On the Potential to Increase the Accuracy of Source Term Calculations for Spent Nuclear Fuel from an Industry Perspective

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1 Introduction One of the many success factors of nuclear projects and in particular of interim storage and final repository projects are: the economic viability of the endeavor and the reliability of the engineering predictions. The better the accuracy of simulation tools and codes is, the smaller are the required error margins of parameters relevant for nuclear and non-nuclear safety assessments and the smaller are the required resources to build the above-mentioned facilities. For





example, the decay heat emitted from storage casks at the time of entry is one factor that determines the minimum spacing between casks in a deep underground repository. The decay heat also determines the minimum required shutdown cooling time before fuel assemblies can be transported to an interim storage facility and final repositories. The gamma and neutron source terms determine the shielding requirements for transport casks and packaging facilities. The planned deep underground repository in Forsmark, Sweden, for example, is designed to have a capacity of 6,000 canisters and requires an excavation mass of about 1.6M tonnes of rock [1]. If the required volume can be reduced by 10 %, due to more accurate predictions of the minimum canister distance, important costs savings for the ~500M€ [2] worth of tunnel investments would follow. Another important cost driver is the waiting period until all spent fuel can be removed from a shutdown nuclear power station. Operation of required safety systems for criticality safety and heat removal cost several 10k€ per day. Therefore, reducing the wait time by several months can make a substantial contribution to the financial performance of a plant decommissioning project.

Besides project costs an equally important success factor is the reliability of engineering predictions regarding the safety parameters of the spent nuclear fuel. A high precision estimate of a safety parameter based on today's knowledge can turn out to be biased and predicted with too optimistic error margins if new research leads to a revision of taken-for-granted methods and data. The consideration of this possibility is especially relevant for the above-mentioned projects, with planning phases that can take many years and execution phases often spanning many decades. The need for cost-optimization on the one hand and the potential of incomplete knowledge on the other hand, can result in an overoptimization of a facility's engineering design which is not sufficiently robust to absorb future revisions of established methods.

This article is structured as follows: firstly, a short review of the state-ofthe-art of source term determination which encompasses nuclide vector determination of spent fuel, gammaand neutron source terms and decay heat is given. Secondly, identification of potential knowledge gaps and options to improve the accuracy of current methods and tools follows. The role of the EURAD task 8, subtask 2 [3] to contribute to this objective is explained. Thirdly, given the current set of data to validate simulation tools and codes the case for using either thin-tailed or thick-tailed statistics to

generate robust engineering predictions is discussed.

Prediction of source terms for spent nuclear

A determination of source terms for spent nuclear fuel can be divided into four knowledge domains. First: initial material composition and geometry. Second: parameter change during irradiation. Third: nuclear data including neutron interaction cross sections, fission product yields, neutron and gamma-ray emission data and radioactive decay data. Forth: nuclide vector generation

during irradiation and decay chains simulation. The domains are shown in **Figure 1**.

From a life cycle point of view reactor operation comes first and criticality safety considerations and the determination of the effective multiplication factor $k_{\it eff}$ were traditionally of higher priority compared to parameters important for backend activities. Therefore, reactor physics tools which determine the neutron field during reactor operation are mostly validated with high quality data often obtained from single effects tests. What constitutes a single effects test depends on circumstances.

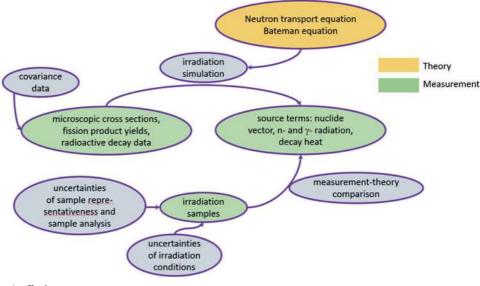


Fig. 1.

Knowledge domains for making source term predictions



Compared to conditions in a commercial reactor here single effects tests are meant to have material compositions, geometries and boundary conditions which are much better defined and are relatively simple configurations compared to the order of 50k of fuel rods in a commercial reactor. There is very little uncertainty regarding irradiation conditions and main emphasis is on validating microscopic data.

In later stages of the reactor life cycle nuclides relevant for burnup

credit receive more attention. First, they are important to predict the reactivity and other safety parameters of a reactor during cycle burnup and core reload. For example: critical boron concentration as a function of full power days, power density peaking and homogenization during irradiation. Second, these nuclides are inputs for safety analyses in which the radioactive inventory is a major parameter (e.g. decay heat during regular shutdowns or dose rate

calculations during accidents). Moreover, they are used as input for safety analyses regarding transport and storage of spent fuel. Finally, as the life cycle ends and interim and final repository activities increase, the priorities among nuclides and radioactive decay modes again changes due to the much larger time scales for these projects.

For example, the SCALE code system, which covers many of the reactor physics and backend analysis fields [4], has been extensively validated with experiments collected in the International Handbook of Evaluated Criticality Safety Benchmark Experiments (ICSBEP Handbook [5]). In these experiments the system configurations are kept as simple as possible: uranium or plutonium systems with a wide range, but accurately defined isotopic vector variations. Other, simple materials include light water as primary moderator, and reflectors consisting of light water as well as graphite, beryllium, molybdenum. The geometrical configurations are often much simpler than in a commercial reactor, they are static and typically no nuclides relevant for burnup credit are included.

