average assembly burnup for PWR assemblies can be determined with an uncertainty of about 2%. It is concluded that the detection of gamma and neutron emission properties of a spent fuel assembly provides valuable information to verify calculational results.

Little BWR data regarding FORK-type or other NDA neutron measurements are available and would add important information to verify the potential of NDA measurements as a quality control tool.

5 Summary

The performance of depletion codes used for the characterisation of spent fuel was assessed. The emphasis was on spent fuel assemblies in view of their handling, transport, storage and disposal. New experimental data from post-irradiation experiments, neutron emission measurements and calorimetry produced within EURAD were taken into account in addition to experimental data available in the SFCOMPO database and reported in the open literature.

At present, most of the depletion calculations dedicated to the characterisation of spent fuel assemblies rely on a 2D lattice representation and an average assembly burnup that is derived from a more detailed 3D core simulation calculation. The predictive power of such codes is better for PWR assemblies than for BWR assemblies. In the case of observables with a linear dependence on burnup and a flat burnup profile, the main uncertainty of the calculated observables is due to nuclear data and the uncertainty of the average burnup followed by the uncertainty of the moderator density and fuel geometry. Note that the uncertainties of the fuel related input data are primarily based on expert judgements and require an experimental verification to confirm these findings.

For fuel cooling times longer than 10 years the combined uncertainty of the calculated decay heat is about 3%. For shorter cooling times the nuclear data uncertainty increases relative to burnup uncertainties. The calculated decay heat for PWR is within the combined uncertainty due to nuclear data and burnup consistent with results of experimental data, which have an uncertainty lower than 2%. For BWR assemblies, differences between estimated and experimental decay heat are somewhat larger than the combined uncertainty due to nuclear data and burnup (i.e. >5%). This is due to the impact of the void fraction. In the absence of detailed information about operating conditions the uncertainty can be multiples of 10%. The predictive power for other observables such as the inventory of higher actinides and neutron emission rate is at present mainly limited due to nuclear data uncertainties, i.e. the uncertainties of the capture cross sections.

The quality of 2D calculations, in particular for observables with a non-linear dependence on burnup and a burnup with spatial dependence, can be improved by providing detailed fuel and irradiation history parameters from a 3D core simulator, which are available from the NPP operators.

Significant differences are observed in calculated observables and their uncertainties using nuclear data from different evaluated nuclear data libraries. In addition, decay data in evaluated data libraries such as ENDF/B and JEFF are not always consistent with the data recommended by DDEP and results of other high-quality evaluation projects. A detailed study of the influence of nuclear data on the calculated

neutron emission and decay heat, reveals that the predictive power of depletion codes can be improved by improving the quality of the nuclear data. This calls for a project dedicated to the production of recommended data for depletion calculations.

To identify errors in the calculation and determine the bias, i.e. estimate of the systematic error that is the difference between the calculated value and the true value, accurate experimental data are required. The work within WP8 of EURAD has shown that some of the PIE data available in SFCOMPO and in the literature suffer from systematic errors. Hence, they cannot be used to determine the bias.

To avoid a systematic error in measured decay heat, careful evaluation of the measurements and the setup is required. To determine a bias in decay heat calculations, presently only the data from the Clab calorimeter can be used. An additional system, ideally mobile and preferably based on slightly different principles/designs, could be recommended to confirm that data derived from measurements with the Clab calorimeter do not suffer from a hidden systematic error. The present set of experimental data should be complemented with results from measurements on other spent fuel types, UOX and MOX fuel with a broader range of initial enrichment, cooling time, burnup and decay heat. Ideally, a reference data book for code validation is produced after a careful quality control and critical evaluation of the experimental data covering a broad range of fuel types.

There is no sizeable difference in different codes using the same nuclear data library as long as the fuel related input data, i.e. design properties and irradiation history, are properly interpreted and implemented. However, the blind benchmark exercise using results of decay heat measurements from the calorimeter at Clab reveals that user effects and errors in the fuel data specifications cannot be excluded. The influence of such errors can be reduced by including NDA measurements on the spent fuel assembly in the quality control procedures and by standardising the procedures on how to calculate the decay heat. Results of EURAD deliverable D8.6 demonstrate that detection systems based on total neutron and gamma-ray emission measurements can be used to verify the quality of the input data and results of depletion calculations. However, more work is needed to assess the performance of such measurements for BWR assemblies.

Traditionally, quantities regarding criticality safety have received more attention compared to parameters regarding the nuclear fuel cycle back-end activities. This is changing with recently initiated international collaborations. For example, in 2020 the Coordinated Research Project (CRP) of the International Atomic Energy Agency, on “Spent Fuel Characterisation" [97] started. In 2021 the WPNCS Subgroup 10 (SG10) [98] on “Nuclear Data Uncertainties Quantification on Spent Fuel Inventory" followed and in 2022 the WPNCS Subgroup 12 (SG12) [99] with activities dedicated to “Spent nuclear fuel decay heat: assessing the confidence level in experimental and computational estimations (SNF-DH)" was created. Besides evaluating existing data, the more important question is if confidence in predictions can be further improved, which are the factors with the highest leverage and if the benefits outweigh the costs. The outcome of this work, in particular the conclusions summarised in section 4, should be a guideline to define activities within these different working groups.

