Sensitivity/uncertainty Analysis Applied to the Phase VII Benchmark

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Abstract. The aim of this paper is to present the results obtained for Phase-VII Benchmark using the nuclear data library JEFF-3.1.1, and the computer programs ACAB (for the inventory prediction) and MCNP (for criticality calculation). Additional calculations have been performed to assess the importance of nuclear data and computing tools. A sensitivity analysis permits to conclude that the uncertainties in decay data libraries are negligible in k_{eff} calculation. But, cross-section data uncertainties and their impact in k_{eff} for long-term disposal have to be assessed in order to reduce the k_{eff} uncertainty. A target accuracy assessment will permit to define a priority list on cross section data uncertainty reduction.

1. Introduction

In November 2008, a Phase VII Benchmark entitled *"UO2 Fuel: Study of spent fuel compositions for long-term disposal"* was proposed by the Expert Group on Burnup Credit of the NEA-OECD [1]. The main objective of this benchmark is to *study the ability of relevant computer codes and associated nuclear data to predict spent fuel isotopic compositions and corresponding k_{eff} values in a cask configuration over the time duration relevant to spent nuclear fuel disposal,* out to 1,000,000 years. The results of this exercise are expected to show differences in international nuclear data sets (decay/branching data to predict the isotopic inventory along decay time and cross sections to predict k_{eff}) and computing tools (inventory and transport codes).

In the present paper, we review our participation in this Benchmark. Our main contribution involves basically, three calculation tools: ACAB code [2] for inventory prediction, MCNP5 for criticality calculation and JEFF-3.1.1 [3] nuclear data library (decay and neutron transport).

In addition, we have performed a sensitivity study both in the inventory calculation and criticality. In the inventory assessment we have studied different decay data libraries (ORIGEN-S, ORIGEN2.2), the impact of numerical solvers and the time-step used in ACAB code. The criticality assessment has involved different isotopic inventories, neutron transport codes (KENO-VI) and neutron transport libraries (ENDF/B-VI).

To complete this analysis the sensitivity capability of MCNP (PERT option) has been used to determine the sensitivity profiles of concentration and multigroup cross-section for the main fuel isotopes. The isotopic uncertainty due to decay data uncertainty and the BOLNA [4] uncertainty data for cross-sections will permit to evaluate a global uncertainty assessment.

2. Benchmark description, nuclear data and computing tools

The Benchmark specifications [1] provide the discharge fuel composition (4.5 initial wt% 235U, 50-GWd/MTU) for calculating time-dependent spent fuel compositions. A total number of 53 nuclides (light element, actinide, and fission product) were designated as Benchmark nuclides. These isotopes were selected according to its relevance to burnup-credit criticality calculations and those that are potential contributors to radiation dose to the public from nuclear waste repositories.

Criticality calculations must provide k_{eff} values for fresh fuel and isotopic compositions from the decay calculations (30 post-irradiation time steps, out to 1 000 000 years) for two cases

involving a first set of 11 actinides and a second case involving 14 actinides and 16 fission products. The criticality model for k_{eff} calculations is a representative cask loaded with 21 PWR-UO_2 17×17 fuel assemblies.

Our participation in this Benchmark has consisted both in predicting the evolution of the isotopes selected in the specifications and in the calculation of k_{eff} for the cask configuration. Times for calculation and reporting rank are from shutdown to 1 000 000 years of cooling time. The nuclear data and computer codes used to perform this Benchmark were:

1) For decay calculations: Nuclear decay data from ORIGEN2.2 and ORIGEN-S, and the evaluated decay data library JEFF-3.1.1. The computer program is ACAB [2] code (NEA-1839) designed to perform activation and transmutation calculations for nuclear applications.
2) For k_{eff} calculations: Nuclear data from JEFF-3.1.1 and ENDF/B-VI. Computer programs MCNPX2.5 and SCALE6/KENO-VI.

In addition to these calculations, an uncertainty analysis is carried out to determine the importance of the cross-section and decay data uncertainties. This uncertainty analysis is divided in two steps:

1) For decay calculations: We have used a Monte Carlo (MC) method to propagate the complete set of decay uncertainties (branching ratios and half-lives) to the isotopic inventory. These uncertainties were processed from JEFF-3.1.1, sampling a set of different decay data libraries to be used with ACAB code. This method allows dealing with the overall/global effect of the complete set of uncertainties, overcoming the limitation of the sensitivity method where only the main depletion/formation chains are considered.
2) For k_{eff} calculations: We have performed the sensitivities profiles using MCNP (PERT option) to obtain the sensitivity coefficients: i) for the isotopic concentration, and ii) for the main reactions and isotopes in the fuel in a 15-energy-group structure. Once, we have obtain those sensitivities, the uncertainty assessment requires a compilation of: i) concentration uncertainties (predicted in the above step), and ii) nuclear cross-section uncertainties. For this last case, the BOLNA [4] multigroup covariance matrices (in 15-energy-group structure) has been considered. It can be said that concerning to actinide reactions they are very likely the most reliable data at present.