For the purpose of criticality safety for transport, storage and treatment of spent fuel the feasibility and reliability of burnup credit has also seen considerable effort [6, 28]. While code-tocode benchmarks are straightforward [7] a comparison with measured nuclide vectors requires much more effort and resources [8, 9, 10]. Firstly, in many cases irradiated fuel comes from commercial reactors and boundary conditions during irradiation are less well known compared to single effects tests for criticality benchmarks, for example. Secondly, a post-irradiation determination of the nuclide composition is resource intensive and usually only done for pellet-sized samples of a fuel assembly. While the average energy generation of a fuel assembly is known with relatively high accuracy, factors such as local parameter variation due to rod or fuel bowing, moderator conditions, neutron field suppression by spacer grids, neutron spectrum shifts induced by neighboring fuel assemblies or shielding by moving control rods increase the uncertainty of the nuclide vector prediction at the pellet-scale and therefore limit validation efforts. Thirdly, nuclide vector determination at a fixed burnup point yields only a single snapshot of the behavior of a non-linear system and

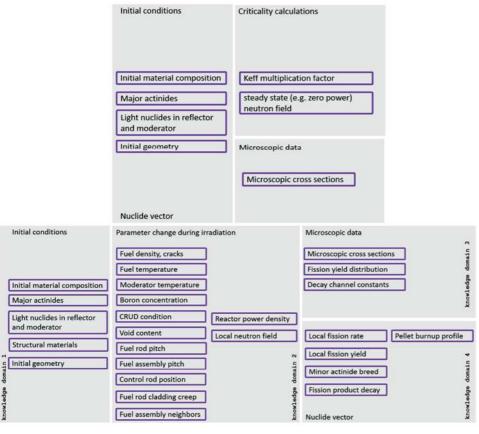
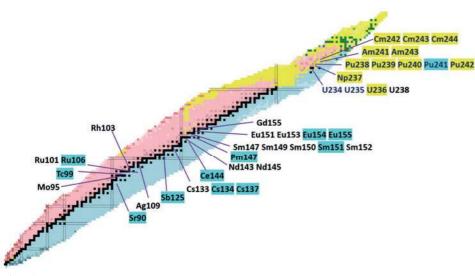


Fig. 2.

Factors influencing accuracy of source term validation for relatively simple (single effects) tests (top) and integral tests like samples from commercial nuclear fuel (bottom).



Tab. 1.Nuclides of interest identified in [49,50] relevant for criticality, burnup credit and dose rate.



therefore limits the ability to extrapolate the validation to different burnup conditions. **Figure 2** summarizes relevant factors influencing the evaluation of samples from commercial reactors. Under ideal validation

conditions irradiation would be done with well-known circumstances in a research reactor and nuclide vectors would be determined for a series of burnup steps to eliminate most of the above-mentioned limitations.

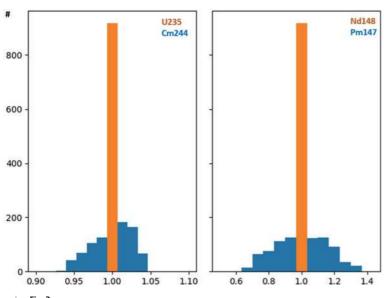


Fig. 3.Concentration of U235, Cm244, Nd148, Pm147 for a reference PWR UO2 assembly at 50MWd/kgU; while the EOL burnup remained fixed; the power history and the cycle durations were randomly changed for the assembly's 4-cycle lifetime.

Table 1 marks the most prominent nuclides for criticality, for burnupcredit and for radiation dose of spent fuel. Which nuclides are more relevant than others depends on time scales and safety parameters. Nuclides contributing to neutron emission are different from nuclides contributing to decay heat. Nuclides contributing to decay heat at reactor shutdown are different from nuclides contributing to decay heat in a final repository. Also, final repositories often have limits on the concentration of particular nuclides mentioned in other environmental regulations which fall outside of the attention of classical source term determination.

Figure 3 shows the relative concentration of some actinides and fission products for a typical 4 wt% U-235 PWR fuel assembly (determined with the SCALE code system). The irradiation history (power and duration) was randomly changed but EOL burnup was kept constant and all values are normalized to the results of the reference irradiation. For some nuclides such as Cm-244 or Pm-147 history effects matter because of the

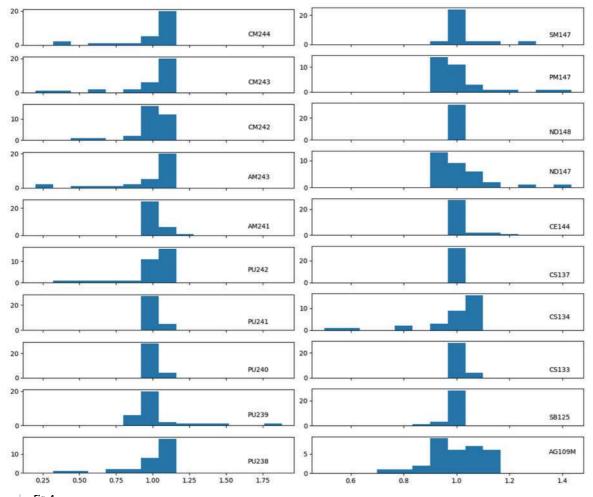


Fig. 4.

