Deliverable 8.7: Recommended procedures to determine SNF source terms

Work Package 8

Spent Fuel Characterisation and Evolution until Disposal (SFC)

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Executive Summary

Based on the conclusions of EURAD deliverable 8.6 (“Performance of sophisticated and best-practice industry codes based on SKB-50 data and data produced in subtasks 2.2 and 2.3 ”), recommendations are formulated to further improve state-of-the-art characterisation of spent nuclear fuel (SNF). The core audience are engineers working on code development and validation, scientists working on experimental methods and measurement evaluation, and practitionieers studying the limitations of current knowledge. In short, the recommendations concern the improvement of nuclear data regarding fission yields and neutron induced capture cross sections of a number of nuclides important for the safety relevant parameters of spent nuclear fuel. Furthermore, recommendations are made concerning a better use of information about the irradiation conditions of spent nuclear fuel that is available from online nuclear reactor core simulators. Introducing redundancy and diversity in the use of computer simulations is also of importance together with an independent, quick verification with non-destructive measurements in an industrial context. Finally, the setup of a dedicated data book for state-of-the-art code validation and a continuation of international collaboration on spent nuclear fuel characterisation is recommended.

Keywords

Recommendation, Burnup, Decay heat, Depletion calculations, Disposal, Gamma-ray emission, Neutron emission, Reactivity, Spent nuclear fuel, Storage, Validation

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Glossary

BU	Burnup
BWR	Boiling water reactor
Clab	Central interim storage facility for spent nuclear fuel in Sweden
EURAD	European joint programme on radioactive waste management
LWR	Light water reactor
MOX	Mixed oxide fuel
NDA	Non-destructive assay
PIE	Post irradiation examination
PWR	Pressurised water reactor
SFC	Spent fuel characterisation and evolution until disposal
SFCOMPO	Spent fuel isotopic composition
SNF	Spent nuclear fuel

1. Introduction

Determination of spent nuclear fuel (SNF) characteristics (i.e. decay heat, neutron and gamma emission, reactivity, radiotoxicity, nuclide concentrations) in industrial applications is routinely the result of calculations. Reliance on calculations is essential since measurements such as post-irradiation examinations (PIE) or calorimetry are too time-consuming to perform for a large number of discharged fuel elements. Moreover, any measurement is only a snapshot of current properties, which will change due to radioactive decay processes. Therefore, validated codes are necessary to obtain a reliable characterisation over the next thousands of years. Validation rests on three pillars: demonstration of the use of state-of-the-art nuclear data, demonstration of predictive power for results of specialised, single effects tests and demonstration of predictive power for measured observables like nuclide composition, neutron emission or decay heat under industrial conditions.

High-quality validated codes avoid too conservative loading schemes of SNF storage configurations and avoid over-engineered casks and canisters for storage and disposal. Thus, it is possible to reduce the environmental footprint of interim storage facilities and underground galleries for geological disposal while improving the economics of the SNF storage and disposal.

2. Main conclusions from deliverable 8.6

In EURAD deliverable 8.6 the predictive power of currently in use computer codes was evaluated by comparing measured and calculated nuclide concentrations, neutron emission, and decay heat of SNF from commercial LWR power reactors. Also, the breadth and quality of data regarding PIE, neutron emission, and decay heat was increased with new measurements. The main conclusions are summarised as follows:

- The effect of nuclear data on nuclide concentrations and decay heat is as important as operating parameters (i.e., irradiation history). This is particularly true for cumulative fission yields (e.g. ^{90}Sr, ^{137}Cs, ^{148}Nd) and neutron capture cross sections for actinides (e.g. ^{242}Pu(n,γ), ^{243}Am(n,γ)).
- The breadth of calorimetric measurements does not equally cover all types and irradiation conditions of SNF and currently only one calorimeter for decay heat measurements of commercially irradiated fuel is in service. Code validation scope is therefore not fully representative for all existing fuel types and irradiation conditions.
- The vast number of experimental PIE programs have different perceived and actual quality due to different experimental methods and irradiation information. For most users of the data, it is not obvious how to distinguish between different levels of quality that (possibly) affects validation.
- Normalisation of transport and depletion calculations strongly affect the main SNF characteristics of interest. This globally affects all calculated nuclide concentrations, as well as derived quantities, like decay heat and gamma-ray and neutron emission properties. Consequently, all calculated quantities are influenced by this normalisation. Hence they included a common uncertainty and might even suffer from a common systematic error.
- Although best estimate calculations for decay heat are very reliable, they are not always used in the industrial context, due to time and effort constraints. Often conservative approaches, based on simplified models are used[1].This leads to less efficient and under-optimised systems for interim storage and geological disposal.
- As observed in the blind benchmark exercise reported in EURAD deliverable 8.6, calculated quantities depend on the interpretation of instructions, even in the perceived case of very precise and detailed definitions. It is important to compare the inputs used for similar codes, as well as “hidden” assumptions (often hard coded or defined by default options). This helps to exclude errors or to understand differences, even if this process is time-consuming.
- Blind benchmarks avoid possible influences from external factors in the simulation decisions. Compared to non-blind benchmarks, it leads to a larger spread of results. This is closer to a realistic situation where no measurements are available, a normal situation in the industrial context. Different codes, different knowledge and competence yield a set of unbiased, *a priori*