Appendix A. Input data and characteristics of the SKB-50 fuel assemblies

Table 1 – SKB-50 main fuel assembly characteristics.

	burnup	discharge	measurement	decay time (d)	fuel type	ID
1	52,768	24.05.2009	19.02.2018	3193	15x15 AFA 3GAA	PWR1
2	49,819	24.05.2009	31.01.2018	3174	15x15 AFA 3GAA	PWR2
3	48,046	16.06.2000	27.05.2019	6919	17x17 F	PWR3
4	46,76	29.05.2008	04.03.2019	3931	17x17 HTP	PWR4
5	46,752	29.05.2008	16.04.2019	3974	17x17 HTP	PWR5
6	45,759	18.06.1999	05.02.2019	7172	17x17 AA	PWR6
7	44,561	15.06.2007	27.02.2019	4275	17x17 HTP	PWR7
8	44,089	01.09.1988			17x17 W	PWR8
9	45,812	27.07.2007	25.01.2018	3835	15x15 W DEN	PWR9
10	43,329	11.06.1998	25.02.2019	7564	17x17 F	PWR10
11	43,345	16.06.2000	19.02.2019	6822	17x17 F	PWR11
12	43,105	01.09.1988			17x17 W	PWR12
13	40,765	25.04.1987	12.02.2018	11251	15x15 KWU	PWR13
14	40,678	13.06.1997	04.04.2019	7965	17x17 F	PWR14
15	40,47	14.08.1987	30.01.2018	11127	17x17 W	PWR15
16	40,339	13.06.1996	18.02.2019	8285	17x17 F	PWR16
17	40,51	26.08.1999	17.04.2019	7174	17x17 F	PWR17
18	39,637	30.05.1995	07.02.2018	8289	17x17 F DEMO	PWR18
19	34,891	04.04.1985	24.01.2018	11983	15x15 KWU	PWR19
20	33,955	30.05.1986			17x17 F	PWR20
21	33,959	30.05.1986	15.04.2019	12008	17x17 W	PWR21
22	31,242	28.06.1986	02.05.2019	11996	17x17 W	PWR22
23	28,542	13.06.1996	26.02.2019	8293	17x17 F	PWR23
24	23,26	30.05.1995	06.02.2018	8288	17x17 W	PWR24
25	19,824	11.05.1984	30.04.2019	12772	17x17 W	PWR25
26	46,501	26.08.2006			SVEA96	BWR1
27	44,25	24.07.2004			SVEA100	BWR2
28	43,932	05.08.2002			SVEA100	BWR3
29	41,626	05.08.2002			SVEA100	BWR4
30	42,145	26.08.2006	18.02.2020	4924	SVEA96	BWR5
31	37,946	12.09.1985			AA 8*8-1	BWR6
32	41,625	24.07.2004			SVEA100	BWR7
33	40,325	28.05.2005			Atrium 10B	BWR8
34	40,542	31.08.2007	11.03.2021	4941	SVEA96	BWR9
35	39,624	26.08.2006	11.02.2020	4917	SVEA96	BWR10
36	31,25	14.08.1992	19.02.2020	10050	AA 8*8-1	BWR11
37	33,737	31.05.2005	12.02.2020	5370	SVEA96	BWR12
38	36,726	31.05.2005	25.02.2020	5383	SVEA96	BWR13
39	30,432	12.09.1985			AA 8*8-1	BWR14
40	29,166	15.07.1989	02.03.2020	11188	AA 8*8-1	BWR15
41	27,269	31.05.1987	24.02.2020	11957	AA 8*8-1	BWR16
42	32,712	15.07.1986			AA 8*8-1	BWR17
43	20,952	14.08.1992	03.03.2020	10063	AA 8*8-1	BWR18
44	30,701	10.06.1989			AA 8*8-1	BWR19
45	26,739	31.05.2005			SVEA96	BWR20
46	27,674	01.07.1987			AA 8*8-1	BWR21
47	20,064	31.05.2005	26.02.2020	5384	SVEA96	BWR22
48	15,715	31.05.2005			SVEA96	BWR23
49	13,219	10.07.1987			AA 8*8-1	BWR24
50	8,897	10.07.1987			AA 8*8-1	BWR25

