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Evaluation Guide for the Evaluated Spent Nuclear Fuel Assay Database (SFCOMPO)

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franco.michel-sendis@oecd.org

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Nuclear Science Committee

Working Party on Nuclear Criticality Safety (WPNCS)

Expert Group on Assay Data of Spent Nuclear Fuel (EGADSNF)

Nuclear Energy Agency

Organisation for Economic Co-operation and Development

ORGANISATION FOR ECONOMIC CO-OPERATION AND DEVELOPMENT

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The NEA Data Bank provides nuclear data and computer program services for participating countries. In these and related tasks, the NEA works in close collaboration with the International Atomic Energy Agency in Vienna, with which it has a Co-operation Agreement, as well as with other international organisations in the nuclear field.

Foreword

The Expert Group on Assay Data for Spent Nuclear Fuel (EGADSNF) of the Working Party on Nuclear Criticality Safety (WPNCS) under the auspices of the NEA Nuclear Science Committee was set up in 2007 with the objective of compiling and evaluating experimental data on the nuclide compositions of irradiated nuclear fuel. Experimental data refer not only to the measured nuclide inventories and uncertainties as determined mainly by destructive radiochemical assay of spent fuel samples, but also the fuel assembly design data, reactor design information, and operating data necessary to develop benchmark models. These data provide an important basis for validating calculation methods (computer codes and nuclear data) used in fuel burn-up analyses applied to spent fuel criticality safety analyses using burn-up credit, thermal analysis, radiation shielding, accident dose consequence analysis, fuel cycle safety, reprocessing, and deep geological repository safety studies. The quality and usefulness of the experimental data for methods validation can be improved by developing complete descriptions of the experiments, providing benchmark specifications, and by performing independent evaluations of the experimental and benchmark data. Evaluations of the experimental data have been identified as an important task to verify the quality of the information in the spent fuel composition (SFCOMPO) database maintained by the Nuclear Energy Agency (NEA) Data Bank.

This guide defines the evaluation document format and data review procedures for evaluators tasked with reviewing the experimental data. Guidance is developed to provide recommended procedures and criteria developed by experts in the field on how to perform standardised reviews, how to identify potential problems in the measurement data and gaps in the experimental description, and provide guidance on how to resolve these issues, when possible, using a consistent technical basis. Procedures for deriving benchmark data and models from the experimental data are also covered by the guide.

Within this report, the following terminology is used:

- *Experimental data* refer to both the measurement data from the radiochemical analysis of spent fuel and the supporting design and operating history data, as provided in original reference reports that may be available from the measurement laboratory or the reactor operator.
- *Benchmark data* refer to the experimental data after review and evaluation that provide a complete experimental description and an assessment of uncertainties has been performed by an evaluator.
- *Benchmark models* are descriptions of the benchmark data for use in computational models developed as part of the evaluation procedure.

The main tasks of the evaluator include evaluating the (1) reactor and fuel assembly design and material composition data, (2) reactor operating history data that describe the operating conditions, and (3) measured spent fuel nuclide data from radiochemical analysis. If the experimental data are found to contain sufficient information to develop a computational model, then (4) one or more benchmark models should be prepared and (5) the calculated

results from the benchmark should be provided, including an assessment of experimental uncertainties.

In cases where experimental descriptions are found to be incomplete it may not be possible to develop a benchmark model. However, in cases when there are minor gaps in data, recommendations are provided for deriving appropriate data or obtaining surrogate data for similar systems. In these cases, approximate or surrogate data are to be clearly identified and any uncertainties associated with the data are to be quantified using uncertainties studies. To the extent possible, the guidance applies widely accepted methods and industry standards for data reduction and derivation of parameters required for modelling and simulation.

The evaluation is to be documented using the following sections and appendices that define the recommended document format:

- Description of the experimental data: This includes original sources of the data to be used in the benchmark model specification. References to primary sources of information on the experiment are provided in Section 1.
- Evaluation of the experiment data: Selection and review of information from Section 1 leading to confirmation or modification of the data as well as accounting for missing information. Errors are identified and corrected and uncertainties from Section 1 are reviewed, modified or estimated when missing in Section 1.
- Benchmark model specifications: Preparation of a benchmark model based on the evaluation of experimental data in Section 2. Biases in the benchmark results due to any model simplifications in the benchmark specifications are quantified and the impact of model uncertainties is estimated.
- Sample calculation results: The benchmarks in Section 3 are applied using a computational method selected by the evaluator. The method and results are briefly summarised. Additional calculation contributions by reviewers may be added.
- References: All published documents used in the evaluation that contain information about the experiments are listed.
- Appendix A: Code input listings for the calculation models are reported in Section 4.
- Other appendices: Additional information of interest to users of the evaluation may be included.

This guide is organised according to the sections of the evaluation report. Additional detailed discussion and information on many review topics are included in Appendix A of this guidance report.

It is recognised that this guidance will not address all of the possible issues that may arise during an evaluation. The importance of using sound technical judgement in these situations cannot be overemphasised. In situations where the guidance does not adequately address the challenges, the evaluator should seek advice of a subject matter expert and bring obstacles to the evaluation to the attention of the expert group where appropriate subject area experts may be assigned to help address issues in a consistent way. Experience gained in the evaluation process will be incorporated in future revisions to the guidance report. In this regard, the guidance report will serve as a living document that is likely to be revised regularly as the evaluation process proceeds, particularly during the early phase of this activity.

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List of authors

P. Ortego (SEA Ingenieria y Analisis de Blindajes S.L., Spain)

D. Boulanger (NIRAS/ONDRAF, Belgium)

I. Gauld (Oak Ridge National Laboratory, US)

M. Gysemans (SCK•CEN, Belgium)

M. Hennebach (AREVA GmbH, Germany)

D. Mennerdahl (E Mennerdahl Systems, Sweden)

J.C. Neuber (Individual, Germany)

C. Tore (SEA Ingenieria y Analisis de Blindajes S.L., Spain)

S. Tittelbach (WTI GmbH, Germany)

S. Van Winckel (ITU, Karlsruhe, Germany)

H.–U. Zwicky (Zwicky Consulting GmbH, Switzerland)

1. Description of the experimental data

Section 1 of the evaluation report should start with a brief description of the experiment that includes a general description of the reactor characteristics, fuel assembly design, nuclides measured, and measurement methods, along with any important or unique features of the experiment. The experimental data in an evaluation report may contain different fuel samples from an experiment, but should not include data from different reactors or assembly designs so that an evaluation report can be uniquely associated with an experimental data set in the SFCOMPO database. A detailed description of the experiment and the available relevant data are provided in subsections of this section.

Only the description of the experiment from primary references or sources of information should be included in Section 1, without reference to models, calculated results, or statements regarding quality of the data. Inconsistencies in data or missing data should be clearly noted. The experimental data include directly measured values, and may include values provided by the fuel vendor or reactor operator that have been calculated from reactor simulations for parameters that cannot be measured directly, but are necessary for a complete experimental description. It is recommended that only experimental data obtained directly from the primary references are included in this section, with the information reproduced with the maximum possible fidelity by using the reported units and decimals. If fuel design or reactor operating information is available in other reports, these may be used with appropriate citations. Other data derived directly from experimental data may be included provided it is clearly noted as derived with the method of derivation given to provide traceability.

The source of each data value should be clearly identified along with any uncertainty (or manufacturing tolerance) assigned in the references. Uncertainties are generally reported by the laboratories for the radiochemical analysis results; however, uncertainty information for reactor operating data are usually not available and fuel design manufacturing data are generally limited due to the proprietary nature of the manufacturing tolerances.

1.1 Design data

1.1.1 Reactor data

The reactor types currently in the database are listed in Table 1. Each reactor is identified by a unique name and unit. The reactors are also categorised by their coolant and moderator type, and fuel types are also identified for the purposes of searching using basic design categories.

Other general reactor characteristics such as active core height, number of assemblies, total heavy metal mass, coolant inlet and outlet temperatures, and specific power may be noted. Although these parameters are typically not required to develop a model of the experiment, this information may be useful for deriving representative values for data not provided directly.

Table 1. Reactor, coolant, moderator, and fuel type categories

Commercial reactor types	Moderator types	Coolant types	Fuel types
PWR	Light Water	Light Water	UO_2
BWR	Heavy Water	Heavy Water	MOX
CANDU	Graphite	CO_2	U (metal)
VVER 440			
VVER 1000			
RBMK			
MAGNOX			
AGR			

1.1.2 Assembly and fuel rod design data

A large amount of design data may be required to fully describe the assembly, including data for the fuel rods, guide tubes, water rods, non-fuel absorber rods, and other assembly components. Also, the location of all fuel rods, non-fuel rods, guide tubes, instrument tube, and any other structural components of the assembly should be described and illustrated. It should be noted, however, that only structural components near the active fuel zone will have an impact on the neutronics, thus the design data can usually be limited to this part of the assembly. Other reactor types may require geometry and dimension data for the coolant channels, pressure tubes, and graphite sleeves etc. Examples of the data typically required for light water reactor designs include:

- fuel pellet outside diameter;
- fuel rod length (total and active);
- fuel pellet inside diameter (e.g. for some VVER and AGR designs);
- cladding inside diameter;
- cladding outside diameter;
- absorber rod dimension (PWR);
- absorber rod compositions (e.g. gadolinium or boron rods) (PWR);
- control blade dimensions and compositions (BWR);
- number of fuel rods;
- number of guide tubes or water rods;
- number of instrument tubes;
- number of absorber rods;
- fuel rod pitch (may be more than one pitch in some assembly designs);
- configuration of rods in the assembly;
- assembly pitch type (square, hexagonal, other);
- assembly pitch dimension;
- guide tube inside diameter (PWR);
- guide tube outside diameter (PWR);

- guide tube material (PWR);
- instrumentation tube inside diameter (PWR);
- instrumentation tube outside diameter (PWR);
- instrumentation tube material (PWR);
- number and position of water rods, internal channel or wings (BWR);
- water rod/channel outer diameter (BWR);
- water rod/channel inner diameter (BWR);
- water rod/channel thickness (BWR);
- water rod/channel material (BWR) ;
- assembly sub-channel and internal material properties (SVEA-BWR and similar designs);
- external flow channel width (BWR);
- external flow channel material (BWR);
- axial elevation of grids or spacers;
- dimension and composition of grid or spacers (if in proximity of measured sample);
- weight and volume of each type of grid or spacer;
- neighbour assembly design types.

Design data are required for all fuel and non-fuel rods in the assembly, not only the measured rod(s). For some designs, the fuel rod enrichment may vary by location in the assembly, and some designs also use axial enrichment variations and partial-length fuel rods. A complete description of the fuel rod characteristics should be listed.

1.1.3 Absorber rod data

Burnable absorber rods in an assembly can have a significant effect on the neutron spectrum of the fuel. Therefore, the design details and locations are critical to develop accurate benchmark specifications. It is important to not only document the design, absorber type and concentrations, number of rods, and locations, but also the duration of the exposure. Absorber rods may be classified as either integral absorbers or discrete absorbers.

Integral absorber rods contain neutron absorbers that are integral to the assembly design and therefore present for the entire life of the assembly. Usually the absorber is gadolinium intermixed with uranium; however erbium has also been used in some designs. The Westinghouse Integral Fuel Burnable Absorber (IFBA) uses an alternate boron-based ZrB_2 absorber on the outside layer of the fuel pellet. Integral absorber rods usually include fuel. However, some assembly designs have used integral absorber rods that do not contain fuel such as B_4C or rods containing stainless steel. It is important to document any integral absorber rods including their design, material compositions, the number of rods, and the location of the rods in the assembly.