Nuclide vector spread for a representative PWR UO2 fuel assembly at 50MWd/kgU; nuclide concentrations are normalized to burnup of each node (i.e. if the nuclide concentration would scale linearly with burnup all values would be at 1.0).

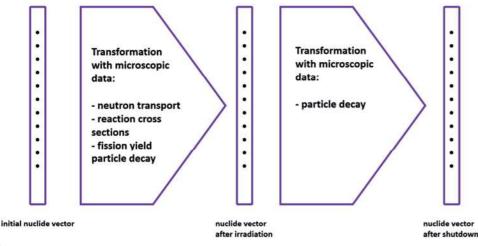


non-linear character of the nuclide generation and destruction chains. Another example is shown in Figure 4. Results for the 32 axial nodes of the same fuel assembly as above were analyzed. In the figure the nuclide concentrations were first normalized with the mean value and then The validation of source terms has scaled with burnup. As expected, the Nd-148 monitor values are concentrated at 1.0. But for many other nuclides the scatter is visibly larger.

This underlines again the difficulty [51]: microscopic cross sections, commercial irradiation.

Potential for improvement of source term predictions

two legs: first, the simulation tools and codes which determine them as input evaluated nuclear data such as ENDF/B [11] or JEFF



Using the principles of particle transport and decay to transform an initial nuclide vector with evaluated, measured microscopic data into a nuclide vector at a future state

LIB	Cumulative yield (%)		
	Sr-90	Cs-137	
JEF-2.2	5.847	6.244	
JEFF-3.1.1	5.729	6.221	
JEFF-3.3	5.676	6.090	
JENDL-4.0	5.772	6.175	
ENDF/B-V	5.913	6.220	
ENDF/B-VII.1	5.782	6.188	
1-sigma	1.20 %	0.40 %	

LIB	<ee>+<eg> / keV</eg></ee>	
	Sr-90 + Y-90	Cs-137 + Ba-137m
decay data	1129	813
JEFF-3.1.1	1107	812
JENDL/FPD-2011	1130	811
ENDF/B-VII.1	1129	806
1-sigma	1.00 %	0.30 %

LIB	Integral, average cross section		
	Sr-90 (b)	Cs-137 (mb)	
TENDL-2017	3.936	1.071	
JENDL-4.0u	4.018	0.926	
JEFF-3.3	3.937	1.040	
ENDF/B-VIII.0	3.987	1.573	
1-sigma	1.00 %	25 %	

Tab. 2. Simple estimate of uncertainty regarding yield, neutron capture of Cs-137 and Sr-90 and decay energy from data of different microscopic data libraries.

to get high quality test data from fission product yields and radioactive decay data. The majority of these data are provided with covariance information [12]. By propagating this input through reactor irradiation simulations and through decay periods the source terms and their uncertainty can be determined [13, 14, 15]. From this perspective the "theoretical" calculation of source terms is a transformation of an initial nuclide vector to a new nuclide vector by means of the laws of particle transport and radioactive decay using evaluated nuclear data, see Figure 5.

Second, the codes for source term determination can be validated with measured nuclide concentrations such as given in the SFCOMPO database [16], with integral measurements of neutron and gamma source strengths of spent fuel [17, 18, 19] and decay heat [20, 21] from irradiated fuel samples and fuel assemblies. If this information would be the only source of validation, a code could be entirely based on empirical parametrizations and could be sufficiently accurate if its application stays within the established parameter range. For example, the classical formulas for decay heat in [22] or [23] are of this kind.

Some of papers published in the literature suggest that SCALE and other sophisticated codes used to predict SNF source terms appear to perform better in terms of accuracy than can be justified by the uncertainty of the fundamental, microscopic input data (see following example of decay heat predictions). In other published results the measurement-theory comparisons show much higher deviations than would be expected from the uncertainty of the microscopic data (see following example on nuclide vector prediction).

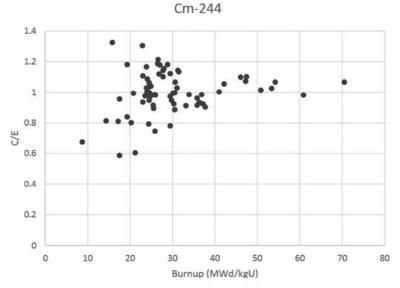
In [24] decay heat measurements on spent nuclear fuel were performed. 50 BWR and 34 PWR assemblies were selected for measurement from the Clab inventory. Shutdown cooling period was 11 to 27 years in these cases. The measurement-theory agreement in this non-blinded study was reported excellent and not larger than the decay heat measurement uncertainty of 2 %. In a followup study [25] the overall decay heat uncertainty from both modeling and nuclear data was estimated at 1.3 %. Research in [26] also concluded that measurement-theory comparisons for decay heat were mainly limited by the



accuracy of the calorimeters used in these experiments. For the assemblies considered in this exercise Cs-137 and Sr-90 are among the main decay heat contributors from the entire nuclide inventory. A simple estimate (by comparing values in different evaluated data libraries) of the uncertainty of their number densities due to fission vield and absorption cross section uncertainty combined with the uncertainty of the specific heat makes the above 1.3 % estimate appear very optimistic (see Table 2). Furthermore, research in [29] with coupled Monte Carlo and burnup calculations and comparisons with data from post irradiation examinations concluded that the inventory of plutonium isotopes can be predicted within 2-4 % of measured values. Given the very good agreement of decay heat measurements with predictions in the above example there is the possibility that a procedure can be formulated about how the irradiation history simulation with its many degrees of freedom must be done to minimize bias. If codes are validated and are used in a parameter range defined by available experiments this can be an acceptable approach from a safety point of view. More attention is necessary if calculations are made for long range forecasts, which cannot be verified before a project receives licensing approval.