Table 2 – Example of PWR standardised input description.

```
<?xml version="1.0" encoding="UTF-8"?>

<CrossSection>

<Title WQTitle="PWR 15x15 AFA 3GAA Uran 4.10" WQName="U-_15_4.1_X_X" WQIdentifier="SKB_50_01" WQPlantName="SKB50" WQRegionName="1" S5Zone="1">
PWR1 H29AI1
</Title>

<!-- pellet diameter in cm; height in cm, density in g/cm3, dishing in mm3, cold data -->
<pellet PelletRadius="0.4565" PelletDensity="10.38" PelletGd2O3Density="0.0" PelletMaterial="UO2" PelletRings="3" PelletDishing="0">
</pellet>

<!-- cladding radius in cm; height in cm, density in g/cm3 -->
<cladding CladdingInnerRadius="0.4650" CladdingOuterRadius="0.5375" CladdingDensity="6.55" CladdingMaterial="Zry-4">
</cladding>

<!-- guidetubes radius in cm; height in cm, density in g/cm3, mass in kg, volume in cm3 -->
<guidetubes GuideTubes="20" GuideTubeInnerRadius="0.5295"  GuideTubeOuterRadius="0.6900"  GuideTubeDensity="6.55" GuideTubeMaterial="Zry-4">
</guidetubes>

<!-- fuel composition enrichment as wgt-percent, densities as particles per cm3 in hot condition kg/cm3 -->
<fuel U235Enrichment="4.10" Gd2O3WeightPercent="0.0" U235Gd2O3Enrichment="0.0">
</fuel>

<!-- reactor data; length in cm; temperatures in degree celsius; pressure in bar -->
<!-- power density: W/gU 214.5W/cm*391.56*236/537 -->
<reactor ReactorType="PWR" ReactorActiveHeightCold="390.0"
         ReactorAverageFuelTemperature="581" ReactorAverageModeratorTemperature="310" ReactorPressure="154"
         ReactorPinPitchCold="1.430" ReactorAssemblyPitchCold="21.56"
         ReactorAverageBoron="500.0" ReactorPowerDensity="36.9116" >
</reactor>

<!-- pin data -->
<pin PinXNumber="15" PinYNumber="15" PinFuelTypes="1" PinCladTypes="2">
</pin>

<!-- fuel pin type layout -->
<fuelpinlayout>
 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
 1 1 0 1 1 0 1 1 1 0 1 1 0 1 1
 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
 1 1 1 1 0 1 1 0 1 1 0 1 1 1 1
 1 1 0 1 1 1 1 1 1 1 1 1 0 1 1
 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
 1 1 1 1 0 1 1 1 1 1 0 1 1 1 1
 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
 1 1 0 1 1 1 1 1 1 1 1 1 0 1 1
 1 1 1 1 0 1 1 0 1 1 0 1 1 1 1
 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
 1 1 0 1 1 0 1 1 1 0 1 1 0 1 1
 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
</fuelpinlayout>

<!-- fuel rod geometry type layout -->
<fuelrodlayout>
 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
 1 1 8 1 1 8 1 1 1 8 1 1 8 1 1
 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
 1 1 1 1 8 1 1 8 1 1 8 1 1 1 1
 1 1 8 1 1 1 1 1 1 1 1 1 8 1 1
 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
 1 1 1 1 8 1 1 1 1 1 8 1 1 1 1
 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
 1 1 8 1 1 1 1 1 1 1 1 1 8 1 1
 1 1 1 1 8 1 1 8 1 1 8 1 1 1 1
 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
 1 1 8 1 1 8 1 1 1 8 1 1 8 1 1
 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
</fuelrodlayout>

<!-- number of fuel assemblies  and names -->
<assemblynames num='1'>
0001
</assemblynames>

<!-- heavy metal mass kgU -->
<assemblymasses>
460.407
</assemblymasses>

<!-- number of cycles and names -->
<cyclenames num='4'>
30 31 32 33
</cyclenames>

<!-- number of cycles, final burnup from plant data in MWd/kgU and EFPD of cycles -->
<cyclelengths num='4' burn='52.768'>
414 362 254 339
</cyclelengths>

<!-- number of cycles, average power in cycles in MW/MTU -->
<cyclepower num='4'>
40.99 45.90 35.05 30.33
</cyclepower>

<!-- number of downtimes, final cooling time and downtime in days -->
<!-- loading     date: 2005-05-04 -->
<!-- discharge   date: 2009-05-24 -->
<!-- measurement date: 2018-02-19 -->
<cyclecooling num='4' cool='3193'>
40 25 49 0
</cyclecooling>

</CrossSection>
```