Discrete absorber rods are used in PWR assemblies. These rods are not an integral part of the assembly design, but instead are inserted into guide or instrument thimble tubes of an assembly during irradiation in one or more cycles. They are frequently removed from the assembly after the first cycle, but may be reinserted in later cycles. Therefore, in addition to

the physical description of these rods, it is important to document when the rods were inserted and withdrawn from the assembly. Common absorbers include boron (B4C), borosilicate glass (Pyrex) compounds, and AgInCd alloys.

1.1.4 Fuel composition data

The initial uranium enrichment is a basic parameter of uranium oxide (UO_2) fuel and is always required. The uranium isotopic concentration is usually given as atom or weight % values. The initial uranium isotopes include ^{235}U and ^{238}U, and should include the initial amounts of the minor isotopes ^{234}U and ^{236}U if available.

MOX fuels are also defined by the Pu content and the isotopic vector which should consider the date (if different than the time of loading in the reactor) due to the decay of ^{241}Pu to ^{241}Am.

1.1.5 Structural material composition data

Other structural compositions may be defined by the density and weight percent of each constituent in the mixture (if provided), by the density and compound, or for structural materials by the material type (e.g. Zircaloy-2 or stainless steel). Other materials including the coolant and moderator must also be defined. These densities may vary in different regions of the assembly. For example, the water density in the coolant flow channel may be less than the density outside the flow channel. Note that material density may also change with time due to temperature variations and changes in reactor operation. Time-dependent information is to be documented with the operating history data (Section 1.2).

1.1.6 Reactor components

A description of reactor component dimensions and compositions is needed, particularly for non-LWR systems. These components include the reactor coolant and moderator, such as heavy water, light water, carbon dioxide (low neutronic importance), and graphite. In graphite and heavy water systems, the reactor volume that is required to be modelled may be much larger than in light water reactors because of the large mean free path of neutrons in these systems, hence their sensitivity to structures located far from the assembly.

1.1.7 Impurities

Impurity levels are generally poorly documented but should be included in the evaluation when information is available. They may be later omitted from the benchmark model since they usually are of low importance to spent fuel analyses and since they are often not known accurately. An exception may be for graphite moderators, where low concentrations of absorbing impurities may have an impact on the neutron spectrum due to the long path length of neutrons in graphite.

Impurities are important when measurements include nuclides that are activation products of the initial impurities. In this case, accurate values of the initial impurity levels are required (not typical or maximum allowed values).

1.1.8 Control blade design data

In BWR designs, control blades are inserted from the bottom of the reactor for reactivity control, and any control blade design information should be documented if blade insertion occurred at the axial elevation and proximity of a measured sample.

1.1.9 Fuel rod relocation

Some experiments involve the relocation, or reconfiguration, of the measured fuel rod from one assembly to another to achieve the desired irradiation characteristics (i.e. high burn-up). In

these special cases, design and irradiation information on both assemblies is required. When a fuel rod is relocated to a previously irradiated assembly, the complete irradiation history of the host assembly is needed to determine the initial fuel compositions of the host assembly at the time of relocation.

1.2 Reactor operating history data

The reactor operating history data includes information for those parameters that depend on the operation of the reactor and may include the specific power, fuel temperature, moderator temperature and density, moderator void for BWRs, boron concentration, absorber rod insertion, and control blade insertion. Parameter values may be provided as average values for the reactor, assembly, and/or sample or as time-dependent values over the irradiation history. Many of these parameters also vary spatially over the reactor. These data are required at the location of the measured fuel sample.

1.2.1 Cycle dates

The start and end dates of reactor operation are required for any cycles that the assembly was irradiated to determine the irradiation times and decay times (between cycles and at time of measurement). For reactors that operate with continuous on-line refuelling (e.g. CANDU, AGR, and RBMK), cycle dates do not apply, and the exposure history is defined by the loading date and discharge date of each assembly in the reactor. In this case, the cycle data are simply a construct to store the assembly at the beginning and end of irradiation dates. The location(s) of the assembly in core may also be given.

1.2.2 Power history

The specific power of the fuel may be reported as either power per assembly, power in the measured rod, or power in the measured sample. If the power in the sample is not provided, approximate values may be derived from the rod or assembly power data. Specific power may be given as cycle-average data, or may be provided as time-dependent data for each cycle. In cases where only the burn-up is provided, average power values may be accurately derived using the cycle or cumulative burn-up and the irradiation time(s).

The actual operating days should be used when available to describe the irradiation power history. However, operating data are sometimes reported as Effective Full Power Days (EFPD).

1.2.3 Temperatures

The fuel, cladding, and coolant temperatures should be provided as available for each sample. These may be provided as either constant values or as time-dependent values. Temperature values for other components of the reactor should also be given including moderator (e.g. graphite).

1.2.4 Coolant density and void

The coolant density is usually available as average or time-dependent values. The densities (and void) vary between the inlet and outlet of the reactor core. These data are required at the axial elevation of each sample. In some cases where data at the sample locations are not provided, they may be estimated in Section 2, using other information, such as the inlet and outlet coolant temperatures, the system pressure, the axial power profile, and the location of the sample in the active fuel length.

1.2.5 Boron level

Soluble boron levels in water moderator should be listed (if applicable). The boron level may be reported as cycle-average values or as time-dependent boron let down curves. Soluble

boron is sometimes enriched in ^{10}B. It is important to record the enrichment level when enriched boron has been used.

1.2.6 Absorber rods and control blades

Any exposure of the fuel assembly to removable discrete absorber rods or control blades should be described, with the time of exposure and duration of exposure. However, these data are only usually required if the absorber insertion reached the elevation of the measured sample.

Exposure to movable control rods (e.g. Reactor Cluster Control Assembly), control blades, or other control elements can similarly affect the neutron spectrum of the fuel. Documentation of the degree of control element exposure, control element design details, and depth of insertion into the core, is required to assess the potential impact at the location of the measured sample and is included in the description if warranted.

1.2.7 Neighbouring assemblies

Information on the neighbour assemblies located adjacent to the measured assembly or measured fuel rod(s) may be available for recent experimental programmes. Frequently, this information has not been documented in earlier programmes because it could not be applied using the available computational analysis methods at the time. When available, information on neighbour assemblies usually includes the assembly design, initial enrichment, and burn-up at the beginning of each cycle.

1.3 Fuel sample data

Fuel sample data includes basic information on the sample and identifies the position in the assembly and rod where the sample was obtained, including:

- assembly identifier;
- rod identifier and rod location in the assembly;
- axial position (height) of the sample in the rod (usually measured from the end of the rod or active fuel region);
- physical size (length) of the sample;
- ^{235}U enrichment for uranium fuels;
- fissile Pu enrichment for mixed oxide (MOX) fuels;
- nominal sample burn-up.

In light water reactors, the elevation of the sample in the rod may be important to estimate the local coolant temperature and density conditions and temperatures of the sample.

1.4 Measurement data

The measurement data include the following radiochemical or radiometric analysis data compiled from the experimental report(s) of the spent fuel isotopic analyses:

- measurement laboratory;
- measured nuclides;
- radiometric or radiochemical analysis techniques (see Table 2);
- measured concentration value;

- concentration units;
- uncertainties;
- confidence level of the reported uncertainties (units of standard deviation, e.g. 1=1 sigma, 2=2 sigma, etc.);
- measurement date;
- reference date (if different than the actual measurement date);
- separation date (may be required if the separation date is significantly different than the date the nuclide contents were measured, to correctly account for nuclide decay).

Measurements may be reported in many different mass, activity, and atom units. Measurement ratios are also frequently reported. The database allows these measurement units to be entered, and also allows special units that are reserved for laboratory-estimated burn-up values, etc. The values should be listed with the precision and units as reported by the laboratory.

Special attention may be necessary to clarify the basis of the measured concentrations. For example, if results are reported per gram uranium, it must be determined if this refers to the uranium content before or after irradiation. In addition, the evaluator may convert the concentrations as reported by the laboratory to other units used more commonly in code calculations, (e.g. mg/g fuel or g/g U initial). Any derived values must be clearly indicated and the method of derivation described.

Table 2. List of common measurement techniques

Measurement method	Abbreviation
Gamma spectroscopy	γ spec
Alpha spectroscopy	α spec
Liquid scintillation counting	LS
Thermal ionisation mass spectrometry	TIMS
Inductively coupled plasma mass spectrometry	ICPMS
Quadrupole ICPMS	Q-ICPMS
Multicollector ICPMS	MC-ICPMS
Isotopic dilution calibration	ID
External calibration	EXT

2. Evaluation of experimental data

Evaluation of experimental data is performed to identify missing data or weaknesses in the data. Any inconsistencies in the published data are discussed and addressed in subsections of this section of the evaluation report.

Data required to develop a benchmark model that is not directly available from the primary experimental reports may be included from other references, or derived from similar data, provided appropriate uncertainties are estimated and assigned. If there is insufficient design or operating data to develop a benchmark model, this should be indicated with the missing data clearly identified. Significant gaps in the experimental description do not preclude using the measurement data in the SFCOMPO database.

The effects of uncertainties in parameter data on the results are to be quantified and discussed. This analysis includes an estimation of the impact on the calculated nuclide concentration due to the uncertainties in fuel design and reactor operation parameter uncertainties. The uncertainty analysis should consider both the reported uncertainties and estimated parameter uncertainties where uncertainties have not been reported. Codes and modelling methods used for the uncertainty analysis should be specified. The adequate combinations of the uncertainties in each nuclide to the different parameters will provide a total uncertainty estimate for the calculated nuclide concentrations. Because of the large number of parameters in the experimental data, each with uncertainties and correlations, the task of combining uncertainties is acknowledged as difficult, and there is currently not a consensus approach on how best to accomplish this task rigorously.

The evaluation procedure does not support the acceptance or rejection of experimental data based on the completeness of information or uncertainties (unless the data are deemed to be unphysical or internally self-inconsistent and therefore in error). The quality of the experimental data as a benchmark may be judged based on how the uncertainties influence the results. This process thereby allows the end user, rather than the evaluator, to determine the acceptability of the benchmark based on the accuracy requirements for their intended application. For example, undocumented fuel impurity data may exclude the experiment for consideration for waste management applications, but the same experimental may be perfectly acceptable for use in criticality safety applications.

Appendix A of this report provides additional guidance and more detailed discussion on data and uncertainties.

2.1 Missing data

Missing design or operating information should be clearly identified and called out in the evaluation report. A recommended procedure to assist evaluators in identifying incomplete information is to develop a model of the fuel and assembly, i.e. for uncertainty analysis (Section 2.9).

Any missing data identified in the evaluation may be requested through the responsible research organisation, report authors, reactor utilities, fuel manufacturers, or researchers involved in the programme. This option may only be practical for programmes that are either

still active or have been recently completed. In some cases, information may be unavailable due to proprietary or other confidentiality restrictions. The evaluator may investigate alternate public sources for the information, e.g. other reports documenting design information for the same assembly design in other references, or determine if the required information may be derived from other available information. Requests for assistance in identifying additional sources of data can be directed to the Expert Group.

If required design information cannot be located, the evaluator may include nominal values based on expert judgment with suitable uncertainty or tolerance range that accounts for the uncertainty in the estimated values. These uncertainties are to be later included in an uncertainty analysis of the benchmark. Typical parameter values obtained from public sources and expert experience are provided with data uncertainties for reference by the evaluator, in Appendix A.