[1] Rochman D., et al., Consistent criticality and radiation studies of Swiss spent nuclear fuel: the CS$_2$M approach, J. Hazard. Mater. 357, 384-392, 2018

predictions. Comparison of results and comparison with measurements yield improved *a posteriori* estimates through the elimination of input errors, clarification of input data and improved calculation models.

3. Recommendations

3.1 Spent fuel assembly characterisation

Depending on the desired degree of confidence in SNF characterisation it is recommended to use different codes and to apply independent model input creation and that evaluated nuclear data libraries are updated to contain recommended data dedicated to SNF characterisation. The degree of diversity and redundancy in use of codes and libaries depends on different circumstances. For example, to advance state-of-the-art simulation codes a broad set of calculations is useful to identify potential improvement. Additionally, taking into account many expert perspectives increases the chances to create a new and advanced scientific consensus. In a regulatory environment, it is up to the competent authority to decide which level of code and input checking is suitable. For example, in Germany it is standard practice that SNF calculations presented by utilities are reviewed through independent calculations performed by authorities or their technical support organisations.

Experience shows that even in the case of very precise and detailed definitions and instructions, different codes and users may still use different “hidden” assumptions. This can happen; in the form of hard coded or default code options, including nuclear data, or because users make different interpretation of instructions. Diversity of codes and users reduces the possibility for undetected errors and facilitates to understand differences and ultimately improve the predictive power.

Compared to a non-blind benchmark or compared to calculations done by a single user, a blind benchmark or fully independent calculations by different users and codes will potentially lead to a larger spread of results, which is closer to realistic circumstances in the industrial context. A blind benchmark adds a component not available in other cases: the user effect and the idiosyncratic dimension of performing and interpreting computer simulations. If measurement outcomes are unknown, independent calculations will increase the confidence that the consequences of epistemic uncertainty are understood.

Computer simulations to determine SNF characteristics depend on input from reactor core monitoring data (during reactor operation). This input can be a common source of error for different methods for which no independent data source is available. There exists the possibility of combining neutron and gamma-ray measurements to obtain independent verification of the correctness of calculations and to enhance confidence in the correctness of code input data. Routine measurements of neutrons and gamma emissions are recommended if verification is deemed necessary. The safety level for fuel assembly characterisation required for storage cask loading is up to the relevant regulatory authority to decide.

3.2 Improvement of experimental data for code validation

Most of the post-irradiation examinations (PIE) data available in the open literature are compiled in the SFCOMPO database[2]. In addition, some measured nuclide concentrations are not publicly available. Both sources of information are used for validation of neutron transport and depletion calculation schemes. The number of experimental programs with PIE (e.g. SFCOMPO, ARIANE, MALIBU, REBUS, PROTEUS) are, naturally, of different perceived and real quality, possibly affecting validation. To facilitate the validation, it would be useful to provide benchmarks associated with the PIE data for a

[2] NEA, Evaluation Guide for the Evaluated Spent Nuclear Fuel Assay Database (SFCOMPO), NEA/NSC/R(2015)8, 2016

selection of the most trusted measurements tailored to specific applications (short- and long-term cooling, transport, storage, fuel type, burnup values, etc.).

It is recommended that from the number of available experimental programs with PIE, a subset of high-quality data should be identified on a rolling basis for state-of-the-art code validation. In addition, it is recommended that uncertainties of publicly available experimental programs to be consistently determined and potential outliers identified. A data book for high-quality code validation should be prepared.