Table 3 – Example of BWR standardised input description.

```
<?xml version="1.0" encoding="UTF-8"?>

<CrossSection>

<Title WQTitle="BWR SVEA 96 Uran 3.14" WQName="U-_11_3.1_X_H" WQIdentifier="SKB_50_35" WQPlantName="SKB50" WQRegionName="35" S5Zone="35">
BWR10 N20960
</Title>

<!-- pellet diameter in cm; height in cm, density in g/cm3, dishing in mm3, cold data -->
<pellet PelletRadius="0.410" PelletDensity="10.506" PelletGd2O3Density="0.0" PelletMaterial="UO2" PelletRings="3" PelletDishing="0">
</pellet>

<!-- cladding radius in cm; height in cm, density in g/cm3 -->
<cladding CladdingInnerRadius="0.4180" CladdingOuterRadius="0.4810" CladdingDensity="6.55" CladdingMaterial="Zry-2">
</cladding>

<!-- waterchannel data  Ri in cm; Ro in cm; geo="-9" square water rod for 9 cells -->
<waterchannel ChannelInnerR="1.485" ChannelOuterR="1.525" geo="-9" ChannelMaterial="Zry-2" pin="8">
</waterchannel>

<!-- slab data  central watter cross thickness cm; central box wall thickness in cm; -->
<!-- thickness water gap between central cross and adjacent pin cell in cm -->
<slab WaterCross="0.125" SlabWallThickness="0.080" GapPitch="0.270" SlabMaterial="Zry-2" pin="9">
</slab>

<!-- fuel composition enrichment as wgt-percent, densities as particles per cm3 in hot condition kg/cm3 -->
<fuel U235Enrichment="3.14" Gd2O3WeightPercent="0.0" U235Gd2O3Enrichment="0.0">
</fuel>
<!-- cruciform control rod data in cm -->
<!-- CrodThickness thickness of half of control rod-->
<!-- CrodStart start position of the cruciform -->
<!-- CrodSteelL length of central steel region -->
<!-- CrodABL length of zone 1 -->
<!-- CrodCRR absorbing cylinder radius -->
<!-- CrodCRP pitch between absorbing cylinders -->
<controlrod CrodThickness="0.352163" CrodStart="0.0" CrodSteelL="2.0066" CrodABL="10.409936"
            CrodCRR="0.21082" CrodCRP="0.578330" CrodMaterial="CRD">
</controlrod>
<!-- reactor data; length in cm; temperatures in degree celsius; pressure in bar -->
<!-- Wall thicknesses in cm, 1/2 values -->
<!-- power density: W/gU 214.5W/cm*391.56*236/537 -->
<reactor ReactorType="BWR" ReactorActiveHeightCold="371.0"
         ReactorAverageFuelTemperature="472" ReactorAverageModeratorTemperature="286" ReactorPressure="70"
         ReactorPinPitchCold="1.240" ReactorBoxInnerDistance="13.74" ReactorBoxWall="0.110"
         ReactorWideWaterGap="0.854" ReactorSmallWaterGap="0.691" ReactorBoxCornerR="1.010"
         ReactorAverageBoron="0.0" ReactorPowerDensity="36.9116" >
</reactor>

<!-- pin data -->
<pin PinXNumber="11" PinYNumber="11" PinFuelTypes="5" PinCladTypes="3">
</pin>
<!-- fuel pin type layout -->
<fuelpinlayout>
 1  1  1  1  1  9  1  1  1  1  1
 1  1  1  1  1  9  1  1  1  1  1
 1  1  1  1  1  9  1  1  1  1  1
 1  1  1  1  1  9  1  1  1  1  1
 1  1  1  1  8  8  8  1  1  1  1
 9  9  9  9  8  8  8  9  9  9  9
 1  1  1  1  8  8  8  1  1  1  1
 1  1  1  1  1  9  1  1  1  1  1
 1  1  1  1  1  9  1  1  1  1  1
 1  1  1  1  1  9  1  1  1  1  1
 1  1  1  1  1  9  1  1  1  1  1
</fuelpinlayout>
<!-- fuel rod geometry type layout -->
<fuelrodlayout>
1  2  3  3  2  0  2  3  3  2  1
2  5  4  2  5  0  5  2  4  5  2
3  4  5  2  2  0  2  2  5  4  3
3  2  2  2  5  0  5  2  2  2  3
2  5  2  5  0  0  0  5  2  5  2
0  0  0  0  0  0  0  0  0  0  0
2  5  2  5  0  0  0  5  2  5  2
3  2  2  2  5  0  5  2  2  2  3
3  4  5  2  2  0  2  2  5  4  3
2  5  4  2  5  0  5  2  4  5  2
1  2  3  3  2  0  2  3  3  2  1
</fuelrodlayout>

<!-- number of fuel assemblies  and names -->
<assemblynames num='1'>
0035
</assemblynames>

<!-- heavy metal mass kgU -->
<assemblymasses>
169.645
</assemblymasses>

<!-- number of cycles and names -->
<cyclenames num='5'>
25 26 27 28 29
</cyclenames>

<!-- number of cycles, final burnup from plant data in MWd/kgU and EFPD of cycles -->
<cyclelengths num='5' burn='39.624'>
332 367 297 363 312
</cyclelengths>

<!-- number of cycles, average power in cycles in MW/MTU -->
<cyclepower num='5'>
27.28 21.01 22.02 28.75 18.85
</cyclepower>

<!-- number of downtimes, final cooling time and downtime in days -->
<!-- loading     date: 2001-08-29 -->
<!-- discharge   date: 2006-08-26 -->
<!-- measurement date: 2020-02-11 -->
<cyclecooling num='5' cool='4914'>
31 47 29 45 0
</cyclecooling>
</CrossSection>
```

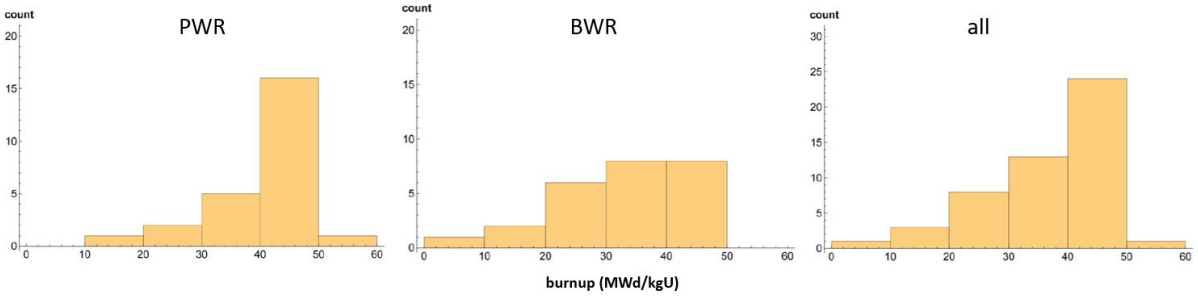

Figure 1 – SKB-50 PWR and BWR and combined distribution of burnup.