2.2 Design data

Fuel design data are frequently given as the nominal dimension and may include manufacturing tolerance. The actual parameter distribution (uncertainty) is typically a Gaussian curve centred within the tolerance range. The distribution can be centred at any point inside that range with the only condition being that the probability curve does not exceed the tolerance limits by a significant amount, i.e. to minimise the number of components that will be rejected by quality control. This information is available to the manufacturer but is normally not included in the experiment reports. Without knowledge of the actual distribution, the evaluator may assume a uniform probability within the tolerance range. The evaluator is referred to [1] for more complete guidance about the interpretation of uncertainties, and Appendix A for typical uncertainty and tolerance values.

If measured fuel samples are located from near grid spacers or the top/bottom of the active region of the fuel, then more detailed design information of the fuel rod plenum and end-plugs, flow nozzles, hold-down springs, and grid spacers may be required to develop an accurate benchmark model. Axial gamma ray scans of the measured fuel rods may be helpful to identify anomalies at the measured fuel sample locations caused by assembly structures.

2.3 Material compositions

A complete description of the initial (un-irradiated) fuel and assembly structure compositions is required for the benchmark specifications. These data are generally well documented and include the density of the material and the elemental fractions. Isotopic distributions are required for elements that are not in natural isotopic abundances (e.g. enriched uranium, boron). Uncertainties may be available for uranium and plutonium (for MOX fuel) isotopic values.

2.3.1 Uranium isotopic distribution

The uranium isotopic distribution includes the atom percent or weight percent concentrations of ^{234}U, ^{235}U, ^{236}U, and ^{238}U. The ^{235}U enrichment is always required as this is a defining parameter of the fuel. Concentrations of minor isotopes ^{234}U (natural), ^{236}U and ^{232}U (present in reprocessed uranium) may be reported. In the event these minor uranium isotopes are not provided, approximate concentrations may be estimated using data for other similar fuel enrichments. Uncertainties in these values typically have a relatively low impact on most other spent fuel nuclide concentrations.

If estimating ^{234}U and ^{236}U concentrations from other sources, the evaluator should consider the origin of the uranium. Different countries use different sources of uranium feed

stock that frequently includes different amounts of reprocessed uranium (the source of ^{236}U and ^{232}U in enriched uranium). Some countries view the ^{236}U as proprietary information for this reason. In several studies involving fuel of Russian origin, the initial concentrations of ^{236}U were found to be many times larger than fuel of US origin. Consequently, using estimates based on fuel data from a different country could lead to large errors in the assumed initial uranium compositions.

2.3.2 Mixed oxide fuel

For MOX (mixed oxide) fuel, the uranium enrichment (usually natural or depleted uranium), the total plutonium mass fraction in initial heavy metal and the plutonium isotopic distribution is required. In addition, the concentration of ^{241}Am (generated by decay of ^{241}Pu after chemical separation) is also usually reported. This value is calculated by the fuel vendor based on the estimated fuel loading date in the reactor. If the actual loading date differs significantly from the estimated date, corrections for decay may be required as ^{241}Am is a neutron absorber.

2.4 Irradiation history

The assembly irradiation history data include the start and end date for each cycle and the cycles that the assembly resided in the reactor. This information is generally considered public and may be available from other sources. For experiments that provide only the operating and decay times it may be possible for the evaluator to determine the dates from other information. The dates corresponding to periods of reactor operation may be different than the dates of fuel loading and discharge from the reactor. After the end of irradiation, the fuel must generally be cooled several days before it can be unloaded from the reactor.

Periods of reactor down time are important to the nuclide concentrations at the time of measurement.

2.5 Reactor operating conditions

Operator data are generated using reactor core physics and fuel management computer codes used by the reactor operator. These data are generated using core calculations and measurements of the reactor conditions, such as coolant temperatures, soluble boron levels, reactor operating power, and the power distribution (reaction rates) in the core as measured by in-core detectors. Some parameters, such as fuel temperature and void, are difficult to determine and have inherently large uncertainties.

The reactor operating data are required for the local conditions at the axial elevation in the assembly where the measured fuel sample was located. Operating data are frequently provided by axial node representing the average data over a given axial range of the assembly. The evaluator may need to perform additional processing (e.g. interpolation) of the operator data to derive estimates of the local conditions at the sample elevation.

Uncertainty information for reactor operating data is usually unavailable. Additional guidance and values for typical uncertainty values are provided in Appendix A. These values may be used in the uncertainty analysis described in Section 2.9.

2.5.1 Specific power

The time-dependent specific power of the fuel sample is required over its irradiation history in the reactor. Attention should be given to providing a detailed representation of the variation of power when available.

The level of detail on specific power documented in experimental reports is very inconsistent. Modern experimental programmes often report detailed time-dependent power

values for the analysed fuel samples. Several older programmes report only the assembly average burn-up at the end of each operating cycle. However, knowing the cycle length, this information may be used to derive the cycle-average assembly power for each assembly. Because the specific power for the sample is usually required as input to the depletion calculations, the evaluator must scale the assembly power to match the burn-up value of the fuel sample as derived from the radiochemical analysis measurements.

2.5.2 Moderator conditions

The water density in light water reactors is required at the elevation of the measured sample in the assembly. Several density values may be required to represent different regions of the assembly having different temperatures (or void fractions). For example, the water moderator conditions inside the flow channel of a BWR assembly may be very different than the conditions outside the channel.

For PWR experiments that do not report local moderator conditions, the water temperature (and density) at the sample elevation may be estimated from the active fuel height assuming a suitable axial power shape for the assembly, the system pressure, and the core inlet and outlet temperatures [10]. However, this approach does not account for the variability in temperatures between low- and high-power assemblies. In general, such an approach should only be used to derive information if data are not available from the operator.

For BWR systems, axial void and temperature data (usually reported by axial node) must be available from the operator. Because the void levels change during reactor operation, the values should be provided in time or burn-up steps that are smaller than the cycle length. Estimating the void conditions or temperature of BWR samples without the assembly data information provided by the reactor operator is not recommended.

For BWR assemblies, it is also important to include the water density in regions of the assembly that are not boiling, e.g. in water rods internal to the assembly, assembly structural components such as water cross regions of the SVEA design, and water external to the channel. Additional detailed discussion of void and uncertainties is presented in Appendix A.

2.5.3 Fuel temperature

Fuel temperatures are not measured directly but are calculated parameters that may be available from the operator or other fuel modelling codes. Fuel temperature is not reported consistently. Fuel temperatures may be reported as the peak (central) and surface temperatures, fuel-volume-averaged temperature, or as effective average temperature (to provide a neutron absorption equivalent temperature value). The effective temperature is required when modelling the fuel as a single region in order to obtain correct resonance absorption rates in the fuel. The effective temperature is generally lower than the average temperature by up to 100 K at low operating powers (~900 K) to more than 200 K at high powers (~1700 K). The evaluator should include the definition of the fuel temperatures so that correct values may be applied in the benchmark specifications.

Approximate methods to obtain fuel temperatures are described in Appendix A. Typical uncertainties are also provided.

2.5.4 Boron concentration

Time-dependent soluble boron levels in water for PWR systems are measured by the operator and are usually available as time-dependent or cycle-average values. The boron levels at the beginning of cycle, at xenon equilibrium, and at the end of cycle (usually near zero) largely define the time-dependent behaviour. However, with the increasing use of burnable absorbers

in PWR fuel designs, the time-dependent variation of boron concentration is therefore not always linear. If the time-dependent boron level variation is not available, the cycle-average boron concentrations have been shown to be equivalent for the purposes of fuel isotopic depletion calculations.

2.5.5 Absorber rods

Because the length of the discrete absorber rods is frequently shorter than the active fuel length, it is important to document the length (if available) and the insertion level to evaluate the potential impact at the axial height on the measured sample.

2.5.6 Neighbour assemblies

Studies performed in [2] suggest a relatively minor influence of the neighbour assemblies on the depletion model for UO_2 fuel, and that a single assembly model with reflective boundary conditions is generally applicable. A negligible impact from neighbour assemblies on fuel rods located internal to the assembly (non-periphery rods) has been observed. For BWR assemblies that have a large water gap outside the flow channels, the impact of neighbour assemblies is usually negligible.

Neighbour assemblies have been demonstrated to influence the nuclide compositions of MOX fuel assemblies, which operate in reactor cores containing a mix of UO_2 and MOX assemblies. The impact is most pronounced on the periphery MOX rods facing the adjacent UO_2 assemblies. Therefore, information on the neighbour assemblies should be included in the evaluation report when available.

When evaluating the impact of neighbour assemblies, it is important to consider the assembly burn-ups at the axial elevation of the measured samples, since the local burn-up of neighbour assemblies is different than the average assembly burn-up.

2.6 Radiochemical assay data

Evaluation of radiochemical analysis data consists of evaluation of the data and uncertainties as measured, and checking any modifications/calculations of the initial analytical results that are frequently performed by the laboratory. These checks may involve relatively straightforward calculations (e.g. unit conversion, decay corrections, adjustment of data to a common reference date), or other tests of the measurement data consistency via different methods (e.g. mass balance, burn-up estimated by different burn-up indicators, comparisons of results obtained by different measurement techniques, comparisons with other data for similar fuels, etc.).

2.6.1 Experimental laboratory reports

The starting point for any evaluation of radiochemical analyses should be the original report(s) on the laboratory measurements. The results of the chemical analyses may also be given in other project reports, but not necessarily with the same analytical detail needed for a proper evaluation of the data. It might be necessary to contact the laboratory in order to obtain the detailed analysis reports (recommended).

2.6.2 Review of analytical procedures

In order to evaluate chemical analysis data, it is important to be familiar with the analytical procedures. This is not an easy task for the evaluator as some (specialised) analytical knowledge is required in order to assess the assay data. A useful source of information is [2], which gives an overview of analysis procedures, from sampling and sample dissolution up to

analytical measurement techniques, with levels of expected uncertainty for each step. The references in that report can be consulted for more detailed and in-depth information.

2.6.3 Measurement uncertainties

Both the measurement instrument and calibration techniques generally have a large influence on the final reported uncertainty, and can lead to variations in achievable accuracy from less than 1% and up to 10% or more. In mass spectrometry measurements, the relative isotopic mass fraction (relative to the element) also plays a significant part in defining the uncertainty, with relative uncertainty increasing with lower isotopic concentrations. Typical instrument uncertainties are described in [2].

The results from any chemical analysis can only be properly evaluated when they are accompanied by their respective uncertainties. What is needed is the total uncertainty from all phases of the measurements. It is important to also understand what is included in the reported uncertainties. Measurement uncertainties can include the uncertainties in various analytical steps, from fuel dissolution, hot-cell work and dilutions, to standards, calibration, measurements and calculations used to process raw measurement data.

The reported uncertainty may include only the measurement uncertainty; the combination of the measurement precision (repeatability plus reproducibility) and measurement accuracy, without consideration of other components that contribute to the overall uncertainty. In many cases, the uncertainty associated with measurements themselves is the biggest contributor to the total experimental uncertainty, but the evaluator should review the original reports to determine what is included in the reported uncertainties and if these reported values are representative of the total experimental uncertainty.

If detailed information regarding the uncertainties is unavailable, then a comparison of the reported uncertainties with the typical uncertainties from the state-of-the-art report [2] may help in assessing the reliability of reported uncertainties. The support of radiochemical analysis experts in the field of spent fuel analysis (preferably those of the laboratory where the measurements were performed) can also be very helpful here.

