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Impact of H in H_2O thermal scattering data on depletion calculation: k_∞, nuclide inventory and decay heat

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Abstract. The impact of the H in H_2O thermal scattering data are calculated for burnup quantities, considering models of a UO_2 pincell with DRAGON and SERPENT. The Total Monte Carlo method is applied, where the CAB model parameters are randomly varied to produce sampled (random) LEAPR input files for NJOY. A large number of burnup calculations is then performed, based on the random thermal scattering data. It is found that the impact on k_∞ is relatively small (less than 35 pcm), as for nuclide inventory (less than 1% at 50 MWd/kgU) and for decay heat (less than 0.4%). It is also observed that the calculated probability density functions indicate strong non-linear effects.

1 Introduction

Thermal scattering data for hydrogen in light water (H in H_2O) are one of the major components of nuclear data affecting reactor and fuel calculations. In light water reactor calculations, such data describe the neutron slowdown by means of thermal scattering on hydrogen atoms, bounded in H_2O. Such interactions are defined by the thermal scattering laws (TSL), and provide information on the energy and angular distributions of the scattered neutrons. The evaluations of TSL (resulting in recommendations for nuclear data users) are regularly updated, based on new theoretical developments [1] or measurements, and are included in nuclear data libraries. Recently, the ENDF/B-VIII.0 and TENDL-2021 libraries have included new evaluations of the H in H_2O TSL [2,3], based on the CAB model [4] (whereas the JEFF-3.3 library kept the previous evaluation from 2004 [5]). In parallel, a growing awareness on the importance of delivering TSL covariance information is currently happening from the library evaluators (see for instance Refs. [6–8]).

Over the past ten years, a number of studies were performed to estimate uncertainties on reactor applications due to TSL. Reference [9] applies the TMC and fast TMC methods [10,11] on TSL for the OPAL reactor, using Serpent and MCNP [12,13]. Similar work was performed with TRIPOLI [14] on fuel lattice benchmarks. Concerning full core calculations with a number of operated cycles, reference [15] presents the impact of specific TSL from the TENDL-2012 library. Another example can be found in reference [16], applying variations to TSL model parameters and propagating random TSL to criticality-safety benchmarks. It was observed in these references that the thermal scattering data affect reactor quantities with non negligible uncertainties, and potentially reflecting non-linear behavior (calculated quantities did not systematically present Normal probability density functions).

More recently, there is an effort in the applied nuclear reactor and fuel community for a better understanding of spent nuclear fuel (SNF) quantities, with the goal of improving the safety and the optimization of the SNF handling, processing and storage. Such long-term work involves the assessment of all sources uncertainties, including the ones from nuclear data on SNF characteristics, such as source terms (nuclide compositions), dose or decay heat. Current efforts are coordinated at the European level with the European project called EURAD, and especially its Work Package 8, on “spent fuel characterization and its evolution until disposal” [17]. At the international level the International Atomic Energy Agency has launched a Coordinated Research Project (CRP) “Spent Fuel Characterization”, including partners from the EURAD project, as well as ones outside the EU. Such interests in better understanding of SNF characteristics indicate the relevance of such studies for countries producing nuclear electricity. The impact of the TSL on SNF characteristics, although only one of many required researches for a better understanding of the SNF behavior, is a necessary step towards a full neutronics characterization of the nuclear waste. In this context, the present

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study will provide required uncertainties (even if small compared to other ones) for SNF quantities.

From a technical aspect, the availability of the new TSL for H in H_2O and the open source CAB model inputs [18], rendered possible to assess once again their impact on simulations relevant for reactor and spent fuel. This is precisely the goal of this paper: providing SNF uncertainties due to recent thermal scattering data and uncertainties, for a better assessment of the SNF neutronics characteristics. The present paper will therefore present first the variation of TSL (with the production of random processed TSL), two types of burnup simulations (one deterministic and one based on Monte Carlo), and finally the calculated uncertainties on k_∞, nuclide concentrations and decay heat. It will be shown that the new TSL uncertainties (or more precisely the uncertainties on the TSL model parameters) moderately affect the quantities of interest. It was nevertheless important to evaluate such impacts, finally answering the question of the TSL impact in depletion calculations.