Also, decay heat codes have been validated at short cooling times against pulse fission experiments (for example [30, 31]) with estimated uncertainties for UOX and MOX fuels of about 7.5 %. The WPEC Subgroup 25 was formed in 2005 to assess and recommend improvements to the fission product decay data for decay heat calculations [32]. It already considered the question if a reduction in the uncertainty in decay heat calculations to about 5 % or better is achievable. One conclusion was that more accurate measurements were required to determine the decay constants of key radionuclides. However, in the recommended list for obtaining better data on 37 nuclides the emphasis was mostly put on nuclides with short decay times.

Already in 1976, the impact of the uncertainties in fission-product yields, half-lives and decay energies on decay heat was studied in [33, 34]. This assessment indicated that decay heat can be calculated to an accuracy of 7 % or better for cooling times > 10 sec. The expected accuracy fell to 3 % for cooling times larger than 10^3 sec.



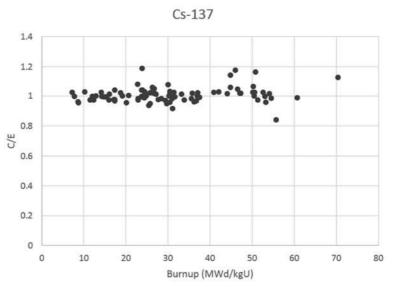


Fig. 6. C/E values for Cm-244 and Cs-137 from [35].

In [35] predictions by the SCALE code system for PWR spent fuel nuclide inventory were compared with results from measurements. In this research a total of 118 fuel samples were analyzed and predictions for 61 nuclides were included. In Figure 6 the C/E ratios (experiment measured over calculated) are shown for Cm-244 and Cs-137 as a function of sample burnup. The C/E values follow no clear trend with burnup. This is the case for most other nuclides. Variations between samples of similar burnup can be as large as variations between samples of large and small burnup and magnitudes can be as large as 10 % and higher.

Even if observables like neutron emission or decay heat can be predicted well through fortunate circumstances of error elimination in some parameter domain, three challenges remain: first, the error cancellation might not occur for those states and time scales which cannot be experimentally verified. Second, for some projects the nuclide number densities themselves are important and the reasons for the observed, relatively large C/E variations must be understood. Third, in order to formulate an improvement strategy of existing codes samples whose irradiation conditions are known with higher accuracy are necessary.

Concerning the second point, the C/E variations in **Figure 6** appear rather random without a trend or bias with burnup. For most nuclides and experiments the stated nuclide measurement uncertainties are very small compared to the observed range of C/E variations. Moreover, nuclear input data such as fission product yield and microscopic cross section uncertainties do not fully explain the observed variations. For example, results in **Figure 7** show the impact of these uncertainties for the fuel



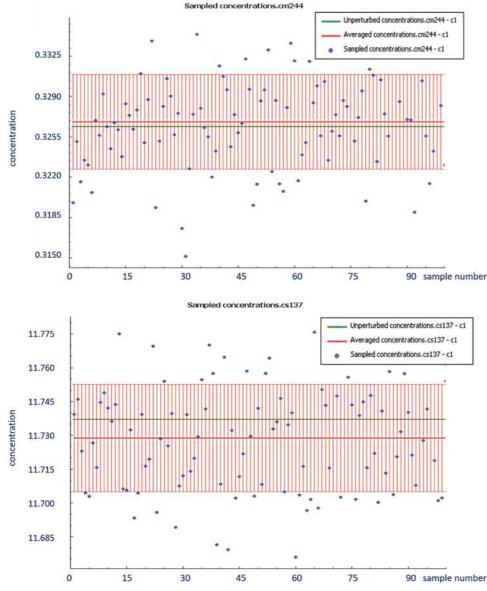


Fig. 7.
Estimating Cm-244 and Cs-137 concentration uncertainties (relative units) due to cross section uncertainties, fission yields and decay parameters for a representative UO2 PWR fuel assembly at 50 MWd/kgU.

example from section 2. Calculations were done with the SAMPLER module from SCALE which uses the therein provided covariance information [36]. Also, this source of uncertainty should manifest itself as a slowly varying bias as a function of burnup, not randomly changing between samples with similar burnup.

Research in [38] made detailed calculations on how the uncertainty of the boron concentration, of the fuel and moderator temperature, of the final burnup, of the initial U-235 enrichment, of the fuel assembly pitch and of the type of fuel assembly neighbors affect C/E results. Assuming expert guesses for plausible input parameter ranges, the results show that expected uncertainties for C/E due to these factors for most of the relevant nuclides are smaller than 5 % (Table 3) and are unlikely to ex-

plain C/E variations in the order of $10\,\%$ or more.