2.6.4 Correlation analysis

Whenever detailed and comprehensive documentation of the complete analytical process allows, it is very useful and instructive to include a correlation analysis of the uncertainties of the complete data set [3]. Although such analysis is currently not common practice, it is worth checking for possibly significant correlations between isotopes of a single element (more probable) and correlations between different elements (less probable). Some examples of the possible impact this can have on validation exercises can be found in [4,5]

2.6.5 Multiple laboratory measurements

Measured fuel contents are sometimes reported based on combining multiple measurements when a nuclide is measured by different analytical techniques (e.g. radiometric and by mass spectrometry), or when the same fuel sample is measured at different laboratories. Although combining measurements may reduce uncertainties, the consequences of combining data may be loss of information depending on the data reduction methods used. Combining of results should only be performed by the measurement laboratory and not by the evaluator. It is usually preferable to work with multiple measurements individually rather than combining the experimental results. However, combined results reported by the laboratory may be included if appropriately identified in the measurement data.

This situation may also occur when different burn-up values are estimated using different burn-up indicators as measured in the fuel sample. In this case, the evaluator should review the consistency of the different burn-up estimates with other measurement data for the sample (e.g. ^{235}U or fission products, particularly the burn-up monitors like ^{148}Nd and ^{137}Cs) to identify potentially discrepant data when the different burn-up estimates are incompatible with the uncertainties. Burn-up values that are compatible, (i.e. *not* significantly different at the chosen confidence level) may be combined. How to combine the results depends on the evaluation of the uncertainties. In most cases, the recommended method of combining results with unequal uncertainties will be to use uncertainty-weighted results (i.e. "weighted mean"). Unequal uncertainties occur because different laboratories most often use different analytical methods, techniques, calibration methods, etc. In a weighted mean, the result with the lower associated uncertainty will get more weight in the final result. This, of course, makes a correct and complete estimation of the uncertainty and confidence interval very important. More details on statistical techniques can be found in textbooks on statistics and chemometrics [6,7]

2.6.6 Reference date

Reference dates that are different than the actual measurement date may be used by laboratories when reporting data to provide a common date for performing consistency checks of the radiochemical analysis data and independent laboratory comparisons. The end-of-life (EOL) date is sometimes used (mostly in older experimental programmes), corresponding to the date the fuel was last irradiated. The data at the time of measurement are preferred (when available) for comparison with code predictions.

Any adjustment of the experimental data to a common reference date must account not only for the decay of the measured nuclide but also possible production from decay precursors. If a decay precursor has not been measured and contributes significantly to the nuclide of interest, then the adjustment to a reference date other than the measurement date is not possible. Data that are decay-time-corrected to a single reference date are useful for consistency checking and may be used as a simplification in the benchmark model provided the time adjustments are minor and any biases are quantified.

The nuclear data (and associated uncertainties) used by the laboratory when performing any data adjustments is another point to check, as the adjusted data values may depend on the source of the nuclear decay data. The nuclear data used should, of course, be consistent throughout the exercise and should be stated by the laboratory.

2.6.7 Separation date

The chemical separation date between mother-daughter nuclides should be considered for nuclides with important decay precursors. The separation date is to be included in the experimental data description when it is significantly different than the measurement date since the decay chains are altered after separation.

2.7 Sample burn-up determination

2.7.1 Burn-up as atom percent fission (%FIMA)

The most suitable (least ambiguous) unit for reporting burn-up from radiochemical assay data is the number of fissions relative to the number of heavy metal atoms initially present in the fuel (percent Fissions per Initial Metal Atom, or %FIMA, also known as atom percent fission or burn-up; see also [2]. The unit is independent of values for the recoverable energy per fission for each fissionable nuclide. The %FIMA value may be converted to units of GWd/tHM [8] should be consulted).

The atom percent fission (%FIMA) value can be derived directly from the analysis results for the compositions of nuclides U, Pu, etc., obtained by destructive analysis as:

$$\%FIMA = F/U = F/(F+U')$$

where F is the number of heavy metal atoms fissioned, U is the number of heavy metal atoms before irradiation, and U' is the measured number of heavy metal atoms at the end of irradiation (e.g. U+Pu+Am+Np+Cm). F is most frequently determined as $F = N/Y_{eff}$, where N is the measured number of fission product atoms of a burn-up monitor nuclide such as ^{148}Nd, and Y_{eff} is the effective fission product yield, i.e. weighted by the yield for each actinide causing fission.

2.7.2 Burn-up as gigawatt days per tonne heavy metal

A common unit for reporting burn-up is the total energy released per unit mass of initial heavy metal (e.g. GWd/tHM). This quantity is not directly measurable. It may be estimated from the %FIMA value (requires an approximate value for energy per fission) or from computer codes by determining the burn-up value that produces the measured quantity of a fission product burn-up indicatory.

2.7.3 Burn-up values from the operator

Burn-up values reported based on operator estimates from reactor code calculations should in general not be used since they may be subject to large uncertainties.

2.7.4 The ASTM E321 – 96 Standard Method for burn-up

The ASTM E321 – 96 Standard Test Method for Atom Percent Fission in Uranium and Plutonium Fuel (Neodymium-148 Method) [8] is widely used for burn-up determination. However, conversion factors for typical fuel characteristics provided in the standard method limit the accuracy of the method to about 3%, and application to higher burn-up will be less reliable. It is recommended that evaluators apply this standard method as it is a useful check of the data. The critical burn-up parameter is that which is directly measured, e.g. the $^{148}Nd/^{238}U$ atom fraction.

2.7.5 Burn-up from other fission products

Although most burn-up determinations use ^{148}Nd, other stable or relatively long-lived fission products may be used that may include $^{143+144}Nd$, $^{145+146}Nd$, ^{150}Nd, ^{139}La, ^{137}Cs and ^{144}Ce. A comparison of the ^{148}Nd burn-up result with the burn-up results using other burn-up indicators is very useful to ensure that isolated analytical problems did not cause large errors in the burn-up estimate.

The use of $^{143+144}Nd$ and $^{145+146}Nd$ (combined because of the large neutron capture cross-sections of ^{143}Nd and ^{145}Nd) has the potential advantage that these isotopes occur at much larger isotopic concentrations than ^{148}Nd (generally <10% of total Nd), resulting in potentially lower measurement uncertainty.

Experience has shown ^{137}Cs to be a reliable burn-up indicator. However, in order to get an accurate burn-up value based on ^{137}Cs, a correct and representative sampling of the fuel is very important as Cs is one of the elements known to migrate in the fuel pellet during irradiation due to the high-temperature gradient in the fuel. Therefore, accuracy of ^{137}Cs as a reliable indicator may be dependent on having a fuel sample large enough to be representative of the fuel pellet. The relatively long half-life of ^{137}Cs (30 years) relative to typical operating times allows accurate corrections for decay during irradiation to be made accurately using only cycle start and end dates, and cycle-average specific powers.

The short half-life of ^{144}Ce (285 days) limits the accurate application of this nuclide as a burn-up indicator to fuels with short cooling times. In addition, a significant fraction of ^{144}Ce produced during the beginning of irradiation may decay by the time of measurement, making the use of this isotope very sensitive to the irradiation history data which may introduce additional uncertainties. Experience with using ^{144}Ce as a burn-up indicator has had mixed success.

2.7.6 Code analysis of burn-up data

Since rigorous computational methods are usually available to the evaluator, there is also the option of using these methods for estimating sample burn-up by the use of more detailed and exact methods than the above-mentioned standards. In this approach, the weighted residuals between calculated and measured concentrations of selected fission product burn-up indicator isotopes are evaluated to determine an appropriate code burn-up value that reproduces the measured concentration(s). However, there is no general consensus on this topic and the evaluator should be aware that the burn-up results will dependent on the selected isotopes, the code and nuclear data.

2.7.7 Discrepancies in burn-up determination

Incompatible burn-up estimates obtained using the different Nd isotopes might indicate analytical problems, such as insufficient separation (Nd-Ce, Nd-Sm) or contamination with natural Nd. Discussions with the analytical experts from the laboratory, when possible, might clarify the discrepancies. However, note that the burn-up results calculated via the other Nd isotopes are not independent of the ^{148}Nd burn-up result because the Nd isotopic vector is usually measured together. Therefore, any bias in the Nd content will impact all Nd isotopes. If the results for the different Nd burn-up values are consistent, they help confirm the consistency of the Nd isotopic assay data.

The evaluator may combine all consistent burn-up results obtained using different methods and indicators to provide a single recommended burn-up value for the sample. The respective uncertainties of the individual results should be taken into account when doing so.

2.8 Additional data verification

2.8.1 Trending analysis

The evaluator can look for correlations in the data by comparing nuclide concentrations like ^{235}U, ^{239}Pu, ^{240}Pu etc. or derived quantities such as depleted ^{235}U, build-up of ^{236}U, etc. for different samples and reactors. These nuclides generally exhibit a smooth build-up or depletion in the fuel over time. Trending analysis of the nuclide concentrations with burn-up, or other measurement results (e.g. ^{148}Nd) may be very instructive when comparing the variance with the uncertainties reported by the laboratory.

Some nuclides are very insensitive to the neutron spectrum while others are highly dependent on the spectrum. Therefore, such correlations must be considered when comparing data from samples irradiated in different neutron spectra. For example, comparison of data from different axial location of the same fuel rod may provide reliable correlations, provided that the axial moderator design is relatively constant or slowly varying. Comparing different fuel rods from the same assembly should consider the similarity of the fuel rod locations and proximity to water rods or neutron absorbers.

2.8.2 Data consistency

The review of data consistency between different samples may help to establish increased confidence in assay data and reported uncertainties. However, it may be difficult to attribute a

lack of correlation to the measurements when comparing data from samples exposed to different neutron spectra and other reactor parameters that can influence each fuel sample differently.

2.8.3 Nuclide correlations

When several members of a decay chain are measured, the relative concentrations of the mother and daughter concentrations may be checked for consistency. For example, the content of ^{241}Am at the time of measurement is dominated by production from decay of the parent ^{241}Pu which contributes typically more than 80% to the ^{241}Am content after 3 years and more than 90% after 10 years. Therefore, ^{241}Am content may be accurately estimated directly from the measured ^{241}Pu content for fuel with long cooling times. Another example is ^{155}Gd. The ^{155}Gd content at the time of measurement is dominated by production from the decay of parent ^{155}Eu. Therefore, any significant deviation (taking into account the respective uncertainties) between the measured ^{155}Gd and the result calculated analytically from the decay of ^{155}Eu is indicative of measurement problems.

2.8.4 Mass balance

Mass Balance (MB) is a straightforward and relevant check of the global quality of the measurement results [2]. This check compares the total mass of individual nuclides or elements from the sample measurements with the mass of fuel sample determined by weighing. Corrections for the loss of actinide mass caused by fission are usually made by estimating the total number of fissions using the measured ^{148}Nd concentration. Deviations larger than 3% are an indication that at least one step in the measurement process was questionable (material loss, inefficient separation, dilution error, etc.). Further analysis of the complete data set should reveal whether this error did affect the as measured content for all the different nuclides or not (depending on the step where the error occurred).

Differences in mass balance may be caused by factors that influence all results by the same bias. In this case, relative results like mg per g ^{238}U final may remain valid and represent more accurate measurement values since absolute mass determination is not required.

2.8.5 Sample size

Samples obtained from very small sections of a fuel pellet may have increased uncertainty caused by inhomogeneity of the fuel due to migration of some species and non-uniformity of the burn-up in a pellet. The evaluator should review the physical size of the sample to determine if it is appropriate for the benchmark model. Note that some samples are not transverse sections of the fuel rod and are designed to measure compositions in different radial regions of the rod. These specialised measurements are generally not considered for evaluation since they require very detailed models.

2.9 Uncertainty analysis

The final step in the evaluation of experimental data is the analysis of uncertainties using a model of the experiment. It is not required to use the exact benchmark model specification to perform the uncertainty calculations, however any large differences from the benchmark model should be noted.