2 Variation of thermal scattering data

As the goal of this work is to assess the impact of the thermal scattering data on quantities obtained from pincell burnup calculations, the Total Monte Carlo method is applied [10]. The principle is relatively simple: repeating the same (burnup) calculation n times, each time with different thermal scattering data. These different thermal scattering data (or TSL), also called random thermal scattering data, are produced by randomly varying parameters of the model used to calculate these TSL. This way, the theoretical knowledge of the TSL evaluators is directly propagated to the quantities of interest, with the minimum number of approximations.

In the present case, the H in H_2O thermal scattering data are produced using the LEAPR module of NJOY (subsequently followed by the ACER module for SERPENT calculations, or by DRAGR for DRAGON calculations). A typical NJOY input is provided in appendix. A number of parameters for the LEAPR input files are varied, based on reference [6], with a number of updates. The original LEAPR input file, from which parameters are randomly changed, is obtained from reference [4] and corresponds to the ENDF/B-VIII.0 evaluation. In total, 9 parameters are modified, as follows:

- σ_s (elastic cross section): ±0.2%
- Δ (scaling factor): ±10%
- C (diffusion coefficient): ±0.5%
- ω_t (translational weight): ±15%
- ω_c (continuous spectrum weight), ω_1 and ω_2 (1$^{\text{st}}$ and 2$^{\text{nd}}$ oscillator weights: correlated with ω_t based on Eq. (1))
- E_1 (first oscillator energy): ±5%, and
- E_2 (second oscillator energy): ±30%.

These parameter uncertainties were determined in agreement with the authors of reference [6], and might differ from the original reference for Δ (24.1% in Ref. [6]),

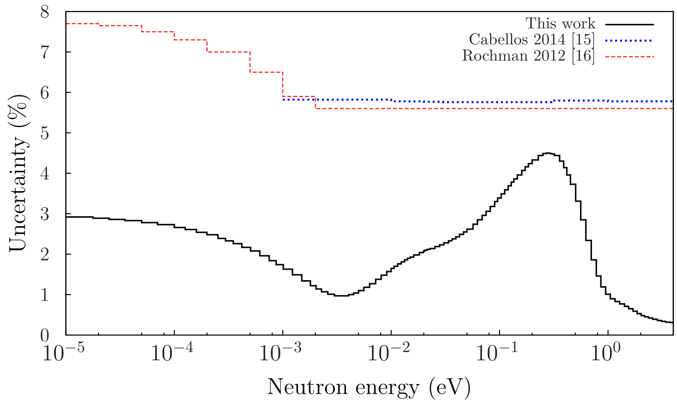

Fig. 1. Uncertainties in the inelastic cross section from this work, compared to previous references.

C (1.5%), E_1 (3%) and E_2 (8%). In the case of the oscillator weights ω_c, ω_1 and ω_2, they are considered correlated with the translational weight ω_t with the following equation:

$$F\omega_t + G(\omega_c + \omega_1 + \omega_2) = 1, \qquad (1)$$

as recommended in reference [6], with F being equal to 1, and G being a normalization factor deduced from the various weights $\omega_t, \omega_c, \omega_1$ and ω_2. All variations follow a Normal distribution, and quoted uncertainties are equal to 1σ (standard deviation) of the input and output variations. The calculated uncertainties on the inelastic scattering cross sections are presented in Figure 1, together with the values from references [15,16]. One can notice that the uncertainties considered in this work are sensibly smaller compared to the previous values used in references [15,16]. Additionally, the uncertainty distribution as a function of the neutron energy are also strongly different.

In total, a large number of samples is produced, leading to processed thermal scattering data in two specific formats: one for Monte Carlo transport simulations (SERPENT), and one for deterministic calculations (DRAGON).

3 Pincell calculation

The samples of TSL are used in the following with two types of neutron transport simulations: a deterministic one (based on the code DRAGON [19]) and a Monte Carlo one (based on SERPENT). Details are provided in the following two sections.

3.1 SERPENT processing and model

The processing of the random TSL for SERPENT is similar to the one for MCNP, and results in the production of an ACE file at a specific temperature (600 Kelvin in the present case). Once a specific LEAPR input file is produced by randomly changing parameters as described in Section 2 (the nominal, or unchanged LEAPR file is from the CAB model), the LEAPR module of NJOY 2016 (version 62 [20]) is used to produce a ENDF-6 formatted file. Based on this ENDF file, the ACER module of NJOY is applied to produce an ACE file at 600 Kelvin. The last step is to perform a SERPENT calculation based on this random ACER file.