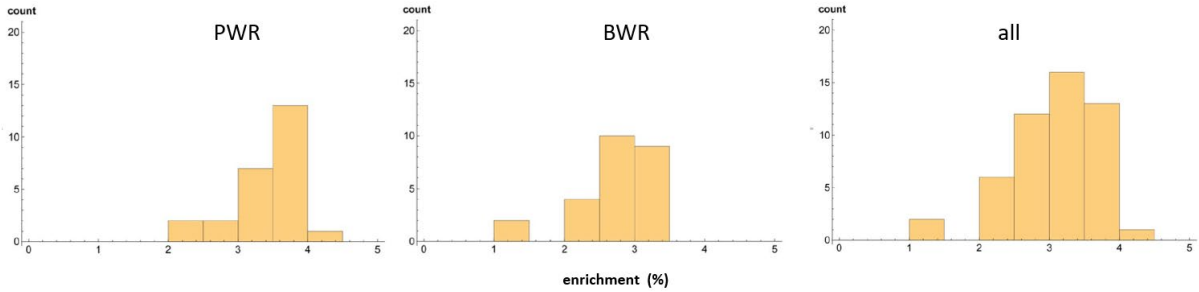

Figure 2 – SKB-50 PWR and BWR and combined distribution of enrichment.

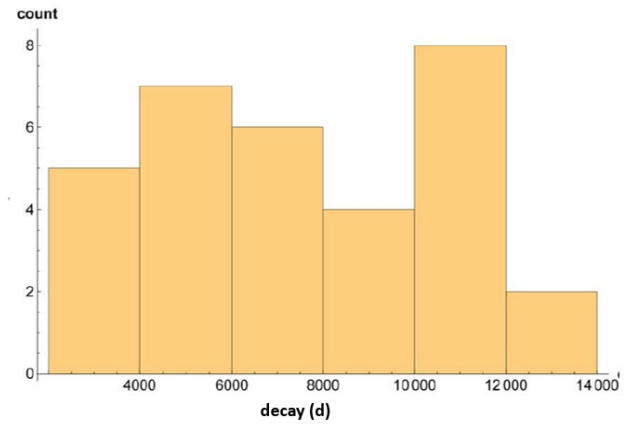

Figure 3 – SKB-50 distribution of cooling times.

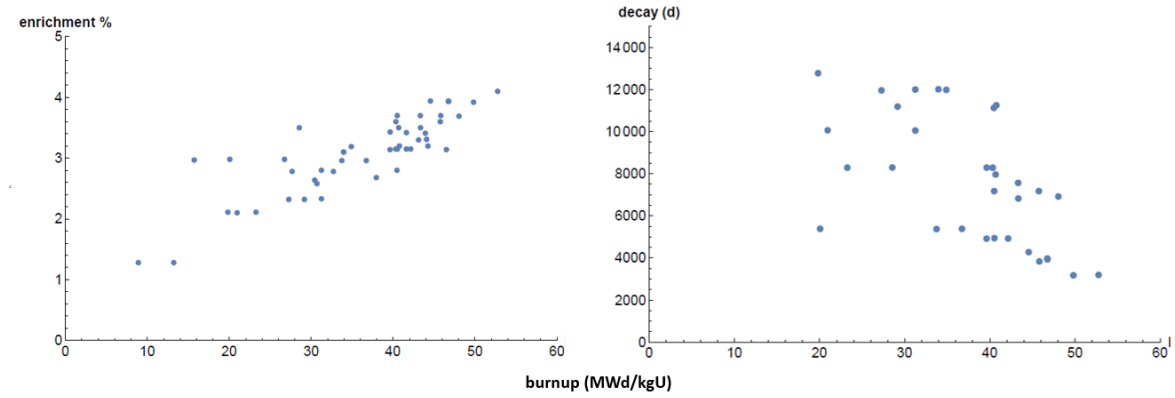

Figure 4 – SKB-50 enrichment and decay time versus burnup (not all of the 50 fuel assemblies have measurement data).