In addition to reported measurement uncertainties, there are uncertainties associated with the design and operating data that also contribute to defining the quality of the experimental data and benchmark. In the case of undocumented or missing data the evaluator is requested to provide surrogate information, if appropriate, based on the best information available, obtained from other sources or based on engineering judgment. However, estimated data may have large

associated uncertainties, and it is the role of the evaluator to assess the importance of these uncertainties.

Unavailability of important design or operating data in the experimental description may introduce such large uncertainties in the model as to preclude the ability to development benchmark specifications or model.

2.9.1 Computational methods

Either deterministic or Monte Carlo codes can be used for the uncertainty analysis. Deterministic methods are sometimes preferable for sensitivity analysis since they provide a value of perturbation effect without the statistical uncertainty associated with Monte Carlo methods. Monte Carlo methods however can support more complex geometry, use of continuous-energy cross-sections, and the statistical uncertainty may be reduced as needed by increasing the number of particle histories.

For Monte Carlo methods, it may be required to increase the perturbation (uncertainty) value beyond the actual uncertainty such that the statistical noise is small compared with the perturbation effect. Once the sensitivity coefficient is calculated (for each nuclide) the results may be scaled to reflect the actual uncertainty. The evaluator is cautioned that such an approach assumes first-order linearity and this should be verified.

The evaluator is cautioned that analysis of temperature uncertainty by perturbation of the temperature values may be inadequate for libraries that tabulate cross-sections at discrete temperatures, e.g. 300, 600 and 900ºK. This issue is more common to Monte Carlo codes that use continuous-energy cross-section libraries.

2.9.2 Single-parameter perturbation

One approach to performing uncertainty analyses is single-parameter perturbation calculations using an appropriate model. This approach is consistent with guidance regarding the calculation tools and methods for performing these sensitivity analyses for critical benchmarks for the International Criticality Safety Benchmark Evaluation Project (ICSBEP), found in [1].

Uncertainty in sample burn-up represents one of the most important sources of uncertainty in calculated nuclide concentrations and must be included in the analysis. Uncertainty in the burn-up derives largely from uncertainty in the measured nuclide content of the burn-up monitor(s) (usually ^{148}Nd or other burn-up indicator).

Other parameters that may be included in single-parameter uncertainty studies are:

- initial heavy metal isotopic composition;
- fuel density;
- fuel temperature;
- moderator temperature;
- moderator density (temperature and void);
- boron concentration;
- power history.

Consensus values for typical uncertainties, when not provided in the experimental reports, are summarised in Appendix A.

The importance of initial fuel compositions, fuel rod data, and fuel assembly design parameter uncertainties is generally small to negligible. A change of the pellet or cladding outer diameter may impact the average moderation of neutrons within the fuel since the volumetric ratio of moderator and fuel depends on those diameters. Any increase in cladding diameter will reduce the moderator to fuel ratio. The sensitivity to the cladding diameter is larger than to the pellet diameter.

Changes in design dimensions that may result from assembly distortion during irradiation due to the high-temperature and high-pressure environment are typically small. These variations are typically unknown and difficult to quantify but may be considered if information on fuel rod distortion is provided.

Uncertainty for operating parameters is not as commonly reported as design data and may pose challenges to uncertainty quantification. Many nuclides exhibit relatively low sensitivity to the operating power history; however, several short-lived fission products exhibit a high sensitivity, particularly to the power history near the end of irradiation.

2.9.3 Mutually dependent (correlated) parameters

Additional care is needed to identify mutually dependent parameters when performing parameter perturbation to avoid unphysical results. For example, in pressurised systems the water density is dependent on the temperature. Therefore these values should be perturbed such that their dependency is preserved.

2.9.4 Combined uncertainty

After the effect of design and operating data uncertainties have been quantified for each of the major contributors to uncertainty, the combined uncertainty for each of the measured nuclides should be estimated. However, there is currently no consensus on the best approach for combining different uncertainties due to the sometimes incomplete reporting of uncertainty information, inconsistent or inaccurate uncertainty estimates, and strong correlations in some parameters. Caution and care are required to ensure that reliable estimates of total uncertainty are obtained.

Combining the individual contributions (see Section 2.9.2) using a summation-of-variances approach may be appropriate but this approach requires independent parameters and assumes that first-order linearity is appropriate when combining uncertainties.

In addition to estimating the uncertainties in the nuclide concentrations, the evaluator may include uncertainties for integral applications such as criticality safety (k_{eff}), decay heat, etc.

3. Benchmark specifications

Benchmark specifications provide the data necessary to construct calculational models that accurately represent the experiment. The data are prepared by the evaluator using the evaluated values for fuel and reactor design parameters, and reactor operating conditions from Section 2. The benchmark model specifications should retain as much detail as necessary to model all important aspects of the actual experiment. When it is necessary or desirable to simplify the representation of the experiment for the benchmark model, the benchmark specifications must include a description of the impact of the simplifications or approximations on the measured values.

Developing the benchmark specification requires a complete benchmark description. Experiments with incomplete assembly design information may preclude the development of benchmark specifications and also sample calculation results, e.g., missing fuel rod enrichment configuration, moderator void information, etc.

3.1 Benchmark model documentation

The benchmark specifications should be documented in this section as: Description of simplifications with an assessment of the magnitude of the simplifications on the measurement results (Section 3.1); design data with geometry and dimensions (Section 3.2); material composition and temperature data (Section 3.3); reactor operating history data (Section 3.4); reactor operating conditions (Section 3.5); and the benchmark values for the measured nuclide values for the fuel and their associated uncertainty (Section 3.6).

3.2 Benchmark model

Two-dimensional models may be used to accurately represent samples in many fuel assemblies. Three-dimensional models are typically not required, but may be used to investigate three-dimensional effects [9] for samples located in regions near grid spacers, part-length rod transition zones, absorber insertion, samples near the end of the fuel rod, or partial control blade insertion.

Models for burnable absorber rods (e.g. gadolinium bearing fuel rods), may require radial subdivision of the rod with concentric material regions in order to allow an accurate representation of the spatial depletion of highly absorbing isotopes in the fuel. Finer spatial divisions of the rod and shorter time steps are considered better approximations. If the gadolinium bearing rod or a fuel rod adjacent to the gadolinium rods is measured, then the requirement for finer divisions and time steps should be verified.

3.3 Benchmark model simplifications

Any simplification or approximation should be clearly described and any resulting bias in the measured nuclide concentrations should be small and noted. Such simplifications may be code specific and nuclide dependent, so it is important to identify the code, libraries, and versions.

The model description should also consider the capabilities and limitation of different methods that may be used to calculate the benchmark, from simple to more advanced calculation tools.

Examples of typical benchmark model simplifications include: using a single assembly (reflected) model when information on the neighbour assemblies is provided; representing detailed time-dependent quantities such as boron level, specific power, or temperature data as cycle-averaged or lifetime-averaged values.

Measurement data adjusted to a common reference date may be included to simplify the use of the data in a benchmark specification for convenience of the comparing measurements with code calculations. If such a simplification is done, the time adjustments should be as small as possible by making the reference date close to the actual measurement dates. Also, any decay precursor nuclides must also be measured and used in the adjustment, or it must be shown that the precursors are not significant.

4. Results of sample calculations

Calculated results obtained using the benchmark model specifications (Section 3) are tabulated in this section. These results are to be regarded as sample calculations because codes usually have several options to represent the benchmark model data and methods to obtain the code solution. These options are not necessarily reviewed or considered consensus options; therefore different users may obtain different benchmark results using the same code and data. Choice of appropriate code input and options to represent the benchmark model described in Section 3 is ultimately the responsibility of the user of the evaluation.

Methodologies, codes, and nuclear data used for the sample calculations and any other recommendation for the calculations are to be described. The model input listing should be included in Appendix A of the evaluation report.

For experiments that report data only at the end of irradiation, it is important that the evaluator understands that these concentrations include the contribution from short-lived precursors to that nuclide. For this reason, the measured end of irradiation (discharge) concentrations for a nuclide do not necessarily correspond to calculated concentrations at discharge. The results from the calculation model should therefore include any short-lived precursors, or, the model should add a short decay time in order to correctly capture the precursor atoms, for comparisons with measurements. The most common nuclide where this occurs is ^{239}Pu. Reported concentrations for ^{239}Pu at discharge always include the contribution from the decay of the precursor ^{239}Np. Other precursor nuclides include ^{95}Nb, ^{99}Mo, and ^{103}Ru.

4.1 Computer codes and nuclear data

4.1.1 Acceptable codes

Validated computer codes suitable for the analysis of spent fuel compositions should be used for the sample calculation(s). Models based on either deterministic or statistical (Monte Carlo) methods may be used for the calculations. When using Monte Carlo codes, it is important to ensure adequate convergence of the model and a sufficient number of histories such that statistical uncertainties are negligible compared to other model uncertainties.

Different computer codes include different nuclides in the fuel model in the neutron transport calculation. It is important that a sufficiently large set of nuclides is included to accurately calculate the neutron spectrum in the fuel, i.e. the large neutron absorbing nuclides. In addition, it is important that the measured nuclides, and their transmutation or decay precursors, also be included such that the most accurate depletion representation of the measured nuclides is achieved.

The results of the analysis will depend to some extent on the specific calculation method and, moreover, the source of nuclear data. The quality of the sample calculations should be assured by adequate validation of the method against measured data or by verification using an independently validated method.

4.1.2 Nuclear data libraries

The nuclear data library used in the calculation model should be clearly identified. Calculated results can exhibit a large dependence on the source of the nuclear data evaluations. It is important to use consistent nuclear data if comparing results with other codes. Use of the most up-to-date nuclear data evaluations is recommended.

4.2 Results

Calculated results for the nuclide quantities (concentrations or activities) should be presented for all measured isotopes.

The results of sample calculations should be reported both as obtained directly from the calculations and in the form of percent difference between the calculated (C) and experimental (E) value, e.g. (C-E)/E*100. Benchmark model uncertainties obtained in Section 3 and measurement uncertainties should also be included here as percentages, for comparison purposes.

A summary of the results should be provided discussing, in particular, any large deviations from the measurements results beyond the estimated uncertainties.

5. References and appendices

5.1 Primary experimental reports

The evaluator should compile a complete list of primary and other relevant reference reports containing the original source information on the experimental data. These references may include reports documenting the reactor and fuel designs, operating history data, selection of fuel samples, and the radiochemical analysis procedures and measurement results. These references are usually cited in Section 2 of the evaluation report.

Reports for many experimental programmes are available at the archive area of the NEA Expert Group website http://www.oecd-nea.org/science/wpncs/ADSNF/reports/.

5.2 Secondary experimental reports

Secondary references should in general not be cited (e.g. code validation studies using the experiments), since they may contain derived or other assumed information. However, secondary references may be useful to identify sources of additional design and operating information, and such supplemental reports should be included.

5.3 Archiving of reports

Legible electronic versions of these reports (preferably as searchable PDF files) should be included as part of the evaluation. Before these reports can be made available through the NEA Data Bank or from the SFCOMPO database, it is important to determine if there are any restrictions on public or third-party use of the reports. Some organisations allow unlimited use of their reports, while others are more restrictive. Approvals for unrestricted use of reports may be required. The evaluator should verify with the originating organisation, in writing, the terms-of-use for any experimental report cited. In some cases, organisations may request the addition of a disclaimer page before the document may be hosted directly by the NEA Data Bank.

5.4 Supplementary information

Supplemental information that is useful, but not essential, to the derivation of the benchmark specification or the sample calculations may be provided in appendices. Appendices are labelled using letters (e.g. Appendix A).

5.5 Appendix A

Appendix A is reserved for the description of the codes, cross-section data libraries, and example input listings used in the sample calculations whose results are given in Section 4. Other appendices may be added as needed.