Apart from the TSL processed file, all other nuclear data evaluations are from the ENDF/B-VII.1 library (cross sections, fission yields and decay data). This library is different than in the case of the DRAGON calculations, and as it will be presented in the following section, calculated uncertainties are not sensibly affected by such differences. The energy limit of 4 eV is the transition point between the use of TSL (below 4 eV) and the free gas model cross section. The considered model is a single two dimensional UO_2 pincell, as presented in references [21,22]. The ^{235}U enrichment is 3.5%, with a fuel density of 10.2 g/cm^3, a pellet diameter of 0.82 cm and a cladding (Zr) thickness of 0.06 cm. The final burnup of the pincell is 54 MWd/kgU, and the irradiation considers three cycles, separately by approximately 25 days each. In addition, after the irradiation, the pincell is cooled down and the decay heat is calculated by SERPENT up to 100 000 years.

The advantage of using a Monte Carlo transport code like SERPENT is its ability to properly handle nuclear data and their processing with a minimum number of approximations, leading to a convenient flexibility. The drawback of any Monte Carlo code is the required computer power in order to lower the statistical uncertainty to a reasonable level. In the case of uncertainty propagation, such level depends on the amplitude of the calculated uncertainties, and in the present case, as the TSL have an impact lower than 30 pcm on k_∞, a large number of neutron histories is required to reach 5 pcm statistical uncertainty: for each burnup step, 40 000 neutrons per batch are used, with 2000 batch (the 50 first ones are dropped). Such requirement limits the number of SERPENT calculations done with random TSL ACE files. As a single burnup calculation (with one random TSL ACE file) takes almost 48 hours on 72 threads, only 20 SERPENT calculations were performed. Such a low number of random calculations does not allow to obtain a precise value of uncertainties, but it still indicates if the impact of the TSL is below 5 pcm, or its order of magnitudes (to separate the statistical uncertainty with the one from the random TSL, it is assumed that the observed variance is the sum of the variance from the TSL and from statistics; this assumption is at the origin of the TMC method with Monte Carlo simulations). As observed in the following sections, the uncertainties derived from the SERPENT calculations are very closes to the ones obtained with a thousand DRAGON simulations.

3.2 DRAGON processing and model

In this work, a thousand WIMSD libraries are generated for DRAGON with a 172 energy group structure. The libraries are produced using the scripts available in the WLUP project [23]. Such libraries only differ by the thermal scattering processed files associated with H in water. The rest of the nuclear data (cross sections, fission yields and decay data) is based on the beta version of the JEFF-4 library, which is under development. Similarly to the SERPENT processing, a specific LEAPR input file is produced for each different WIMSD library; it is produced by randomly changing the LEAPR input parameters and running NJOY 2016 to generate a ENDF-6 formatted file [20]. The ENDF-6 file is then included in the WIMSD library generation process.

The pincell model considered in this work assumes an ^{235}U enrichment of 3.2% with a pellet diameter of 0.82 cm and a cladding thickness of 0.06 cm. The moderator contains 500 ppm of soluble boron. The transport calculations are performed using the collision probability theory. For self-shielding calculations the fuel region is subdivided into three concentric subdivisions of equal volume. For ^{238}U, the self-shielding effect is calculated for each subdivision. Depletion calculations are performed with the default depletion chain provided in the WIMSD libraries. A total of 202 nuclides are taken into account, and a reference depletion history is generated with 81 steps from 0 to 100 MWd/tHM.

The advantage of using a deterministic code like DRAGON is its ability to perform quick calculations. Each output sample took approximately 1h on a single core (the most time consuming step is to run the LEAPR model of NJOY). The drawback of any deterministic code with respect to Monte Carlo depletion calculation, is the inherent additional bias introduced by the discretization of the transport equation (space and energy).