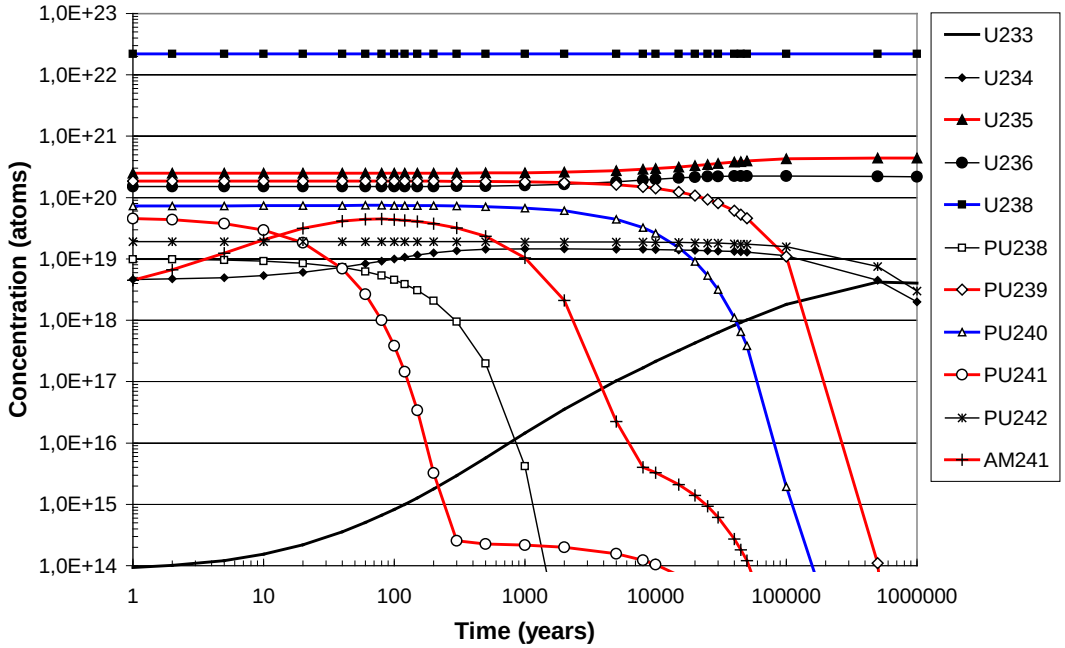
3. Benchmark results

3.1. Decay calculations

First, we predict the isotopic inventory as a function of cooling time with ACAB code. Figure 1 shows the evolution for the main actinides in the fuel predicted using the JEFF-3.1.1 decay data library. The main conclusions are:

- U233 increasing during the cooling time. The decay chains responsible of this generation are: *Pu241 (β-)Am241(α)Np237(α)Pa233(β-)U233* and *Np237(α)Pa233(β -)U233*.
- Pu241 ($T_{1/2}$=14.3 y) disappears in 100 years and Pu238 ($T_{1/2}$=87.7 y) in 1000 years.
- Am241 ($T_{1/2}$=433 y) has a maximum at 100 years, and disappears in 1.0E+4 y. The main contribution is due to: *Pu241(β-)Am241*
- Pu240 ($T_{1/2}$=6.56E+3 y) disappears in 1.0E+5 y. and Pu239 ($T_{1/2}$=2.41E+4 y) in 1.0E+5 y.
- U235 increases the concentration in a factor of 1.76, the main reaction is *Pu239(α)U235*

FIG 1. Evolution of the main actinides selected in the Actinide-only burnup-credit nuclide set. Calculation performed with ACAB code and JEFF-3.1.1 decay data library.