6. Quality control and approval of the evaluation

6.1 Evaluator qualifications

The evaluation should be performed by a person or persons with expertise in the actual reactor design and operation. Knowledge of the specific design and operations will contribute to the quality of the experimental data and reliability of the benchmark specification.

An advanced understanding of the radiochemical laboratory analysis techniques is considered necessary to evaluate the measurement data. Therefore, it is recommended that the evaluator engage specialists to review the measurement data should measurement data questions arise.

6.2 Peer review process

Each evaluation should undergo an independent review by an expert working in the same group or organisation as the evaluator. An independent review by an expert external to the group and ideally external to the evaluator organisation is also required. All reviewers will require access to the original experimental and supporting reports. An open discussion should be established between evaluator and the independent reviewer to ensure the quality of the evaluation.

6.3 Documentation

The evaluation report should include the names, organisations, and review dates of the evaluation author(s), internal reviewer(s), and external reviewer(s).

6.4 Approval of the evaluation

The evaluation will be presented to an *Evaluation Review Task Group* for review before receiving final approval. Members of the *Evaluation Review Task Group* are appointed by the Expert Group on Assay Data of Spent Nuclear Fuel.

Upon approval by the *Evaluation Review Task Group*, the status of the experimental data in the SFCOMPO database will be updated from “unevaluated” to “evaluated”. Any revision to the experimental data based on the evaluation will then be included in SFCOMPO.

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Appendix A. Supplemental information to the Evaluation Guide

This appendix provides supplemental information fuel on assembly design manufacturing data and reactor operating data provided by the operator, and includes typical uncertainties associated with some of these parameters. Although this information is not strictly considered as guidance for the evaluator, it provides additional insight into the source and nature of the data and their associated manufacturing tolerances and uncertainties. This information may be useful to the evaluator for estimating values of uncertainty that are not documented in the experimental reports.

Table A.1 summarises typical tolerance and uncertainty values for the several important fuel design and reactor operating conditions. These values are based primary on experience with commercial light water reactor designs, and may be applied for uncertainty analysis when they are not provided in the experimental reports. A description of these parameters is provided in subsections of this appendix.

Table A.1. Values of typical uncertainties and manufacturing tolerances

Parameter	Uncertainty/tolerance
Fuel pellet diameter	± 20 μm
Fuel cladding diameter/thickness	± 40 – 50 μm
Fuel pellet height	± 1 – 2 mm
Fuel pellet density (UO_2 fuel = 95% TD)	± 1% (10.3 – 10.6 g/cm^3)
Pellet dishing and chamfer volume	± 50%
Stoichiometry U:O (UO_2 fuel)	2.00 ± 0.01
Stoichiometry M:O (MOX fuel)	2.00 ± 0.02
Stoichiometry M:O (UO_2-Gd_2O_3 fuel)	2.000 ± 0.015
Enrichment (^{235}U wt%)	± 0.05%
Enrichment (MOX fissile content wt%)	± 1%
Fuel impurity content	< 5000 ppm
Fuel impurity as effective boron content	1 ppm boron
Core power	± 2%
Core water inlet temperature	± 2° C
Water moderator temperature	± 2° C (at sample position)
Water moderator density (PWR only)	± 0.005 g/cm^3
Void fraction (nodal value)	± 6%
Void fraction (local value)	< 25%
Fuel temperature (if temperature is reported)	± 50^{0}C
Fuel temperature (if temperature is estimated)	± 100^{0}C
Boron content in water	± 10 ppm

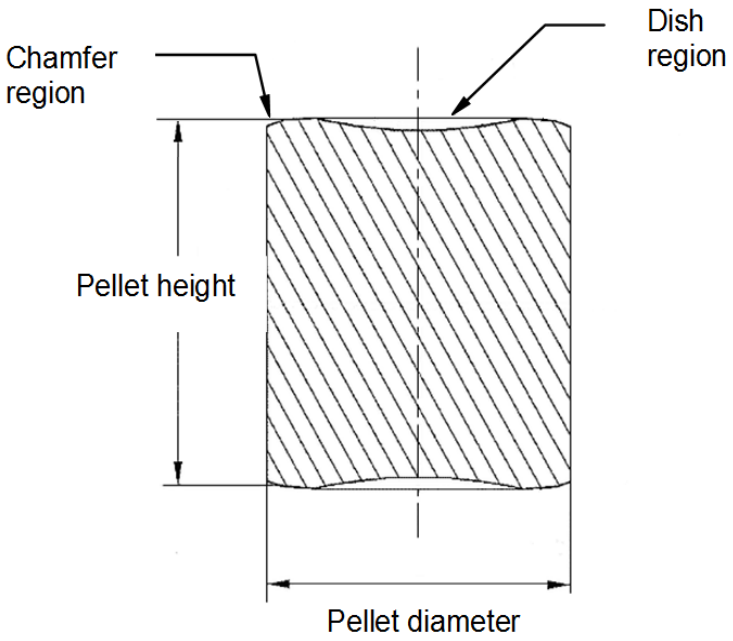
Fuel rod design data

Fuel pellet data

Fuel pellet dimensions (refer to Figure A.1) can include:

- outer pellet diameter;
- inner pellet diameter (VVER and AGR fuel designs);
- dish radius and mean depth or volume fraction;
- chamfer width and height or volume fraction;
- pellet height.

Figure A.1. Fuel pellet design data



LWR fuel pellets are cylinders fabricated from powder compacted by cold pressing and then sintered to the required density, an operation which causes shrinkage of the material. The sintered pellets are then rectified to obtain the required dimensional values necessary to guarantee a required gap between the fuel pellet and the cladding. The tolerance on LWR pellet nominal diameter ranges typically between 10 and 20 µm [1,2], while the usual drawing tolerance values are 200 µm [3]. Therefore the diameter uncertainty will be 10 to 20 times larger when only the nominal value of the diameter is provided or when the specification tolerance is available, i.e. when the pellet is not well characterised.

The inner fuel diameter is only applicable to VVER fuels having an internal hole in the pellet centre. The fuel pellet length/diameter is designed to minimise pellet geometric distortions caused by the temperature profile in the fuel pellet during irradiation. A dish is generally present at one or both faces of a fuel pellet to accommodate differential axial

expansion (due to thermal expansion and gaseous swelling) along the pellet radius, resulting from large radial temperature gradients in the pellet. Chamfers are generally present as well; they ease the pellet introduction in the cladding, reduce problems with chipping of the pellet, and lower the pellet-cladding interaction at pellet ends which results from the pellet hourglass distortion (i.e. stresses are reduced by sectioning the pellet in regions where the maximum deformations occur).

Explicit modelling of the pellet dish and chamfer volume (see Figure A.1) is usually neglected in neutronics codes due to its low impact on the neutronics calculations, but it should be taken into account as an effective reduction of fuel density in the calculation model since the calculation codes usually model the fuel pellet and rod as a perfect cylinder. The reduced fuel volume is dependent on the design but it ranges generally between 1 and 3% of total pellet volume. The dish and chamfer volume does not need to be considered when the fuel density is derived from the fuel stack density (given as either pellet cylindrical density or linear weight), since the stack density already includes these density reductions. If a dished/chamfered design is present but a value is not given in the reported information, a 50% uncertainty in the volume (e.g. ~1% of the total pellet volume) should be considered in estimating the effective fuel density.

Fuel pellet height generally ranges between 9 and 15 mm, with higher tolerance than that on the pellet diameter (generally ±1 to 2 mm). Therefore, the exact number of pellets loaded in the fuel rod is not known and the active fuel length can vary by several millimetres within the rods of a given fabrication campaign.

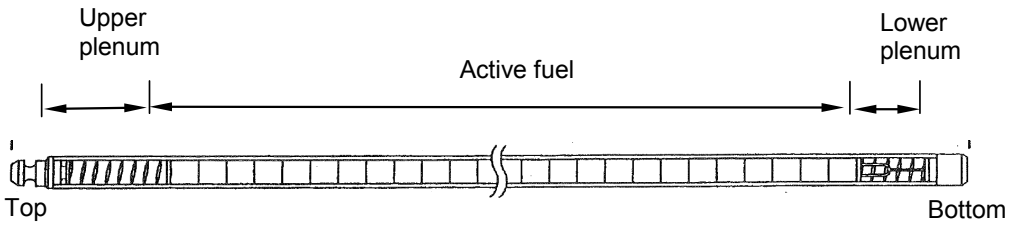
Fuel rod dimensions

Information on fuel rod dimensions may include:

- outer cladding diameter;
- inner cladding diameter;
- cladding thickness;
- upper plenum length;
- upper end plug length;
- bottom plenum length;
- bottom end plug length.

The fuel rod dimensions are illustrated in Figure A.2. Information on the plenum and end plug length may be useful for determining the exact axial position (elevation) of the measured fuel sample when distances are measured from the end (top or bottom) of the fuel rod rather than from the active fuel length. This may be required to estimate the coolant temperature at the sample elevation, since heating of the coolant occurs primary in the active fuel region, not over the entire fuel rod.

Figure A.2. Axial description of a typical fuel rod



The cladding is designed to withstand the pressure difference between the reactor system and the fill pressure introduced during manufacturing, (about 1 MPa in BWR fuel and 2-3 MPa in PWR fuel). For current LWR designs, the nominal cladding thickness generally ranges between 0.55 and 0.75 mm, and up to 0.9 mm for older designs [4,5]. Given the transparent nature of zirconium-based clad materials to neutrons, the inner clad diameter is not neutronically important. The outer clad diameter however, is very important due to the displacement of water moderator that can alter the fuel-to-moderator ratio.

The minimum clearance between the pellet and the cladding at fabrication is specified on the basis of pellet expansion requirement, cladding creep properties and pellet loading considerations. The gap is important for heat transfer considerations that define the fuel temperature during irradiation. For most of the current LWR designs, the nominal radial gap ranges between 0.075 and 0.135 mm. Typical uncertainty on cladding outer/inner diameters and thickness is around 40-50 μm.

A published analysis of cladding tube fabrication [6] shows the variability (i.e., the difference between the minimum and the maximum tube-averaged values) in the outer/inner diameter and thickness for a specific tube lot. The cladding tube-averaged dimensions remain within 15 to 30 μm. For measurements on a single tube, the variability can reach up to 75 μm (resulting from ovality).

Tolerance values of 200 to 300 μm are typically given for the clad outer diameter for PWR and BWR fuel rods respectively [3]. Therefore, there is a large difference in uncertainty depending on whether the uncertainty is given for the specific manufacturing lot, or if nominal dimensions and manufacturing tolerances are provided.

During fuel irradiation there is a continuous variation of the outer clad diameter. Initially, the clad yields under the coolant pressure and the outer clad diameter decreases with a minimum value defined by the pellet diameter and the clad thickness. Later in fuel life, pellet swelling increases the clad diameter to a magnitude depending of the mechanical characteristics of the pellet and clad, and also the power history (i.e. with or without large power transients). Depending on the power history, the cladding diameter may even exceed the as-fabricated diameter. While this is generally not the case for typical burn-ups and standard reactor operations, it should be considered for assay data from high-burn-up fuel rods.

Fuel pellet density

The volumetric fuel pellet density is usually given as an absolute density or relative to theoretical density (TD). The design value of fuel density balances the desire for increased fuel loading in the reactor for longer cycle operation and the need to keep some void fraction in the pellet for limiting the effects of swelling due to gas fission products. The fuel pellet is usually fabricated with a dishing and chamfer that reduces the effectively fuel density compared to the

fuel full volumetric density. It is this effective fuel density that is usually used in neutronics codes such that the average linear fuel density (stack linear density) is preserved. It is important to clearly identify, if possible, whether the fuel density value is the actual density or the effective (linear) density.