Appendix B. SKB-50 blind test results

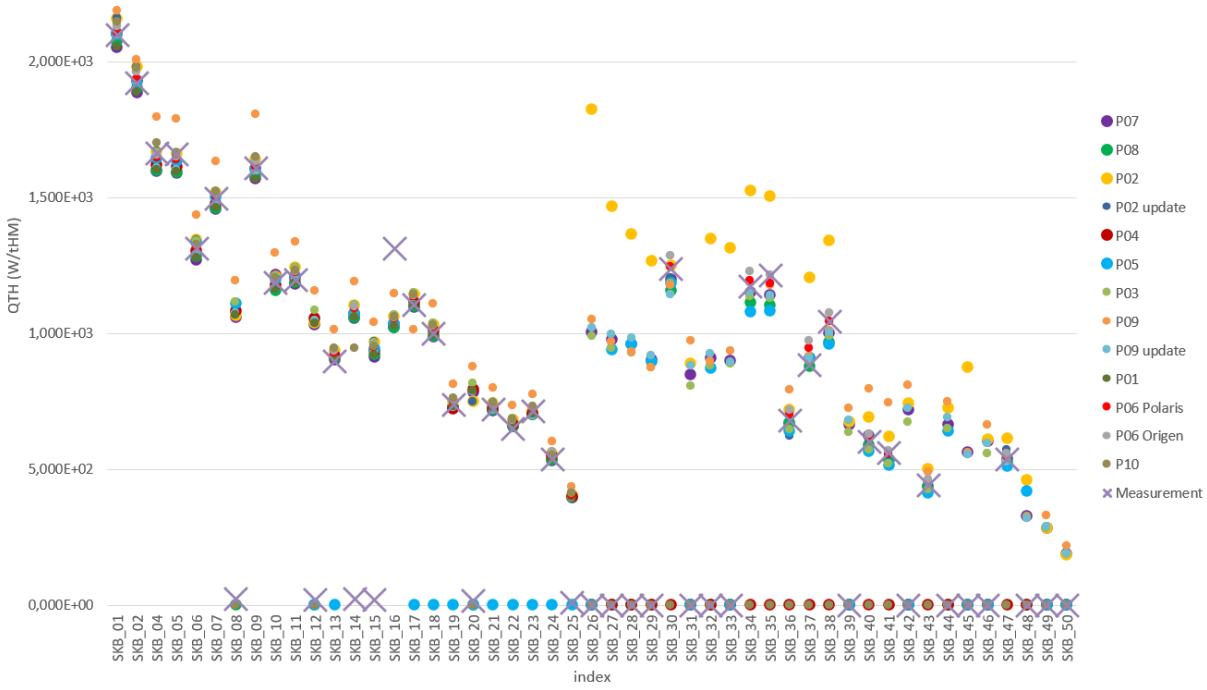

Figure 5 – Calculation and measurement results of all participants for all submitted cases before un-blinding.

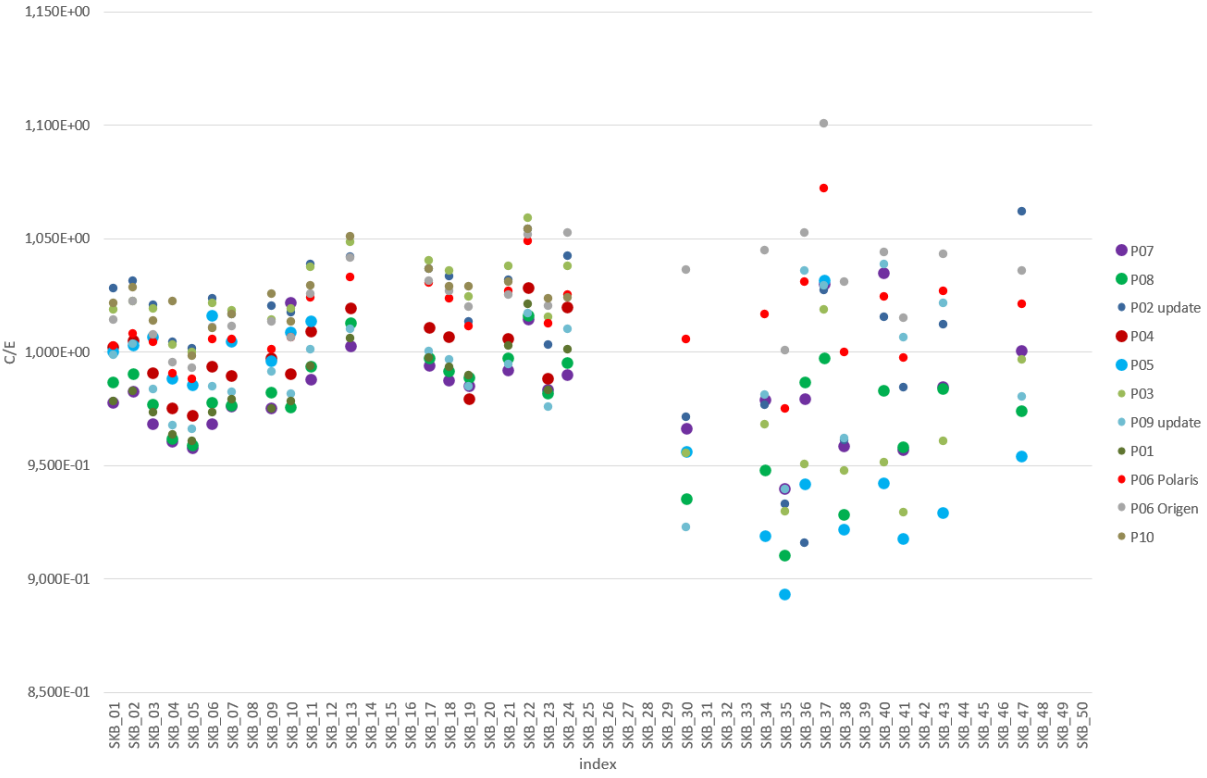

Figure 6 – C/E results of all participants after re-evaluation and re-submission as described in the text.

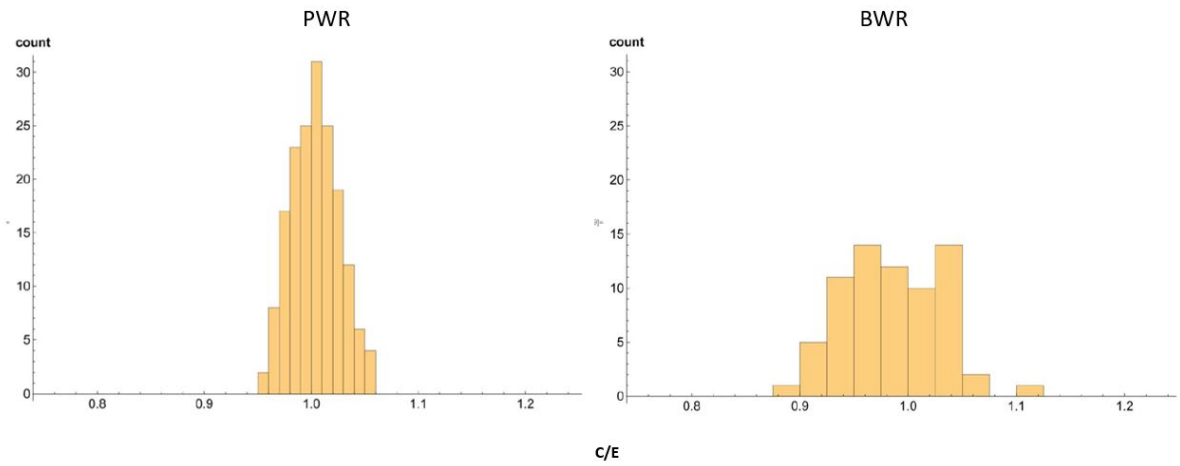

Figure 7 – PWR and BWR C/E histogram results.