4 Results

Based on the simulations and models presented in the previous sections, a number of quantities are calculated, related to the burnup and cooling of the UO_2 pincells. As explained, in the case of the DRAGON simulations, a thousand calculations are performed, leading to probability density functions for k_∞ and a number of nuclide densities. As the number of simulations is relatively large, quantities such as uncertainties (one standard deviation), skewness and kurtosis can be obtained with a high degree of confidence. In the case of the SERPENT calculations, although only 20 random burnup calculations were performed, other quantities can be accessed, such as a larger number of nuclide concentrations, as well as the pincell decay heat. It is clear that 20 random calculations do not allow to obtain converged results. As an example, the standard error on the standard deviation is about 20% with these 20 calculations.

4.1 k_∞

In the case of a pincell, the calculation of k_∞ is a convenient indicator of the change of characteristics as a function of burnup. As mentioned, two types of models are used: a single burnup sequence (or pseudo cycle) with DRAGON, up to 100 MWd/kgU, and a more realistic case, considering three consecutive cycles with

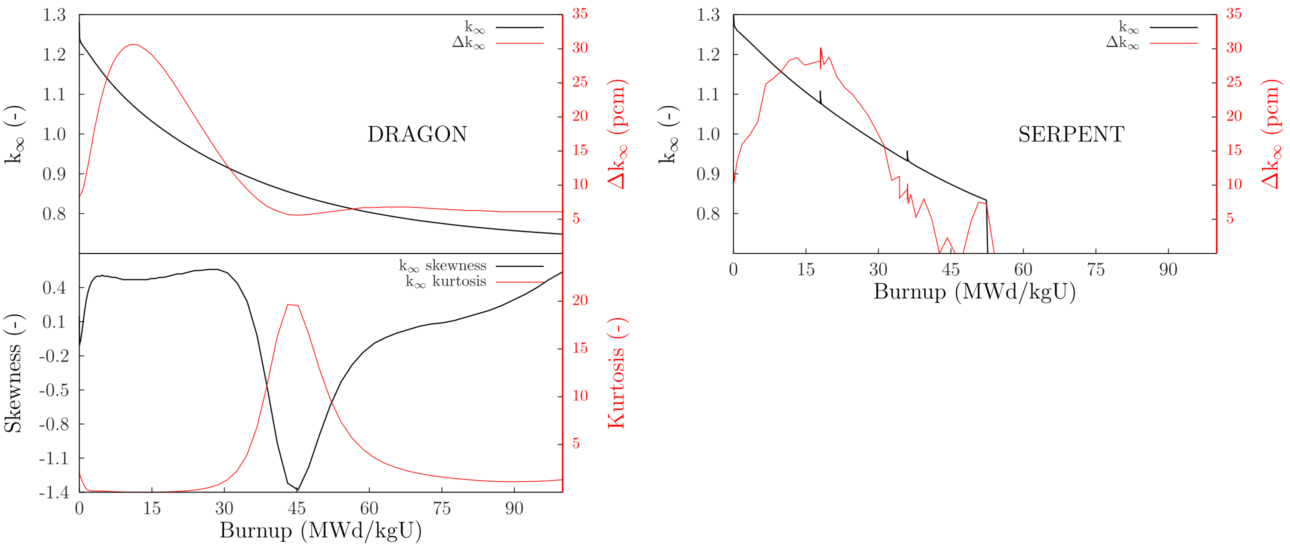

Fig. 2. Calculated k_∞, with its uncertainty, skewness and kurtosis as a function of the pincell burnup value, using DRAGON and 1000 random cases (left) and SERPENT and 20 random cases (right).

SERPENT, up to 58 MWd/kgU. Results in terms of average k_∞ (average with respect to the perturbations of the TSL) are presented in black in Figure 2 top left and right. One can see that both k_∞ are relatively similar, and indicate the usual decrease of reactivity of a burned fissile material. Two local "peaks" can be observed for the SERPENT case close to 20 and 35 MWd/kgU, indicating the end of cycles. In the same top figures are plotted in red the uncertainties due to the variations of TSL: 1000 times for the DRAGON calculations, and only 20 for the SERPENT case. Given the differences in models and numbers of random cases, both uncertainties are nevertheless similar. In the case of SERPENT, the figure indicates the uncertainties due to the TSL variations, after the subtraction of the statistical uncertainty (or more precisely its variance). Therefore it is not possible to observe uncertainties due to TSL smaller than the statistical uncertainty of 5 pcm.