Fuel linear density may be available in the experimental reports. When details of the pellet dimensions (dishing etc.) are not provided, it may be possible to estimate the effective fuel density using the active fuel (stack) length and the mass of fuel in the stack (rod or assembly).

For UO_2 fuels, the as-fabricated nominal pellet density is typically 94-97% of theoretical density (TD), where

TD (UO_2) = 10.96 g/cm^3.

MOX fuels contain PuO_2 dispersed in a UO_2 matrix and therefore similar values of pellet density are observed. The theoretical density of MOX fuel is given in [7] as:

TD (MOX) = 10.960 – 0.049 y,

where y is the molar fraction of PuO_2 in the mix.

Additional considerations are required for fuel that contains gadolinium or erbium oxide, or has a zirconium boride coating. When gadolinium is present, the fuel density decreases because of the lower density of Gd_2O_3 powder compared to UO_2. A simple rule [7] gives the theoretical density for Gd_2O_3 bearing UO_2 as:

TD (Gd_2O_3-UO_2) = 10.960 – 0.031 g,

where g is the weight fraction of gadolinium oxide in the Gd_2O_3–UO_2 mixture.

Typical manufacturing tolerance values for the fuel density are 1.0-1.5 % TD (2% TD for the upper limit). Note that within a given fabrication campaign, the pellet density can show a variability of 1 to 2% TD. A much smaller tolerance, 0.20% of TD, or ±0.01 g/cm^3, was reported in ARIANE project [8]. These smaller values are more typical when measurements of pellet density are available for the specific fuel manufacturing lots used in a fuel rod and assembly.

Information on the oxygen-to-uranium atom ratio of the fuel oxide (stoichiometry) may be provided, and in these cases may be considered. For pure UO_2 fuel, about 88.15% of the fuel mass is uranium. However, since impurities and U_3O_8 are used by commercial fuel manufacturers to control fuel density, the stoichiometry value can be slightly higher than 2.0. LWR fuel specifications for stoichiometry [9] are typically:

UO_2 fuels O: U of 2.00 ± 0.01,

MOX fuels O: M of 2.00 ± 0.02,

UO_2-Gd_2O_3 fuels O: M of 2.000 ± 0.015,

An atom ratio of 2.00 can usually be assumed if specific stoichiometric information is missing.

Fuel compositions

In experiments that report only the initial ^{235}U enrichment, values for the other minor isotopes of ^{234}U and ^{236}U may sometimes be estimated from other data. The minor uranium isotope ^{234}U is present in natural uranium and its content increases in the enrichment process with ^{235}U. The isotope ^{236}U does not exist naturally but is introduced during fuel processing when reprocessed

uranium is mixed with natural uranium. Some experimental programmes have not reported ^{236}U to protect sensitive fuel recycling information.

If these minor isotope values are not reported, empirical formulae are given in [10] that may be used to estimate the ^{234}U and ^{236}U values. It is important to note that the initial concentrations or ^{234}U and ^{236}U can be highly dependent on the origin of the fuel, as different countries use different amounts of reprocessed fuel in their fuel production.

A typical nominal tolerance for ^{235}U initial enrichment for enrichment values higher than 2% is about 0.05% in the absolute enrichment. This value is large and can impact the isotopic composition of the irradiated fuel. Since as-built enrichment values are usually available from the reactor operator, this tolerance is considered to be bounding of the initial enrichment of the fuel. The enrichment is usually much closer to the nominal value. Generally, all of the fuel pellets in the same assembly (and even in different assemblies of the same core reload) are produced from the same uranium batch. Therefore the uncertainty given in any as-built report is usually valid for the measured sample and also for all the other fuel rods in an assembly.

The information required for mixed oxide (MOX) fuels includes:

- uranium isotopic distribution;
- total Pu content;
- Pu isotopic distribution;
- the ^{241}Am content (produced by ^{241}Pu decay after reprocessing);
- reference date of the reported ^{241}Am content (usually the estimated loading date).

The variability of the plutonium isotopic composition depends on the reprocessed fuel types (PWR/BWR/AGR/MAGNOX) and fuel burn-up. For a given MOX fabrication campaign, the fissile fraction is generally within 1% (relative) of the nominal value.

For MOX fuels both the total Pu content and Pu isotopic vector of at least the main four isotopes are usually available. The total Pu content is given relative to initial heavy metal (U+Pu). MOX fuel is characterised by a spatially dependent plutonium concentration in the fuel pellet that, on a microscopic level, can range from near zero to 100%, although for modern MOX fuel, local concentrations generally do not exceed 20-30%. Plutonium distribution in the fuel pellet is very dependent on the fabrication process. Consequently, for measurements performed on small sections of a fuel pellet, the potential uncertainty caused by variability in the Pu distribution is a consideration.

There may also be significant variation of the plutonium content at the pellet-to-pellet level. The degree of macro-homogeneity depends on the sophistication of the MOX blending technology. For typical modern MIMAS production, the variability in Pu content of the pellets (difference between min-max content at pellet level) is about 1% (relative).

Fuel containing gadolinium

Many LWR fuels use burnable absorbers to control the reactivity of the fuel during initial irradiation (low burn-up). Gadolinium oxide is widely used as an absorber, although erbium is used as well. The gadolinium content is given as weight percent of Gd_2O_3 in the fuel. The use of gadolinium in BWR fuel has been routine for many decades, and the use in PWR assemblies has become more commonplace.

The concentration of Gd_2O_3 in BWR fuel rods has increased from 3% to about 6% to manage cycle length extensions. The number of rods containing gadolinium has also increased

with the evolution of fuel and assembly designs, but the ratio of gadolinium rods to total number of rods in the assembly has not changed appreciably over time, with typical ratios being 1/8 to 1/10. Assembly designs with respect to gadolinium content vary by reactor and cycle, and actual values may differ from these trends.

PWR assemblies may also contain gadolinium rods in order to flatten the power distribution, reduce the necessary boron concentration at beginning of cycle, and manage increasing cycle length and low leakage reactor core loading patterns strategies. The use of gadolinium rods in modern PWR assemblies is less prevalent than in BWR assemblies, with typically only 1/20 to 1/30 rods in the assemblies containing gadolinium.

Fuel cladding materials

The fuel cladding information can include:

- alloy type (or Nb, Sn, Fe, Cr, Ni, O content);
- cladding dimensions;
- thickness of internal/external layer with different alloyed material (if any);
- material density;
- material impurities (Hf, N and Cl).

The base material for present-day cladding is zirconium. Usual alloys are Zircaloy-2 and Zircaloy-4 with a variable content of tin (1.2 to 1.7%) and smaller quantities of Fe, Cr and Ni (generally below 0.20% each). Russian zirconium contains mainly Nb as the alloy, and other modern alloys such as ZIRLO and M5 contain Nb in proportions 0.8-1.4% (with a commensurate reduction in Fe, Cr, and Sn which is reduced to 0.9-1.3%). The Zr content is about 98% for all of these alloys. Some older zirconium alloys contained a significant quantity of hafnium, and in the 1960`s stainless steel was used for cladding [11]. The neutronic impact of these older materials can be important.

Minor changes in clad composition may occur during irradiation. First, zirconium oxide build-up can increase the clad thickness up to 100 μm for fuels rods with burn-ups above 40-45 GWd/tM. Newer zirconium alloys like ZIRLO and M5 have a much reduced corrosion layer (< 30 μm). Second, hydriding of the base cladding material (which is correlated to the zirconium oxidation process) can introduce 100-200 ppm H in corrosion-resistant materials and up to 800 ppm H at high burn-up for Zr-4 material. These changes are generally not included in a calculation model, however, in the event that severe oxidation is reported, it could be included in the uncertainty analysis.

Fuel impurities

The tolerance for the total impurity content is typically around 5000 ppm; however, the actual content is usually much lower, in the order of hundreds of ppm. Fuel impurities are important in reactor neutronic calculations (contributing to neutron absorption in the system), but they generally do not have a significant impact on the isotopic compositions.

Impurity content is frequently given as the maximum concentration rather than precise values. The concentration for some elements is defined by the lower limit of detection for the measurements. A frequent practice for reactor analysis is to define impurities in terms of an equivalent boron content (EBC), thereby bypassing the need to consider individual impurities. An EBC value of 1 ppm boron (relative to fuel weight) is typical for core management calculations.

Impurities can have a role in the radiochemical analysis measurements. For example, a Nd impurity concentration of 100 ppm could contribute to the concentrations of minor isotopic species such as ^{142}Nd. The impurity level of rare earths such as Eu, Sm and Gd is normally below 1 ppm. These issues are usually checked and addressed by the measurement laboratory.

The most abundant impurities are light elements as N, C, Si, and tool-originated metals such as Fe, Ni, Cr, in concentrations of 100 to 300 ppm. However, these impurities and their activation products typically have no impact on most spent fuel applications such as burn-up credit or long-term disposal. More important for burn-up credit applications is the possible presence of heavier metals also present in tools such as Mo and Ag that could lead to interference with fission products such as ^{95}Mo and ^{109}Ag. Again, these complexities are typically addressed by the measurement laboratory and are beyond what can usually be resolved by the evaluator.

For waste management applications, some nuclides of radiological importance are generated by the activation of impurities rather than by fission (e.g. ^{36}Cl and ^{14}C). For such nuclides, it is important to have precise information on the initial impurity content.

Typical concentrations and maximum allowed impurity content in fuel [8,11,12] are presented in Table A.2.

Table A.2. Typical and maximum allowed contents for impurities in fuel (ppm fuel weight)

Element	Typical	Maximum
Fe	10-50	1200
Cr	10-12	500
Si	10-35	500
N	20-53	75
Cl	5	25
Al	10-50	300
Ni	5-25	300
Mo	10	150
C	<10	100
Ca	6-25	100
W	<2	50
Ti		40
V	0.2-0.5	-
F	<1	25
Pb	0.5-4	20
Mg	2-4	20
Mn	<1	20
Sn	1	20
Zn	2-15	20
Cu	1	10
Co	<2	6
In		3
B	0.2-0.6	1.5
Cd	<1	1.0
Ag	0.1-0.5	0.5
Total rare earths	0.1-0.3	0.6

Fuel assembly design data

Fuel rod pitch

Fuel rod pitch is defined by the centre-to-centre spacing of fuel rods in an assembly. The SVEA-BWR design includes four subassemblies of either 4x4 or 5x5 rods separated by water filled wings. In some assembly designs, the fuel rod pitch for corner rods may be different than the pitch of other rods in the same assembly. In these cases, multiple fuel rod pitch values are required to fully define the assembly.

The uncertainty in the pitch value is generally not available but is constrained by the assembly dimensions. The impact of pitch variations on the neutron spectrum (therefore spent fuel compositions) is limited since it is averaged over many fuel rods due to the neutron moderation process. Fuel rod bowing is observed and pitch variations up to 200 μm are reported in the literature. However, even if this value is assumed for an individual rod, the impact on the neutron spectrum is mitigated by the contribution from other rods, and an effective variation of only 40 μm is likely more representative.

Fuel assembly pitch

The fuel assembly pitch defines the thickness of water gaps existing between adjacent fuel assemblies. In PWR assemblies, the gap has a significant impact on the moderation of the peripheral fuel rods but the effect decreases for the inner rods. In BWR assemblies, the gap is much larger as it includes the additional moderator outside the flow channel, resulting in more moderation between assemblies.

For BWR assemblies, the centre-to-centre assembly spacing in the core may not be uniform in order to accommodate the control blades that reside between assemblies, outside of the flow channel. This non-uniform spacing gives rise to both a narrow gap and a wide gap between adjacent assemblies.