Currently, only one calorimeter is used worldwide, i.e. the calorimeter installed at the Clab facility in Sweden. Improved analysis procedures have been presented as part of the EURDAD deliverable 8.4. These procedures reduced the uncertainty of the decay heat measurements by a factor 2 to less than 2%. Nevertheless, the availability of only one calorimetric system to produce experimental data for code validation is not ideal. An additional system is needed to confirm that data derived from measurements with the Clab calorimeter do not suffer from a hidden systematic error. Additionally, the SNF assemblies measured with this calorimeter do not fully represent all SNF types from different countries due to different irradiation conditions, enrichments, designs, or fuel types. Therefore, it is recommended that the present calorimetric data is complemented with results from at least another calorimeter and that the breadth of calorimetric measurements on SNF types is increased (the type here refers to, not only UOX or MOX but also to initial enrichment, cooling time, burnup and decay heat).

In general, it is recommended that for a given sample different experimental methods are combined to enhance the quality of data, ensure consistency, and enable simultaneous validation of multiple observables.

3.3 Improvement of nuclear data

Evaluated nuclear data libraries should be updated with focus on SNF characterisation. This requires dedicated nuclear data programms to improve the most important reactions and quantities relevant for SNF characterisations, based on traceable evaluation and validation procedures.

As observed during various steps within this project, nuclear data is one of the most important components in the estimation of SNF characteristics as confirmed in previous studies and in a number of publications within WP8 of EURAD (see references in deliverable 8.6). The first priority is given to fission yields and their covariances and some cross sections for neutron induced capture reactions. If most of the depletion codes are using independent fission yields, the information from cumulative or mass yields is to be considered, in order to improve the quality of both independent yields and their covariances. Efforts in this direction are currently ongoing in the nuclear data community.

The quality of recommended neutron induced capture cross sections for minor actinides, e.g. ^{242}Pu, ^{243}Am, which are important in the built-up of neutron emitters such as ^{244}Cm should be improved. A second priority concerns the use of “consistent” nuclear data within transport and depletion modules. It basically means using a unique source of recommended nuclear data for both types of calculations. Presently, this is not made due to practical limitations (processing steps, different developers, mixing of data sources), which can lead to inconsistencies or differences in results, thus rendering the analysis difficult to make.

For most nuclides the production or depletion is a non-linear process. Therefore, fuel assemblies with the same average assembly BU can have a different nuclide inventory. Systematic errors due to a normalisation to the average BU can only be avoided by using observables that are directly proportional to the BU or neutron fluence.

Also, normalisation to a BU tracer, such as the ^{148}Nd concentration, globally affects all calculated nuclide concentrations, as well as derived quantities (e.g. decay heat). Consequently, all calculated quantities are correlated to this normalisation and include a common uncertainty and potentially a common systematic error.

It is also recommended that the consequences of normalisation of depletion calculations to specific BU indicators like ^{148}Nd is reconsidered. For example, results normalised to burnup from core monitoring data could be compared to results normalised to ^{148}Nd.

3.4 Improvements with the help of core simulator data

It is recommended that a maximum amount of data available from online core monitoring is used for SNF characterisation.

One important part of predicting SNF characteristics is the simulation of the irradiation condition of the fuel. Modern online core monitoring tools usually perform a detailed 3D core power simulation based on actual plant parameters. Core monitoring predictions are regularly verified and possibly adapted with the help of in-core power map measurements. Therefore, information about the fuel conditions after final discharge is much richer than just average fuel assembly BU. In particular, 3D power and BU profiles are available, as is the history of control rod insertion, soluble neutron absorbers, moderator temperature, and void fraction. Due to the nature of the 3D simulations, the intra-fuel assembly power gradients, as well as the neutron spectrum modulation from neighbouring fuel assemblies, are known. While the quality of predictions of core power distributions has been steadily improved, there has been less focus on specific SNF characteristics.

Since the consequence of uncertainty of irradiation conditions is currently comparable to the effect from nuclear data uncertainty, they cannot be unambiguously separated for fuel data available from most samples from commercial operation. This has been observed especially for BWR cases, studied in the blind benchmark of WP8 work and describedin EURAD deliverable 8.6. Hence, the use of detailed information from online core monitoring beyond average BU is one possibility to increase the confidence in a fuel assembly’s irradiation condition description.