As observed, the uncertainties due to the TSL are not larger than 35 pcm. This amount can be compared to the impact of other nuclear data (cross sections, spectra, emitted particles, fission yields) as presented in references [24–28]: up to 800 pcm, depending on the considered library covariance information, up to 300 pcm due to fission yields only [29]. The amplitude of the impact of the TSL on k_∞ is therefore small compared to the impact of other nuclear data. It is also interesting to remark that even with 20 SERPENT simulations, and after the removal of the 5 pcm statistical uncertainty, the uncertainties from SERPENT are close to the ones from DRAGON (for values higher than 5 pcm). It is also interesting to notice that the uncertainties reach a maximum close to 10-15 MWd/kgU, then decrease to a plateau of about 5 pcm. This is not relevant for application, but can be related to a similar shape observed for the impact of the ^{238}U(n,γ) cross section on k_∞ as presented in reference [30]: although the ^{235}U enrichment considered in this reference was 4.8%, a noticeable decrease in the uncertainty was observed around 50 MWd/kgU, followed by an increase at higher burnup. This was interpreted as the rise of the effect of ^{239}Pu, slowly overcoming the integrated fission rate of ^{235}U. Similar to the present case, this was linked to a shift towards higher energy for the neutron fluence.

One can also observe that the effect of the TSL is highly non linear, as the skewness and kurtosis of the k_∞ distributions strongly vary as a function of burnup values. Only the values derived from the DRAGON calculations are presented here, as not enough SERPENT samples were obtained. Non-linear effects for burnup calculations were already observed, as in the case of the ^{238}U(n,inl) cross section [31], usually due to large cross section or fission yield uncertainties. In the present case, the CAB model uncertainties do not strongly impact k_∞, but the small variations still induce non-linear changes in k_∞. Again, as the uncertainty are relatively small, these observations are not fully relevant for applications, such as SNF characterization.

4.2 Nuclide inventory

The nuclide inventory (or concentration) as a function of the pincell burnup values can be obtained from both the SERPENT and DRAGON calculations. A number of examples for important actinides are presented in Figures 3–5 (from the DRAGON and SERPENT calculations) and in Table 1 for actinides and fission products (from the SERPENT calculations). As for k_∞, the skewness and kurtosis can be obtained from DRAGON only. One can observe that both results from SERPENT and DRAGON are relatively similar, even if some small differences exist (probably within statistical standard errors). Two additional observations can be made. The first one is that the uncertainties due to the thermal scattering data are relatively small. For amounts of isotopes after 10 of 20 MWd/kgU, the uncertainties are not larger than