As already mentioned, one possible explanation is that irradiation conditions on the scale of pellet-sized samples have much higher uncertainties than typically assumed. But they should also average out over the irradiation lifetime. Another explanation is that the experimental uncertainties of the radiochemical nuclide inventory data may be biased due to systematic effects depending on the laboratory or method that is used. A third explanation is that burnup monitors like Nd-148 are not sufficiently reliable to establish similarity between samples and that more variables are necessary to create meaningful classes of samples.

Finally, unrecognized sources of uncertainty [37] have been introduced among researchers responsible for

providing evaluated nuclear data to address the issue that uncertainties based on existing covariance information sometimes appear to be inconsistent and underestimated with observed scatter of predicted mean values for cross sections or benchmarks. In the context at hand irradiation conditions at pellet-scale or lack of an adequate set of irradiation history variables could be examples thereof.

4 Options for improvement of source term predictions

One of the simplest methods used in industry practice to reliably predict source terms (i.e. conservatively overpredict concentration or source strength) uses the minimum from a set of C/E results and applies this value as penalty factor in future calculations. For example, the C/E values in Figure 6 suggest that the calculated Cm-244 concentration is underestimated at most by a factor of 0.6. All future calculation results would be multiplied with a penalty factor of 1.7. The disadvantage of this approach is that it depends only on a single minimum value which could also be an outlier. Another downside is that in this approach no information is generated for situations which are not covered by the existing validation database. Also, any burnup dependence of the penalty factor is ignored. Moreover, the information of all the other samples' C/E result is discarded.

An appropriate statistical analysis framework is necessary to account for all the information which is available in the data. The main condition to decide is whether the observed, seemingly random variations of the C/E results are thin- (optimistic approach: statistical independent sample irradiation and evaluation conditions, averaging over C/E results converges to true bias) or thick-tailed (conservative approach: sample irradiation and evaluation conditions are not independent, outliers are important pieces of information).

If the C/E variations are relatively small or within plausible uncertainty margins one can assume that the randomness comes from a Gaussian distribution with unknown mean and variance. There are various statistical tests available to check if this assumption should be rejected. **Table 4** shows, for example, that C/E results for Cm-244 are more likely to be Gaussian distributed than results for Cs-137. If there is sufficient confidence

	Fuel pitch (δ =0.005cm)	Surrounding (depleted vs reference)	Enrichment (δ =0.05wt%)	Fuel-T (δ=50K)	Moderator-T (δ=2K)	Burnup (δ=2%)
Cm-244	1.2	3.0	2.4	0.1	0.7	9.0
Cm-243	1.2	2.0	1.1	0.4	0.7	5.3
Cm-242	1.0	1.0	0.6	0.4	0.4	3.3
Am-243	0.5	2.2	1.7	0.3	0.4	6.1
Am-241	1.2	2.0	0.5	0.9	0.6	0.2
Pu-242	0.1	1.0	1.3	0.2	0.0	4.4
Pu-241	1.2	1.0	0.0	0.7	0.6	1.2
Pu-240	0.4	0.0	0.3	0.2	0.3	1.6
Pu-239	1.4	0.0	0.5	0.7	0.6	0.1
Pu-238	1.1	1.0	0.2	0.2	0.6	4.3
Np-237	0.7	1.0	0.4	0.3	0.3	2.2
U-236	0.0	0.0	1.0	0.1	0.0	0.7
U-235	1.0	1.0	3.1	0.6	0.5	4.0
U-234	0.1	1.0	0.5	0.2	0.1	1.5
Eu-155	1.3	1.0	0.2	0.2	0.5	3.1
Eu-154	0.6	1.0	0.4	0.0	0.3	3.7
Eu-153	0.1	1.0	0.2	0.0	0.1	2.5
Sm-152	0.3	0.0	0.0	0.0	0.2	1.5
Sm-151	1.5	1.0	0.7	0.5	0.9	0.5
Sm-150	0.1	1.0	0.0	0.0	0.1	2.3
Sm-149	1.1	1.0	1.1	0.7	0.9	0.3
Sm-147	0.2	0.0	0.5	0.1	0.2	0.1
Pm-147	0.2	0.0	0.5	0.2	0.1	0.5
Gd-155	1.4	1.0	0.1	0.2	0.5	3.0
Cs-137	0.0	1.0	0.1	0.0	0.0	2.0
Cs-134	0.3	1.0	0.4	0.1	0.2	4.0
Cs-133	0.1	1.0	0.2	0.0	0.0	1.6
Ag-109	0.2	1.0	0.7	0.3	0.1	2.8
Rh-103	0.1	0.0	0.1	0.2	0.0	1.3
Ru-101	0.0	1.0	0.0	0.0	0.0	2.0
Tc-99	0.1	0.0	0.1	0.0	0.0	1.7
Mo-95	0.1	0.0	0.2	0.0	0.1	1.7

Tab. 3. Relative uncertainties (%) due to irradiation boundary condition changes estimated in [38].