For decay calculations, we have performed a decay sensitivity analysis assessing the importance of decay nuclear data and numerical solvers implemented in the inventory codes. The main pathways for the formation/depletion of relevant nuclides were calculated for each initial isotope at discharge. Timeframes relevant to long-term disposal (1000 000 y) were considered.

i) The impact of different nuclear decay data libraries.
We have processed the JEFF-3.1.1 decay data library for the ACAB code using the PROCDECAY program [2]. In addition, ORIGEN2.2 and ORIGEN-S decay data libraries were converted into ACAB format. We have found significant differences comparing JEFF-3.1.1 with ORIGEN2.2, while the agreement between JEFF-3.1.1 and ORIGEN_S is good. Major differences between JEFF-3.1.1 and ORIGEN-S are shown in Table I.

Table I. Major differences between JEFF-3.1.1 and ORIGEN-S decay data contributing to the differences in the isotopic prediction for this Benchmark.

	JEFF-3.1.1	ORIGEN-S	Diff (%)
$T_{1/2}$ Ni^{59} (s)	2.3980E+12	2.3670E+12	-1.29
$T_{1/2}$ Se^{79} (s)	1.1900E+13	9.3000E+12	-21.85
$T_{1/2}$ Sr^{90} (s)	9.0850E+08	8.8830E+08	-2.22
Yield (Zr^{93} to Nb^{93m})	9.7500E-01	1.0000E+00	2.50
$T_{1/2}$ Nb^{94} (s)	6.3070E+11	6.4060E+11	1.57
$T_{1/2}$ Mo^{93} (s)	1.2620E+11	1.1045E+11	-12.55
$T_{1/2}$ Tc^{99} (s)	6.7530E+12	6.6620E+12	-1.35
$T_{1/2}$ Sn^{126} (s)	7.2580E+12	3.1558E+12	-56.52
$T_{1/2}$ I^{129} (s)	5.0810E+14	4.9540E+14	-2.49
$T_{1/2}$ Eu^{155} (s)	1.5000E+08	1.4770E+08	-1.53
$T_{1/2}$ Th^{229} (s)	2.3160E+11	2.4870E+11	7.38
$T_{1/2}$ U^{236} (s)	7.4790E+14	7.3910E+14	-1.17
$T_{1/2}$ Pu^{236} (s)	9.0190E+07	9.1520E+07	1.47

ii) Importance of numerical solvers to predict the inventory
The selection of time step intervals for calculations in ACAB(ORIGEN) code is important. For short-lived nuclides the matrix exponential method is not enough, and for these nuclides

ACAB uses the Bateman method. It is known that solving chains with long-lived and short-lived isotopes are time-step dependent. ACAB has been implemented with other mathematical solver (LSODE) to avoid this problem. Only differences in Pb210 and Ra228 were identified, ~6% and ~3%, respectively. In addition, an analysis of a reduced time-step calculation (ACAB pulsed option) has shown discrepancies (< 10%) in Sb126, Pb210, Ac227, Th229, Pa231 and U233.

3.2. Criticality calculations

For criticality calculations, a representative PWR cask model is selected. MCNP and KENO-VI, with different nuclear data libraries, were used to compare the predicted k_{eff}. An extensive work has been done to guarantee the same modelization for the MCNP and SCALE inputs. Table II shows the different cases for criticality calculations.

Table II. Different cases for inventory prediction and criticality calculations.

Cases #	Isotopic prediction: ACAB code using different decay library	k_{eff} prediction: different neutron transport libraries and codes	k_{eff} (fresh fuel)	k_{eff} (shutdown)
1 (Ref.)	JEFF-3.1.1	MCNPX-JEFF-3.1.1	1.15057±0.00035	0.95819±0.00033
2	JEFF-3.1.1	MCNPX-ENDF/B-VI	1.14631±0.00053	0.95228±0.00050
3	JEFF-3.1.1	SCALE6-ENDF/B-V-44g	1.14688±0.00009	0.95737±0.00008
4	ORIGEN-2.2	MCNPX-ENDF/B-VI	1.14631±0.00053	0.95228±0.00050
5	ORIGEN-S	MCNPX-JEFF-3.1.1	1.15057±0.00035	0.95819±0.00033

The k_{eff} evolution versus cooling time for the actinides only case presented in Figure2 shows that: i) the k_{eff} has a maximum value at shutdown, ii) a minimum at 100 years, and then, iii) the k_{eff} increases to another maximum around 30.000 years cooling time, this second maximum is always below the k_{eff} at shutdown.