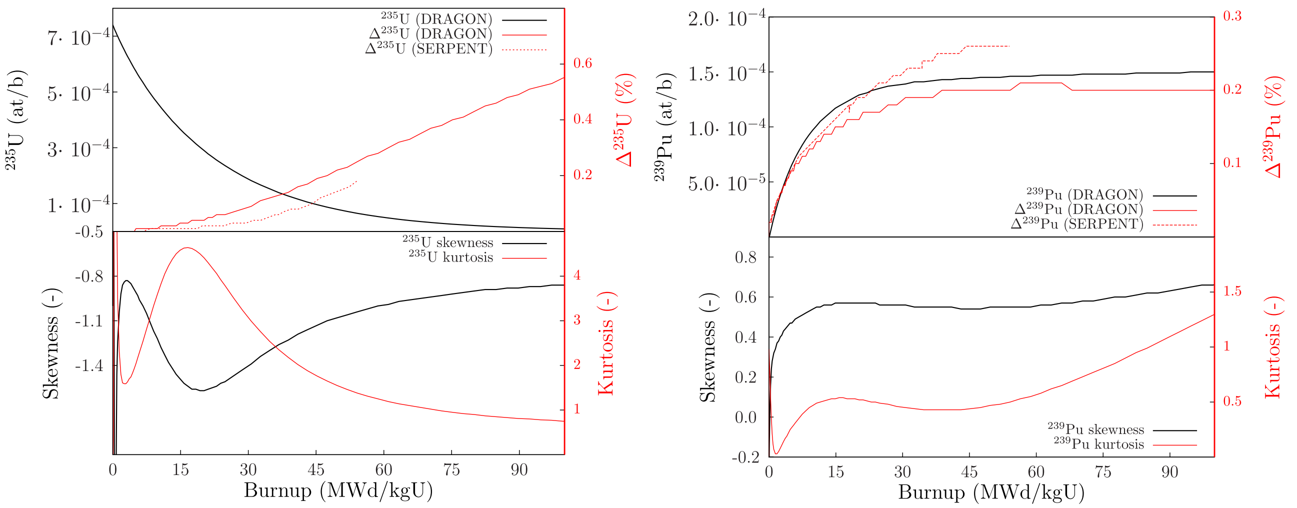

Fig. 3. Calculated concentrations for ^{235}U and ^{239}Pu with their uncertainties (DRAGON and SERPENT), skewness and kurtosis as a function of the pincell burnup value (DRAGON only).

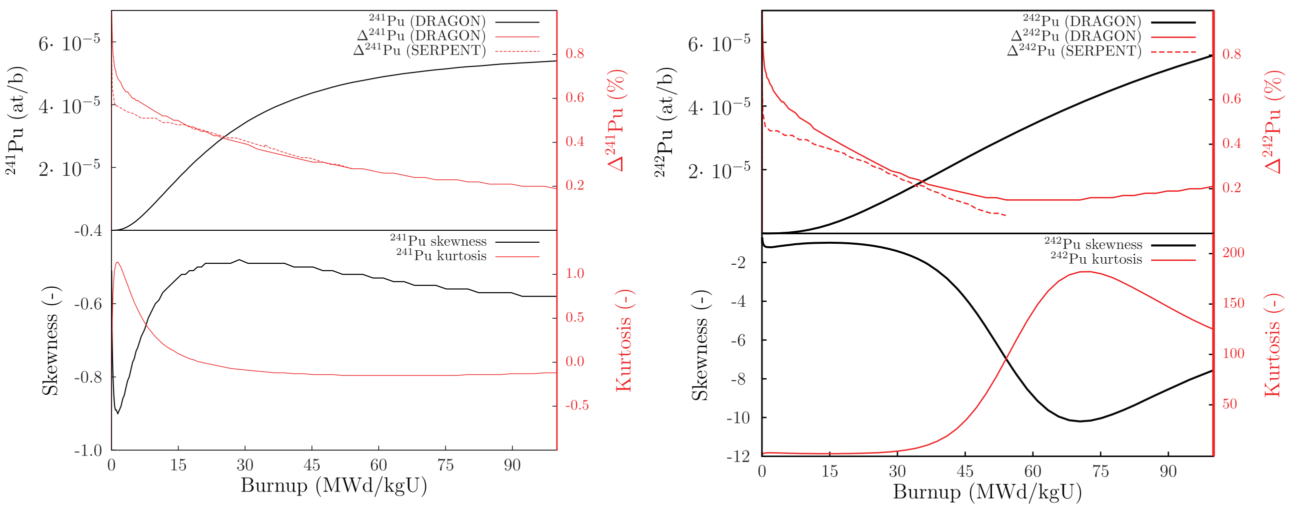

Fig. 4. Same as Figure 3, but for ^{241,242}Pu.

1%. In the case of concentrations at 50 MWd/kgU (see Tab. 1), the maximum uncertainties for heavy actinides are less than 1%, and for fission products, they are almost negligible or less than 0.5%. Such values can be compared to the impact of other types of nuclear data. For covariance information from recent libraries (ENDF/B-VIII.0, JEFF-3.3 or JENDL-4.0) [2,5,32], uncertainties for nuclide concentrations are 5 to 10 times larger, due either to fission yields, or cross sections (together with fission spectra); see for instance reference [33]. Consequently, the impact of the TSL on nuclide concentrations are a second-order effect compared to other sources of uncertainties.
The second remark concerns the non-linear effect of the TSL on the nuclide concentrations. As for k_∞, even if the uncertainties are small, the values of the skewness and kurtosis indicate non Normal distributions for the concentrations, with values changing as a function of the pincell burnup. Again, this might not be of practical interest, but shows that depletion calculations might be prone to various non-linear effects.