3.5 Improvement of national and international decay heat standards

A result of EURAD deliverable 8.6 has been that different observables of spent fuel are not always determined with the same code or nuclear data library. Hence it is recommended by the WP8 partners that methods to determine fuel characteristics (nuclide inventory, neutron and gamma source strength, decay heat, reactivity, long-term radiotoxicity and inventory of mobile long-lived radionuclides) use a consistent approach.

This work package aimed at improving best estimate calculations, by providing guidance for developing calculation schemes and assessing uncertainties (and errors). Nonetheless, best estimate calculations are not always used in the industrial context due to poor data availability, time, effort constraints, and regulatory requirements. In this case, conservative approaches based on standard methods (e.g. ANSI or ISO standards) are used. It inherently leads to less efficient and under-optimised systems (e.g., cask loading), possibly increasing various costs related to SNF storage and disposal. The advantage of best estimate calculations needs to be emphasised from an economical point of view, but also from a scientific aspect. SNF decay heat as well as its reactivity rely on the SNF nuclide concentrations, and the use of standard methods for decay heat calculations does not allow to link them. This is an unnecessary decoupling between these two aspects of the SNF characterisation, leading to reduced consistency.

3.6 Improvement by use of non-destructive assay methods

Calorimetric measurements are time-consuming and can hence not be recommended to be performed for all fuel assemblies. However, measurements of neutron and gamma source strength can relatively quickly and cheaply be performed during routine handling of the fuel. The research has shown that decay heat and other relevant properties can be correlated with the intensity of neutron and gamma emission[3]. Hence, routine measurement of neutron and gamma emission allows for an independent verification of relevant fuel properties, avoiding misloadings and mistakes in datarecords.

Hence, it is recommened that additionally to the information in the data book of a fuel assembly, non destructive methods, like decay heat measurements and measurements of neutron and gamma emission, are used as a matter of redundancy and diversity to verify the stated SNF properties. Given the large number of fuel assemblies handled in industrial applications verification can be done with different levels of detail, for example randomly, class-wise or for each fuel assembly individually. The degree of confidence or level of conservatism is situation dependent and must be decided by the owner of the fuel assemblies together with the competent regulatory authority.

3.7 Improvement by international collaboration and independent verification

It is recommended that as a matter of redundancy and diversity regarding computer model creation and use, interpretation of experimental data, and application of computational methods and nuclear data, international collaboration is continued to further improve the state-of-the-art of SNF characterisation.

Many organisations have quality control and quality assurance policies to eliminate trivial mistakes, thus releases results with a high degree of confidence in their correctness. However, rarely results are derived independently within the same organisation. This EURAD work package has for example shown that the use of different nuclear data libraries can have a larger effect on spread of calculation results than decay heat measurement uncertainty. It was also demonstrated in EURAD deliverable 8.6 that the uncertainty introduced by the effect of user interpretation of fuel assembly specifications and different choices of code options can be of the same order of magnitude as the nuclear data or measurement uncertainty. Collaborative exercises such as the blind benchmark of this work package have:

- speed up the knowledge distribution between experts,
- improved the competence of experts by contemplating a spectrum of opinions and practices, and
- offered a framework for a structured process for expert opinion convergence.

Therefore, collaboration across organisational boundaries and international cooperation will further enhance and accelerate current state-of-the-art knowledge in SNF characterisation.

4. Conclusion

Management and analyses of SNF entails dealing with all types of uncertainties, which occurs from manufacturing to irradiation and until discharge. It also entails the consequences of uncertainties in nuclear data. These uncertainties are propagated until all the fuel's radionuclides have decayed below detectable limits.

Given the need to ensure feasibility and safety of long-term storage and disposal of SNF, it is warranted to further pursue a systematic approach to evaluate and improve nuclear data, to improve experimental methods and to obtain more accurate information about the fuel's irradiation history. The objective is to consistently predict decay heat, neutron and gamma-ray source intensity, reactivity, and radiotoxicity based on reliable estimates of the underlying nuclide vector. During this research, it was shown that current overall uncertainties cannot be improved by improving one single factor. Instead, a handful of factors contribute roughly equally and need improvement for further progress. These factors concern nuclear data relevant for SNF characterisation, experimental methods to measure observables, obtaining reliable fuel input data, and using validated simulation methods.

[3] Solans V., Spent nuclear fuel analysis for improved safety, Thesis, Uppsala University, Sweden, 2023

This research has shown that the aspiration of an improvement of the state-of-the-art is realistic and doable and a necessity if interim and final storage safety margins shall be improved in the future.