FIG 2. The calculated k_{eff} values for actinide case. (I= Decay data library for the isotopic inventory, NT= neutron transport library for k_{eff} calculation)

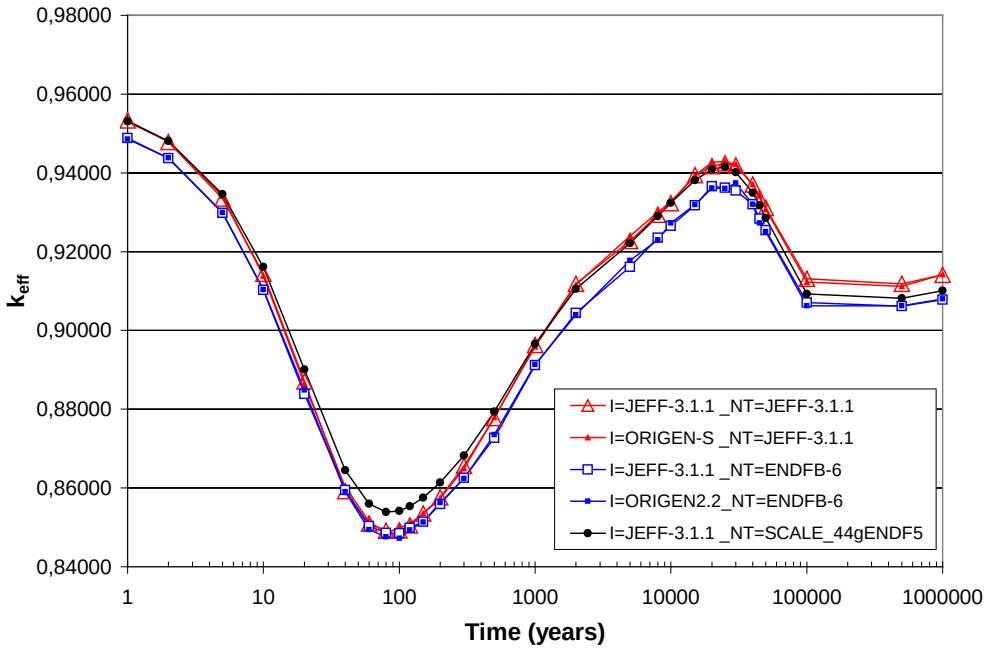
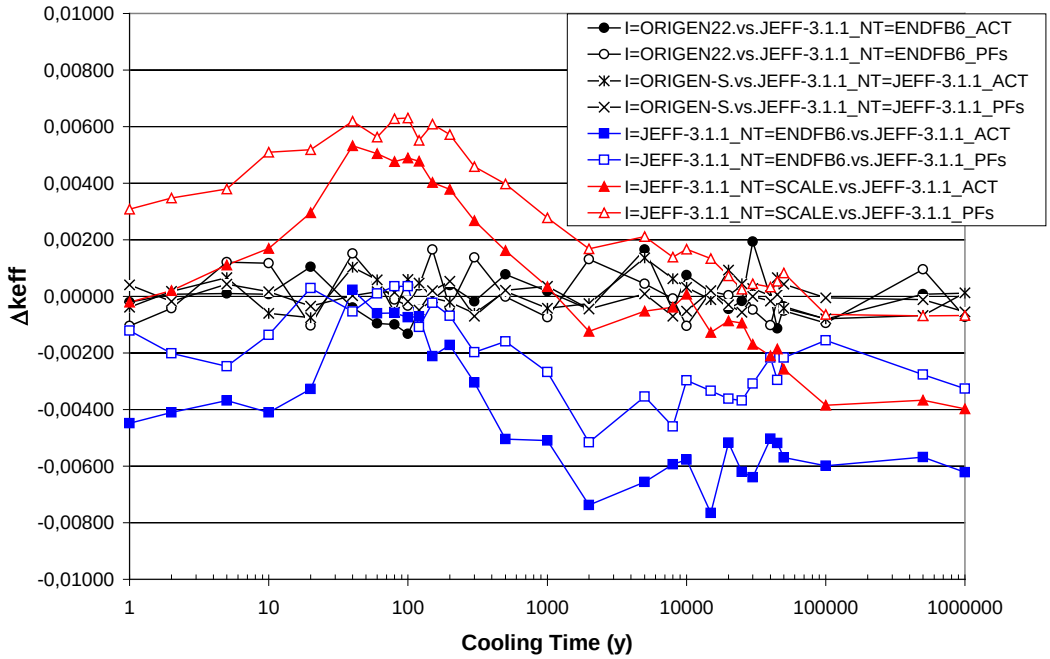


FIG 3. Differences for the calculated k_{eff} values. Inventory predictions with ACAB code for ORIGEN2.2, ORIGENS and JEFF-3.1.1 decay data. Criticality calculations with MCNP (JEFF-3.1.1 and ENDF/B-VI) and SCALE code. Differences between the actinide-only (ACT) and actinide+fission products (PFs) burnup-credit nuclide sets have been shown.