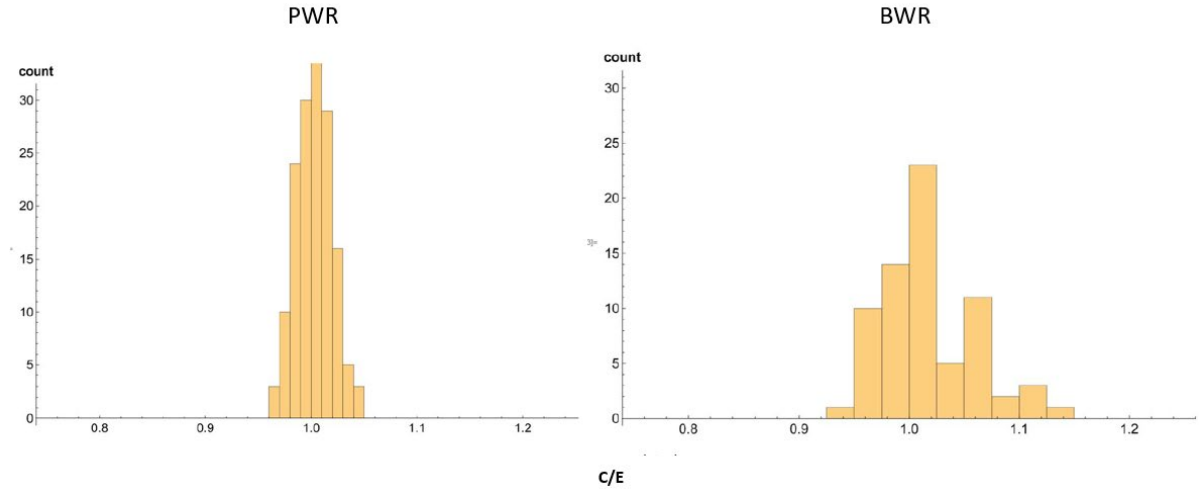

Figure 8 – PWR and BWR C/E histogram results determined with correction factor as described in text.

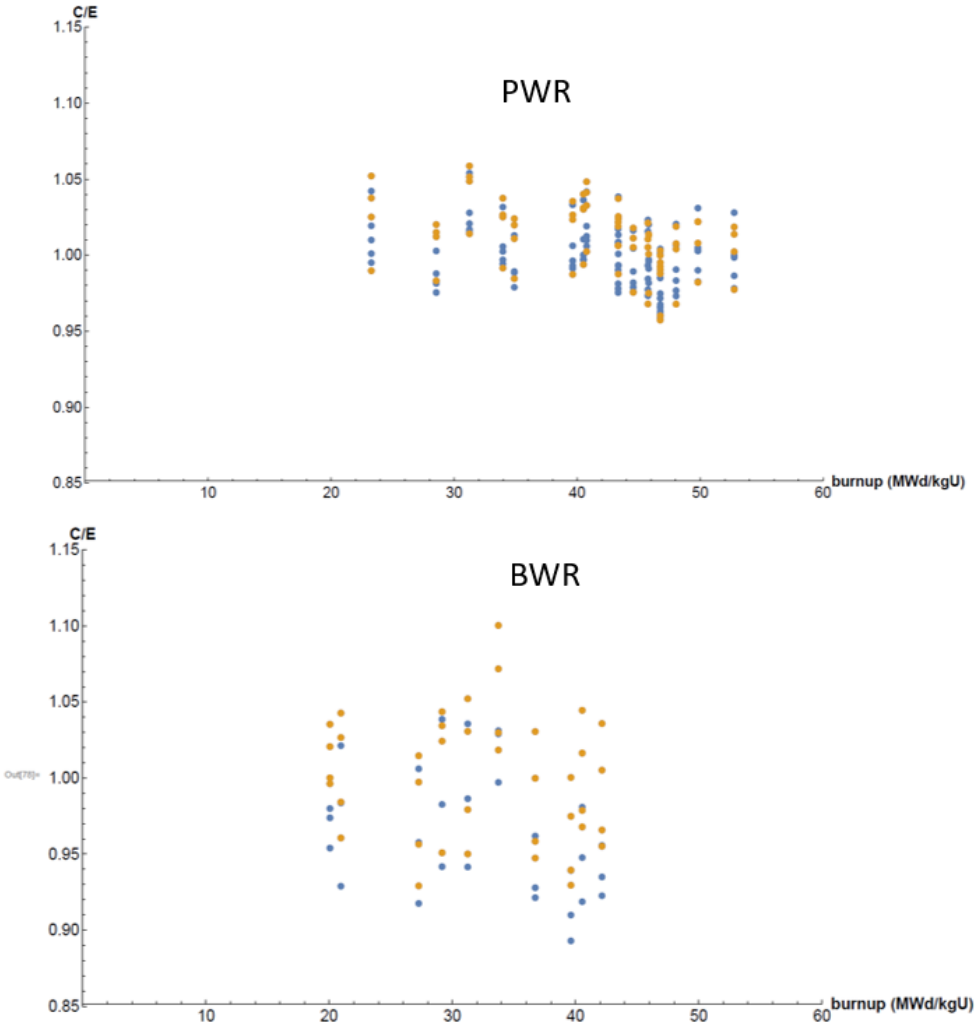

Figure 9 – PWR and BWR C/E results with all SCALE6 related results marked in orange.