4.3 Decay heat

The last quantity of interest studied in this paper is the decay heat of the pincell, obtained from the SERPENT calculations, from the discharged time (end of irradiation, and cooling time of zero year) up to 100 000 years. The decay heat was not calculated with DRAGON, and consequently only the average decay heat and its uncertainty (one standard deviation) is presented in Figure 6. It is not a surprise to observe that a small number of isotopes contributes to the decay heat (not considering short cooling periods of less than a fraction of one year): ^{90}Sr/^{90}Y, ^{137}Cs/^{137m}Ba, ^{134}Cs, ^{244}Cm, and ^{238,239,240}Pu.

As mentioned, the number of samples is relatively small, but it still allows to calculate the order of magnitude of the impact of the TSL; as presented in Figure 6, such impact varies with cooling time, but does not exceed 0.4%. The justification for the observed variations is still not clear, and additional calculations would be necessary. It nevertheless shows that the decay heat is not sensibly

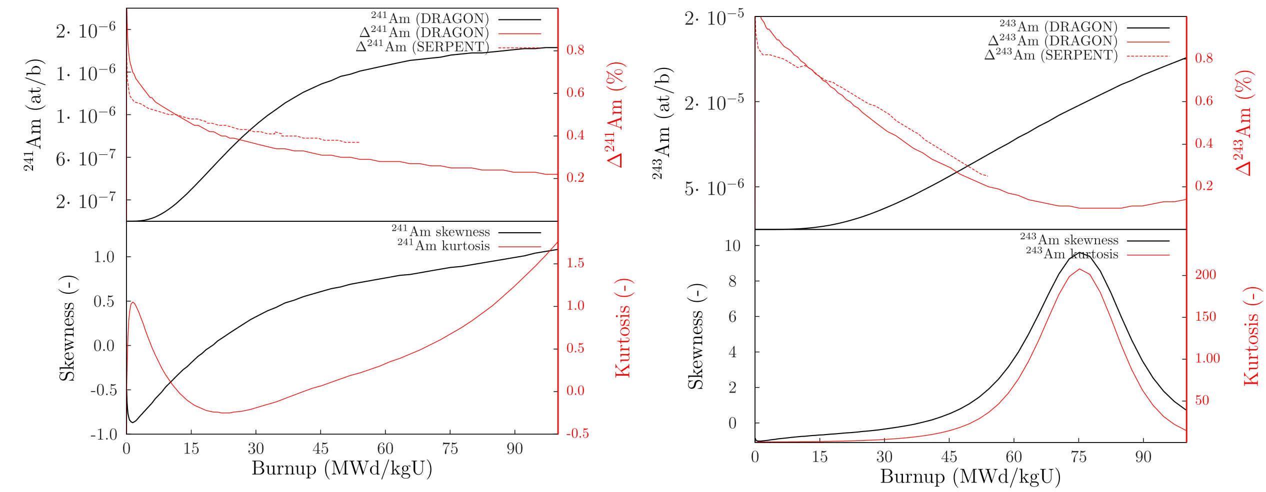

Fig. 5. Same as Figure 3, but for ^{241,243}Am.

Table 1. Uncertainties in isotopic concentrations (ΔC) in% (1σ) due to thermal scattering data of H in H_2O at 50 MWd/kgU obtained from SERPENT calculations.

	ΔC		ΔC		ΔC		ΔC		ΔC		ΔC
^{234}U	0.02	^{235}U	0.14	^{236}U	0.02	^{238}U	0.00	^{237}Np	0.08	^{238}Pu	0.20
^{239}Pu	0.25	^{240}Pu	0.70	^{241}Pu	0.30	^{242}Pu	0.10	^{241}Am	0.32	^{243}Am	0.25
^{244}Cm	0.80	^{245}Cm	0.88	^{246}Cm	0.82	^{88}Sr	0.01	^{90}Sr	0.01	^{95}Mo	0.01
^{99}Tc	0.00	^{101}Ru	0.00	^{106}Ru	0.03	^{103}Rh	0.22	^{109}Ag	0.04	^{125}Sb	0.00
^{133}Cs	0.00	^{134}Cs	0.01	^{135}Cs	0.07	^{137}Cs	0.00	^{144}Ce	0.00	^{142}Nd	0.05
^{143}Nd	0.01	^{144}Nd	0.04	^{145}Nd	0.01	^{146}Nd	0.01	^{148}Nd	0.00	^{150}Nd	0.01
^{147}Pm	0.01	^{147}Sm	0.02	^{148}Sm	0.02	^{149}Sm	0.18	^{150}Sm	0.01	^{151}Sm	0.13
^{152}Sm	0.01	^{154}Sm	0.06	^{153}Eu	0.06	^{154}Eu	0.15	^{155}Eu	0.45	^{154}Gd	0.15
^{155}Gd	0.20	^{156}Gd	0.03	^{158}Gd	0.10						