Cm-244		
	Statistic	P-Value
Anderson-Darling	0.208448	0.87023
Baringhaus-Henze	0.341385	0.790368
Cramér-von Mises	0.0295401	0.858128
Jarque-Bera ALM	0.147449	0.928628
Kolmogorov-Smirnov	0.00851119	0.952135
Kuiper	0.0155151	0.93949
Mardia Combined	0.147449	0.928628
Mardia Kurtosis	-0 .239727	0.810542
Mardia Skewness	0.1006	0.751111
Pearson x2	51.712	0.170192
Shapiro-Wilk	0.999592	0.90984
Watson II2	0.0284101	0.836886

Cs-137		
	Statistic	P-Value
Anderson-Darling	0.734219	0.0541662
Baringhaus-Henze	0.706856	0.0646831
Cramér-von Mises	0.121485	0.0568223
Jarque-Bera ALM	7.19179	0.0466512
Mardia Combined	7.19179	0.0466512
Mardia Kurtosis	1.58167	0.113726
Mardia Skewness	3.27423	0.0703758
Pearson x2	14.9452	0.0924521
Shapiro-Wilk	0.968223	0.0621728

Tab. 4. Statistical tests to check if distributions of C/E for Cm-244 and Cs-137 in Figure 6 are consistent with a Gaussian distribution.

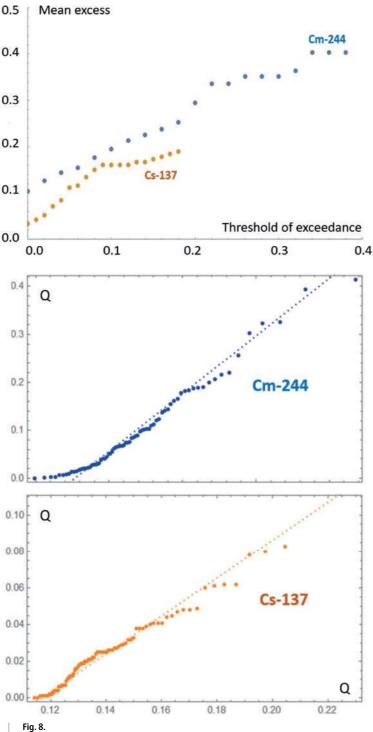
governing the tests, the unknown mean and variance can be estimated with the usual maximum likelihood method and the confidence interval by using a Student-t distribution [39]. For the shown example of Cm-244 the 95 % confidence intervals are: $\mu \in [0.96, 1.03], \sigma \in [0.12, 0.17],$ Cs-137: $\mu \in [0.99, 1.02], \sigma \in [0.04,$

in the existence of a Gaussian process 0.06]. The results for μ can be inter- 1966 [41] and in ENDF/B-VII.1 and preted as systematic bias and can be used to improve codes with empirical factors or to confirm that updated, microscopic cross sections result in improved C/E values. For example, the path to Cm-244 is through neutron capture of Pu-242. In the thermal energy range most evaluations refer to cross sections from 1971 [40] and

JEFF-3.2, for example, evaluations differ up to 20 %. Hence this cross section would be a suitable candidate for further improvement.

In previous research using Bayesian updating [42,43] it has been demonstrated that a combination of information from measurements of microscopic data and from integral





Distribution of excesses for Cm-244 and Cs-137 (top) and Q-Q plot using a Generalized Pareto distribution as reference.

tests like the above can lead to an improvement of microscopic data. One of the objectives of the EURAD work package 8 subtask 2 is to provide highly accurate integral test results and provide recommendations for nuclear data that need to be improved.

The other alternative to interpret a relatively thin database is to embed it into a thick-tailed model (i.e. a model which allows higher probabilities for events outside of conventional domain). This can be reasonable for three purposes: first, observed outliers

cannot be discarded and are a hint for unidentified sources of uncertainty. Second, in some applications simulation tools must make predictions in parameter ranges which are not accessible by current experiments and prudence and conservatism is important. Third, the system belongs to the complex class of systems in which often small changes of boundary parameters can have over proportionally large effects on results [44,45]. In these cases, the methods of extreme value theory can be applied

[46,47,48] to cover the large variations of output parameters. In short, the C/E data can be used for the preparation of a set of upper-order statistics and from it the characteristic of threshold exceedances can be deduced. The main distributional model for exceedances over thresholds is the generalized Pareto distribution $G_{\xi,\beta}(x)$. For a given level u, a number of N_u datapoints will exceed the threshold and the excesses are used to fit the parameters of G by maximum likelihood. The threshold is typically determined from a mean excess plot, see Figure 8 top (u≈0.2 for Cm-244 and u≈0.1 for Cs-137 in this example). The bottom of Figure 8 shows the Q-Q plots for both nuclides together with the reference line from fitted $G_{\xi,\beta}$. The advantage of this approach is that all the information of the existing datapoints is used and that very conservative, quantitative estimates can be given how likely unseen outliers or extreme values are. The disadvantage is that there is no explanation why the outliers exist. Extreme value theory assumes that more often than not unknowns in irradiation conditions, code theory and nuclear data and radiochemical sample analysis do not fortuitously cancel each other out.

5 Conclusion

A large database of single effects tests and integral tests has been built for source term validation since the start of the civil nuclear programs. Efforts were mainly focused on criticality safety, burnup credit and decay heat. There is little coherence between these efforts and requirements concerning long-term storage only recently received higher priority. Increasing the accuracy of existing source term predictions faces several hurdles:

- Different source terms and different time scales require setting different priorities on nuclides. Resource constraints exist to complement existing data.
- High quality tests for measurement of source terms are scarce and significantly improving knowledge about irradiation boundary conditions for most samples of commercial fuel appears unrealistic at the moment.
- Many integral tests show relatively large differences between measurements and theory which cannot easily be explained by known uncertainties of microscopic data and irradiation conditions.