Uncertainties in the assembly pitch may occur when there is a known or suspected fuel deformation or bowing. This was a significant problem in PWRs during the late 1990s with assemblies deformed in an S-shape, creating significant gaps with adjacent assemblies. In extreme cases, maximum gap widths of 25 mm have been estimated [13,14], however, these large gaps were limited to relatively short operation periods. A maximum value of its impact on power distribution has been estimated [15].

In BWR fuel, the observed fuel deformation does not usually affect the fuel assembly itself but rather the outer flow channel. This deformation is dependent on several factors but is basically driven by the neutron flux gradient during irradiation. This deformation is so routine that the channel is usually modelled with some degree of deformation for obtaining the normal operation assembly constants in fuel core management analyses [16,17].

However, without specific deformation data for a measured fuel assembly, obtained by post-irradiation examination of the fuel, it is difficult to generalise these effects in any uncertainty analysis.

Guide and instrumentation tubes

The modelling of the guide tubes and instrument tube in PWR fuel assemblies is important for obtaining a good neutron spectrum for the sample. The outer diameter of the guide tube is slightly smaller than the rod-to-rod pitch because they are used for the mechanical support of the grids. A guide tube thickness of 0.5 or 0.6 mm is typical. The centrally located

instrumentation tube is usually smaller than the guide tubes, with a diameter similar to that of the fuel rods.

In modern fuel designs, the same zirconium-based alloys used in fuel cladding are also used for the guide and instrumentation tubes.

In BWR fuel designs, water rods that contain water moderator without any void have a similar neutronic effect as PWR guide tubes. The water rods have evolved towards larger rod diameters that now replace seven or eight fuel rods or a square channel replacing nine fuel central rods. Since there is not a large pressure, their thickness is similar to guide tubes, i.e. between 0.6 and 0.8 mm.

Assembly grids or spacers

The global characteristics of the grids may be available, i.e. the volume and the mass of each material present in a grid spacer. While their exact position (elevation) is frequently not provided, it can sometimes be accurately inferred from an axial gamma scan of the fuel rod, if available. The geometrical details of the spacers are most frequently considered proprietary. However, these details are usually not required for modelling.

The main consideration for the evaluator should be to estimate the position of the nearest grid spacer relative to the sample location. If the grid-to-sample distance is less than the moderation distance, about 5 cm, then their presence could impact the nuclide compositions of the sample and should therefore be considered in the model (i.e. assess the moderator volume displaced by the grid).

Assembly channel

The importance of the assembly flow channel in BWR fuel is related to the separation of voided and non-voided moderator. Some BWR designs have several sub-channels inside the assembly separated by additional wings with regions of non-voided water inside (e.g. SVEA design).

The value of channel thickness typically ranges between 2 and 3 mm. In the 1990s there was an effort to reduce the thickness of the channel walls by reinforcing and increasing the thickness at the corners.

Operating conditions

Information on the operating conditions mainly originates from the reactor operator or fuel vendor and is essential for developing a model. Many parameters such as power distribution, void fraction, and fuel temperatures are determined using computer codes and models, with in-core monitoring data, since they cannot be measured directly.

Operation-based burn-up

The fuel assembly burn-up is normally estimated by the reactor operator-based on the results of the core management neutronic core simulator, generally three-dimensional proprietary codes as SIMULATE, ANC, PANACEA, etc. The accuracy of assembly burn-up estimates provided by a utility will depend on the reactor and the core management codes, but is generally between 3 and 5%. However, these codes are developed mainly to provide an accurate estimate of the limiting linear power that normally occurs in the central region of the core. For measured fuel samples from an assembly that has been located at core periphery or at other low power regions for one or more cycles, the burn-up uncertainty can be larger. Similarly, larger uncertainties in operator-based burn-up can be expected for samples obtained

from the low-power ends of a fuel rod. Pin-power reconstruction calculations that can be performed by the operator to estimate local burn-up of a fuel rod at the elevation of the measurement will introduce additional uncertainties.

For these reasons, the operator-based burn-up is generally not used, and sample burn-up is most frequently estimated from the measured concentrations of stable or long-lived fission products. Nuclides such as ^{148}Nd, ^{139}La, ^{137}Cs are widely used as burn-up monitors. The uncertainty in burn-up estimates based on nuclide measurements depends on the accuracy of the measurement, but typical values of around 2% can be achieved [8]. A recent analysis of high burn-up fuel [18] gives a burn-up uncertainty of 1.8% at the one-sigma level based on averaging of four measurements.

Moderator temperature and density

The water density at the elevation of the fuel sample position should be available to the evaluator in order to prepare an accurate model. The neutron spectrum in the fuel is very dependent on the water density and has a large impact on the nuclide composition in the fuel. A decrease in moderator density produces a hardening of the spectrum and corresponding increased production and consumption of plutonium, and reduced consumption of ^{235}U.

For PWRs, the reactor pressure is fixed and the density variations are only due to the water temperature change between the inlet and outlet of the core. If the only information available is the core inlet water temperature, the corresponding temperature and density at sample location can be accurately estimated by a simple heat balance between core inlet and sample position knowing the axial power distribution in core. Given a well-defined axial position of a sample the moderator temperature and density can be estimated with relatively low uncertainty; typically about several ºC in temperature and 0.005 g/cm^3 in density.

For BWRs, the moderator temperature is constant along the entire fuel height, except for the short sub-cooled region at the core entrance. Above the sub-cooled region, it is difficult to determine accurate values of the coolant density due to the large variations in steam/liquid fractions. For samples in these regions the moderator conditions cannot be reasonably estimated and it is essential to have values of the void fraction from the reactor operator.

Void fraction

The void fraction in a BWR is defined as the fraction of flowing moderator volume occupied by steam. The non-void moderator inside the water rods, inside the internal channel and other channel structures present in some assembly designs, and outside the flow channel, is not included in the void definition.

For many modern experimental programmes the operator will provide nodal void fraction as a function of date or effective full power days (EFPD), or burn-up, for all axial nodes of an assembly with time steps significantly shorter than the cycle length. The uncertainty in the void fraction determination has been estimated by comparison of calculated to measured planar average void fractions. Values are given [18] for the standard deviation of 5.3 and 6.3% for the codes COBRA/BWR and THERMIT, respectively, with an uncertainty in the measured void fraction reported as 2% [19,20]. Additional uncertainties in the calculation of void fractions should also be considered. A margin of 2ºC for coolant temperature at the core inlet and 2% for total core power are representative values. A total uncertainty of 6% can be considered for the average axial void.

Within the assembly flow channel there is a planar (radial) distribution of the void, and the exact void fraction in the vicinity of any single fuel rod is not known even by the reactor

operator. There are indications of significant heterogeneity in the radial void fraction distribution in regions near the channel or water rods. It is suggested [19] that there can be 25% less void near corner rods for some conditions. However, the radial variability can depend significantly on the axial location with the assembly. These results indicate that the void in the BWR flow channel is not uniform and that uncertainty in local void near any fuel rod may be much larger than the uncertainty in the average node void level provided by the operator.

Periphery rods and rods located close to water rods are moderated mostly by the un-voided water external to the channel or internal to water rods, and therefore are not as dramatically affected by these uncertainties. Also, void-enhanced turbulence increases the homogeneity of the void distribution between rods. In this sense, void fraction data corresponding to samples from the lower sub-cooled region or at the fully developed annular boiling regime region are more reliable in terms of reduced void fraction heterogeneity.

For BWRs, experiments that do not report void information, there are no easy options for the evaluator to make an assessment of this important parameter. Without information from the reactor operator or access to full core simulator containing adequate void correlations, it is not possible to obtain reliable benchmark specification for the experiment.

Fuel temperature

The fuel can experience significant temperature fluctuations during operation due to changes in the assembly power, expansion of the fuel, changes in thermal conductivity associated with irradiation, and creep-down (compression of cladding due to the reactor and fuel rod internal pressure differential). The temperature of the fuel pellet surface is strongly influenced by the fuel and clad gap that varies in width during irradiation. The gap exists at low irradiation of the fuel that leads to a pellet-surface to coolant gradient of 150ºC at 200 W/cm. At higher irradiation, the gap is completely closed due to swelling of the fuel and the gradient decreases to about 100ºC.

The fuel temperature gradient between pellet centre and pellet surface is directly proportional to the linear power with limited dependence on the pellet radius. For fresh UO_2 fuel, a typical value of fuel pellet temperature gradient is 350ºC for a linear power of 200 W/cm while for highly irradiated fuel a gradient of 550ºC is more representative. This behaviour of fuel temperature suggests that the evaluator can estimate fuel temperatures by comparing the values against data for other rods containing the same fuel that have a similar linear power to the rod of interest.

The most significant variable affecting fuel temperature apart from the linear power is the fuel matrix thermal conductivity. Therefore, there is a significant difference between a UO_2 rod, a mixed oxide rod or a gadolinium fuel rod. The fuel conductivity is highly affected by the build-up of other chemical fission product species and hence the gradient increases with fuel burn-up.

Fuel temperature is not measured in commercial reactors but is calculated with codes, using either simplified models created solely for the radial temperature or more detailed and complex thermo-mechanical models such as FRAPCON, FALCON, TRANSURANUS, FEMAXI, COMETHE, etc. In most cases, the fuel temperature will be given by the plant operator as a volume-average temperature or as neutron-absorption equivalent (effective) temperature. If the radial temperature profile, or peak and surface temperatures are provided, weighting factors can be used for obtaining an effective fuel temperature [21].

A typical uncertainty for the reported fuel temperature is 50ºC at the level of one standard deviation. When fuel temperature data are not given and must be estimated, the uncertainty should be increased significantly, e.g. 100ºC.

Boron concentration

The presence of dissolved boron in the moderator of a PWR changes the neutron flux spectrum in the fuel and therefore influences the plutonium production and the concentration of highly absorbing isotopes. The critical boron concentration is an important parameter for reactor operation and its value during each cycle is normally available from the operator.

Start-up to full power operation of the reactor typically requires one or two days of low power operation for testing, during which the critical boron concentration is very high. The boron concentration then exhibits an abrupt decrease because of the build-up of ^{135}Xe in the first few days of operation. After that, the decrease is very linear and proportional to fuel reactivity decrease due to the depletion of fissile atoms and the build-up of fission products and other neutron absorbers. Therefore, the boron concentration value at a burn-up of typically 200 to 300 MWd/tU, commonly referred to as BOL-EqXe (beginning of life – equilibrium xenon), should be used instead of the critical concentration at the strict beginning of cycle.

The maximum boron concentration uncertainty of 10 ppm is appropriate if the critical boron concentration is reported.

Neighbour assemblies

Information on the assemblies adjacent to the measured assembly is often not available to the evaluator. However, the nuclide compositions of the fuel may be influenced by the physical characteristics and the accumulated burn-up of the neighbour assemblies and can be important particularly when the sample rod is located at the assembly periphery. However, sensitivity studies on the influence of neighbours in a UO_2 core have shown the impact to be relatively minor for typical discharge fuel that has been irradiated in several different core locations with different neighbours. However the impact may be larger for low burn-up fuel that has resided in only one or two core locations. Also, in a hybrid core with both UO_2 and MOX assemblies, the UO_2 assemblies can have a significant effect on the compositions of the MOX assembly.

Information on the neighbour assemblies, if available from the reactor operator, typically includes the initial enrichment and accumulated burn-up of each neighbour assembly in each cycle. Other assembly parameters such as the number of water rods, guide tubes, exposure to burnable absorber rods, even fuel rod dimensions, are not essential because of operation requirements to use fuel assemblies with very similar neutronic characteristics in order to avoid large power differences between assemblies.

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