Table 4 – Blind test statistics of each participant.

Participant	**Code**	**ND library**	**C/E**			
			PWR		**BWR**	
			Average	St. dev	Average	St. dev
P08	CASMO5	ENDF/B-VII.1	0,986	0,015	0,960	0,029
P01	DARWIN2	JEFF-3.1.1	0,986	0,016		
P05	MCNP/CINDER	ENDF/B-VII.1	1,002	0,010	0,940	0,037
P02	MCNP/EVOLCODE	JEFF-3.3	1,025	0,014	0,986	0,044
P06	SCALE 6.2.3: TRITON/ARP/ORIGEN	ENDF/B-VII.1	1,020	0,017	1,040	0,026
P06	SCALE 6.2.3: Polaris/ORIGEN	ENDF/B-VII.1	1,014	0,016	1,017	0,025
P07	SCALE 6.2.3/TRITON/NEWT	ENDF/B-VII.1	0,984	0,017	0,983	0,031
P03	SCALE 6.2.3/TRITON/NEWT	ENDF/B-VII.1	1,026	0,015	0,961	0,028
P10	SCALE 6.1.3/ORIGEN-ARP	ENDF/B-V	1,025	0,013		
P04	Serpent 2	ENDF/B-VII.1	0,999	0,016		
P09	Serpent 2	JEFF-3.3	0,991	0,014	0,992	0,041

Table 5 – Summary of results on Clab 2006 C/E results.

Ref.	Year	Code	Library	PWR		BWR	
				<C/E>	σ	<C/E>	σ
Ilas and Gauld	2008	SCALE 5.1	ENDF/B-V	1,011	0,012	1,003	0,025
Ilas et al.	2014	SCALE 6.1.2	ENDF/B-VII.0	1,002	0,012	0,997	0,024
Ilas and Burns	2021	SCALE 6.1	ENDF/B-VII.0	1,013	0,013	1,002	0,012
	2021	SCALE 6.2.4	ENDF/B-VII.1	1,008	0,012	1,009	0,024
Ilas and Burns	2022	SCALE 6.3	ENDF/B-VIII.0	1,006	0,014	1,007	0,024
Shama et al.	2022	SCALE 6.2.3	ENDF/B-VII.1	1,019	0,012	1,003	0,025
		SCALE6.2.3 (POLARIS)	ENDF/B-VII.1	1,015	0,012	1,010	0,026
Shama et al.	2022	CASMO5 2.03	ENDF/B-VII.1 (201)	1,009	0,013	1,008	0,025
Rochman et al.	2023	CASMO5 2.03	ENDF/B-VII.1 (201)	1,008	0,013	1,007	0,026
		CASMO5 2.03	ENDF/B-VII.1 (201)	0,986	0,013	0,987	0,026
		CASMO5 2.13	ENDF/B-VII.1 (202)	0,986	0,013	0,986	0,026
		CASMO5 3.05	ENDF/B-VII.1 (202)	0,987	0,013	0,986	0,026
		CASMO5 3.05	ENDF/B-VIII.0 (300)	0,986	0,013	0,986	0,020
		CASMO5 3.05	JEFF-2.2 (300)	0,978	0,012	0,978	0,025
		CASMO5 3.05	JEFF-3.1.1 (200)	0,972	0,012	0,971	0,025
		CASMO5 3.05	JEFF-3.2 (202)	0,977	0,012	0,976	0,026
		SNF 1.6	ENDF/B-VII.1 (201)	1,003	0,015	1,014	0,035
		SNF 1.07	ENDF/B-VII.1 (202)	0,984	0,015	0,992	0,034
Yamamoto	2016	CASMO5	JENDL-4.0	1,016	0,013	1,001	0,024
Hannstein et al.	2023	MOTIVE	ENDF/B-VII.1	1,008	0,010	1,003	0,022
			ENDF/B-VIII.0	1,004	0,010	0,998	0,022
			JEFF-3.2	0,987	0,010	0,981	0,023
Ebiwonjumi et al.	2019	STREAM	ENDF/B-VII.0	1,000	0,017		
Haeck et al.	2014	VESTA 2.1	JEFF-3.1	0,978	0,013		
		VESTA 2.1	ENDF/B-VII.0	0,995	0,013		
San-Felice et al.	2012	DARWIN	JEFF-3.1.1	0,978	0,011		
Mills and Sutton	2009	FISPIN	JEF-2.2	0,995	0,013		
		FISPIN	JEFF-3.1.1	0,985	0,012		
Rochman et al.	2023	DIN 2014		1,027	0,027		
		ANS 2014		1,121	0,043	1,170	0,036
		RG-3.54 2018		1,075	0,018	1,063	0,027

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