Among others, research in the EURAD WP8 subtask 2 addresses these issues by:

- Reevaluating data from samples from commercial fuel for which irradiation boundary conditions are known with relatively high accuracy.
- Detailed sensitivity analysis to define reliable uncertainty margins for nuclide inventory and corresponding source terms predictions and identify nuclear data requirements to improve the predictive power of codes.
- Identifying a potential for improvement of the robustness of industry-standard code predictions. Both by embedding existing C/E results into a suitable statistical framework and by comparison with latest, sophisticated codes.

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References

- SKB Technical Report TR-11-01, Long-term safety for the final repository for spent nuclear fuel at Forsmark, Main report of the SR-Site project, Stockholm, March 2011.
- SKB Technical Report TR-17-02, Basis for fees and guarantees for the period 2018–2020, Stockholm, April 2017.
- EURAD Deployment Plan 2019-2024, https://www.ejp-eurad.eu/sites/default/files/2020-01/4.%20 EURAD%20Deployment%20Plan.pdf
- B. T. Rearden and M. A. Jessee, Editors, SCALE Code System, ORNL/TM-2005/39, Version 6.2, Oak Ridge National Laboratory, Oak Ridge, TN, 2017.
- International Handbook of Evaluated Criticality Safety Benchmark Experiments, NEA/NSC/DOC(95)03, Nuclear Energy Agency/OECD, Paris, France, 2016.
- M.C. Brady et al, International Studies on Burn-up Credit Criticality Safety by an OECD/NEA Working Group, Intl. Conference on the Physics of Nuclear Science & Technology, Long Island, NY, 5-8 Oct. 1998.
- Burnup credit criticality safety benchmark Phase VII, UO2
 Fuel: Study of spent fuel compositions for long-term disposal,
 NEA No. 6998, Nuclear Energy Agency/OECD, Paris, France,
 2012.
- G. Ilas, I. C. Gauld, and B. D. Murphy, Analysis of Experimental Data for High Burnup PWR Spent Fuel Isotopic Validation – ARIANE and REBUS Programs UO2 Fuel, NUREG/CR-6969, ORNL, Tenn., February 2010.
- G. Ilas, I. C. Gauld, F. C. Difflippo, and M. B. Emmett, Analysis of Experimental Data for High Burnup PWR Spent Fuel Isotopic Validation - Calvert Cliffs, Takahama, and Three Mile Island Reactors, NUREG/CR-6968, Oak Ridge National Laboratory, Oak Ridge, TN, February 2010.
- I.C. Gauld, U. Mertyurek, Validation of BWR spent nuclear fuel isotopic predictions with applications to burnup credit, Nuc. Eng. Des., Vol. 345, pp.110-124, 2019.
- M. B. Chadwick et al., ENDF/B-VII.1 Nuclear Data for Science and Technology: Cross Sections, Covariances, Fission Product Yields and Decay Data, Nuclear Data Sheets, Vol. 112, pp. 2887–2996, 2011.
- 12. M. Salvatores et al., Needs and Issues of Covariance Data Application, Nuclear Data Sheets, Vol. 109, pp. 2725–2732,
- D. Rochman et al., Nuclear Data Uncertainty Propagation Total Monte Carlo vs. Covariances, J. Korean. Phys. Soc., Vol. 59, pp. 1236-1241, 2011.
- D. Rochman, C. Sciolla, Nuclear data uncertainty propagation for a typical PWR fuel assembly with burnup, Nuc. Eng. Tech., Vol. 46, pp. 353-362, 2014.
- D. Rochman et al., Nuclear Data Uncertainties for Typical LWR Fuel Assemblies and a Simple Reactor Core, Nuclear Data Sheets, Vol. 139, pp. 1-76, 2017.