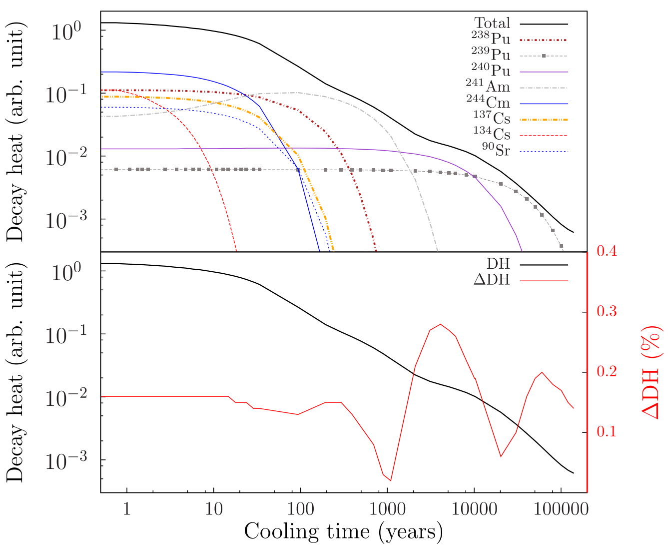

Fig. 6. Decay heat, contributors and its uncertainty due the variations of the thermal scattering data, for the UO_2 pincell obtained with SERPENT.

affected by the thermal scattering data, given that the impact of other nuclear data are not less than 1% for cooling time longer than 1 year and burnup higher than 50 MWd/kgU [33,34].

5 Conclusion

The impact of the H in H_2O thermal scattering data has been assessed in burnup calculations, considering models of a UO_2 pincell. Simulations were performed with the codes DRAGON and SERPENT, and uncertainties for k_∞, nuclide inventory and decay heat were calculated. Sampled (random) thermal scattering data were produced by varying the model parameters in the LEAPR input file of NJOY, following the TMC approach. In conclusion of this study, it was found that the uncertainties due to H in H_2O thermal scattering data are relatively minor (less than 35 pcm for k_∞, less than 1% for nuclide densities at 50 MWd/kgU, and less than 0.4% for the decay heat), especially compared to the impact from other nuclear data. A number of non-linear behavior was observed, but given the small amplitude of the uncertainties, such effect has a limited impact for the SNF characterization.

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Author contribution statement

The authors have equally contributed to the various steps of technical work and to the preparation of the paper.

Appendix A: Typical NJOY input

A typical NJOY input to produce an ACE file is presented in the following

```
ln -s tsl-HinH2O.endf tape24
ln -sf n-001_H_001.endf tape30
ln -sf tsl-HinH2O.endf tape34
./proc.njoy 293.6 hh20 00 njoy-2016.62, with

cat proc.njoy:
#!/usr/bin/env bash

#
# Process thermal scattering file using 0.1%
tolerance,
# 32 angular bins and 200 energy bins.
#
# Parameters:
#  $1: temperature
#  $2: name
#  $3: suffix for acer
#  $4: NJOY executable
#


cat>input <<EOF
moder
30 -31
reconr
-31 -32
'pendf tape for h-1 from endf/b-viii.0'/
125 3/
.001/
'1-h-1 from endf/b-viii0'/
'processed by the njoy nuclear data processing
system'/
'see original endf/b-viii.0 tape for details of
evaluation'/
0/
broadr
-31 -32 -33
125 1/
.001/
${1}
0/
thermr
34 -33 -35
1 125 32 1 2 0 2 2 221 2
${1}
0.001 5.0
acer
-31 -35 0 60 61
2 1 1 .${3} 0
'* H(H2O)                                     *'/
125 ${1} hh2o 3
1001 0 0
221 200 0 0 1 5.0 0
stop
EOF

${4} < input

echo 'saving output and pendf files'
cp tape60 lib_${2}.ace
cp tape61 lib_${2}.xsdir
```

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