- F. Michel-Sendis et al., SFCOMPO-2.0: An OECD/NEA database of spent nuclear fuel isotopic assays, reactor design specifications, and operating data, Ann. Nucl. Energy, Vol. 110, pp. 779–788. 2017.
- B.B. Bevard at al., Review of information for spent nuclear fuel burnup confirmation, NUREG/CR-6998, Oak Ridge National Laboratory, Oak Ridge, TN, 2009.
- A. Tanskanen, Assessment of the neutron and gamma sources of the spent BWR fuel, STUK report STUK-YTO-TR 170, Helsinki, 2000.
- A. Rimpler, Bonner sphere neutron spectrometry at spent fuel casks, Nucl. Instruments Methods Phys. Res. Sect. A Accel. Spectrometers, Detect. Assoc. Equip., Vol. 476, pp. 468–473, 2002
- G. Ilas, I.C. Gauld, SCALE analysis of CLAB decay heat measurements for LWR spent fuel assemblies, Ann. Nucl. Energy, Vol. 35, pp. 37–48. 2008.
- T. Yamamoto, D. Iwahashi, Validation of decay heat calculation results of ORIGEN2.2 and CASMO5 for light water reactor fuel, J. Nucl. Sci. Technol., Vol. 53, pp. 2108-2118, 2016.
- 22. ANSI/ANS-5.1-2005, Decay Heat Power In Light Water Reactors, ANSI, Washington, DC, 2005.
- DIN-25463-1:1990-05, Decay heat power in nuclear fuels of light water reactors; non-recycled nuclear fuels, DIN e.V., Berlin, 1990.
- SKB report R-05-62, Measurements of decay heat in spent nuclear fuel at the Swedish interim storage facility, Clab, Stockholm, 2006.
- G. Ilas, H. Liljenfeldt, Decay heat uncertainty for BWR used fuel due to modeling and nuclear data uncertainties, Nucl. Eng. Des., Vol. 319, pp. 176–184, 2017.
- I.C. Gauld et al., Validation of SCALE 5 decay heat predictions for LWR spent nuclear fuel, NUREG/CR-6972, Oak Ridge National Laboratory, Oak Ridge, TN, 2010.
- I.C. Gauld et al., Uncertainties in predicted isotopic compositions for high burnup PWR spent nuclear fuel, NUREG/CR-7012, Oak Ridge National Laboratory, Oak Ridge, TN, 2011.
- 28. IAEA-TECDOC-1241, Implementation of burnup credit in spent fuel management systems, International Atomic Energy Agency, Vienna, 2001.
- H.R. Trellue, M.L. Fensin, J.D. Galloway, Production and depletion calculations using MCNP, LA-UR-12-25804, Los Alamos, NM, 2012.
- M. Akiyama, S. An, Measurements of Fission-product Decay Heat for Fast Reactors, Proc. Int. Conf. on Nuclear Data for Science and Technology, pp. 237-244, Antwerp, Belgium, 1007
- J.K. Dickens, T.A. Love, J.W. McConnell, Fission-product Energy Release for Times Following Thermal-neutron Fission of 239Pu and 241Pu Between 2 and 14 000 Seconds, Nucl. Sci. Eng., Vol. 78, pp. 126-146, 1981.
- NEA/WPEC-25, International evaluation cooperation volume 25, Assessment of fission product decay data for decay heat calculations, Report NEA no. 6284, Nuclear Energy Agency/ OFCID Pagis 2007
- F. Schmittroth, Uncertainty analysis of fission-product decay-heat summation methods, Nucl. Sci. Eng., Vol, 59, pp. 117-139, 1976.
- F. Schmittroth, R.E. Schenter, Uncertainties in fission product decay-heat calculations, Nucl. Sci. Eng., Vol. 63, pp. 276-291, 1977
- G. Radulescu, I.C. Gauld, G. Ilas, SCALE 5.1 Predictions of PWR Spent Nuclear Fuel Isotopic Compositions, ORNL/TM-2010/44, Oak Ridge National Laboratory, Oak Ridge, TN, 2010.
- W.J. Marshall et al., Development and Testing of Neutron Cross Section Covariance Data for SCALE 6.2, Proceedings of International Conference on Nuclear Criticality Safety, Charlotte, NC, 2015.
- R. Capote et al., Unrecognized sources of uncertainties (USU) in experimental nuclear data, Nuclear Data Sheets, Vol. 163, pp. 191-227, 2020.
- NEA/NSC/WPNCS/DOC(2011)5, Spent nuclear fuel assay data for isotopic validation, State-of-the-art report, Nuclear Energy Agency/OECD, Paris, 2011.
- Student, The probable error of a mean, Biometrika, Vol. 6(1), pp. 1-25, 1908.
- 40. T.E. Young et al., The low-energy total neutron cross section of plutonium-242, Nucl. Sci. Eng., 43, pp. 341-342, 1971.
- G.F. Auchampaugh et al., Neutron total cross section of Pu242, Phys. Rev., Vol 146, p.840, 1966.
 A.J. Koning, Bayesian Monte Carlo method for nuclear data
- evaluation, Eur. Phys. J. A, Vol. 51, 184, 2015.
 43. E. Alhassan, Bayesian updating for data adjustments and multi-level uncertainty propagation within Total Monte Carlo, Ann. Nucl. Energy, Vol. 139, 107329, 2020.
- 44. A. Majdandzic et al., Spontaneous recovery in dynamica networks, Nature Physics, Vol. 10, pp. 34-38, 2013.
- S.V. Buldyrev et al., Catastrophic cascade of failures in interdependent networks, Nature, Vol. 464, pp. 1025-1028, 2010.

- 46. P. Embrechts, C. Klüppelberg, T. Mikosch, Modelling extremal events for insurance and finance, Springer-Verlag, Berlin, 1997.
- 47. J. Pickands, Statistical inference using extreme order statistics, Ann, Statist., Vol. 3, pp. 119-131, 1975.
- E.J. Gumbel, Statistics of Extremes, Columbia University Press, New York, 1958.
- I.C. Gauld, G. Ilas, G. Radulescu, Uncertainties in predicted isotopic compositions for high burnup PWR spent nuclear fuel, ORNL/TM-2010/41, Oak Ridge National Laboratory, Oak Ridge, TN, 2010.
- G. Zerovnik et. al., Observables of interest for the characterization of spent nuclear fuel, JRC Technical Report JRC 112361, Luxembourg, 2018.
- 51. R. Jacqmin, M. Kellett, A. Nouri, The JEFF-3.0 Nuclear Data Library, PHYSOR 2020, Seoul, Korea, 2002.

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