In Figure 3 we have compared those 5 cases, and we conclude that:

i) The isotopic calculations performed with ACAB code with different decay data libraries do not affect the k_{eff} prediction (< 200 pcm).

ii) We have found significant differences between JEFF-3.1.1 and ENDF/B-VI. For the actinide-only case we have found 400 pcm at shutdown and 600 pcm at 1.0E+6 years. At 100 years the difference is negligible, and the maximum difference (~760 pcm) at 1.0E+04 years. For actinide+fission products case the differences are not so important, and the maximum difference (+500 pcm) occurs at 2.0E+3 years.

We have analyzed these differences performing additional MCNP evaluations from the JEFF-3.1.1 reference case, by substituting individual isotopes with those of the ENDF/B-VI data library. Table III shows that U238 and Am241 are the isotopes that induce the major change in k_{eff}. The calculation result with ENDF/B-VI underestimates the k_{eff} prediction using JEFF-3.1.1. This discrepancy can be explained by the differences in the resolved resonance parameters between ENDF/B-VI and JEFF-3.1.1, resulting in lower U^{238} resonance absorption. Additional work should be done to better characterize these differences.

Table III. Δk_{eff} (ENDFB-VI-JEFF-3.1.1) predicted by substituting individual isotopes with those of the ENDF/B-VI in the reference k_{eff} calculation performed with JEFF-3.1.1.

	Shutdown	100 years	1E+06 years
U233	-0.00034	-0.00020	-0.00034
U234	-0.00040	-0.00002	0.00009
U235	0.00060	0.00137	0.00219
U236	-0.00111	-0.00033	0.00043
U238	-0.00581	-0.00478	-0.00611
Pu238	0.00030	-0.00001	0.00000
Pu239	0.00072	0.00208	0.00079
Pu240	-0.00198	-0.00071	0.00051

Pu241	0.00199	0.00113	-0.00030
Pu242	-0.00121	-0.00017	0.00011
Am241	-0.00032	0.00552	-0.00030

iii) Regarding SCALE and MCNP (with JEFF-3.1.1)
   a. For the *actinide-only* case we have predicted similar values both at shutdown and in the second maximum. At 100 years (in the minimum k_{eff}) SCALE has a difference of +500 pcm, and -400 pcm at 1.0E+6 years cooling time.
   b. For *actinide+fission products* case the difference at shutdown is +300 pcm and in the minimum the difference reaches 610 pcm

4. Sensitivity and uncertainty analysis

4.1. Decay calculations

In this section we describe uncertainty results in the inventory calculation computed by the Monte Carlo technique. The JEFF-3.1.1 decay data library has been processed to obtain the information of half-live relative errors (see Table IV) and the uncertainty in the different decay modes. In this case, decay constants and branching ratios are treated as random variables, and we have assumed a normal probability distribution for these variables. The Monte Carlo procedure involves a collection of random decay data libraries generated by Monte Carlo sampling, following inventory calculations with ACAB code.

Table IV. Half-live and relative errors (in %) from JEFF-3.1.1 decay data library.

Isotope	$T_{1/2}$ (y)	Err(%)	Isotope	$T_{1/2}$ (y)	Err(%)	Isotope	$T_{1/2}$ (y)	Err(%)
C 14	5.7007E+03	0.53	CS135	2.2999E+06	13.04	U233	1.5926E+05	0.13
CL 36	3.0101E+05	1.00	CS137	3.0040E+01	0.10	U234	2.4571E+05	0.12
CA 41	1.0299E+05	3.88	SM147	1.0600E+11	1.89	U235	7.0379E+08	0.07
NI 59	7.5988E+04	6.58	SM149	2.0002E+15	0.00	U236	2.3700E+07	0.84
SE 79	3.7709E+05	5.04	SM151	8.9994E+01	6.67	U238	4.4680E+09	0.07
SR 90	2.8789E+01	0.21	PB210	2.2159E+01	0.54	NP237	2.1399E+06	0.47
ZR 93	1.5299E+06	6.54	RA226	1.5999E+03	0.44	PU238	8.7713E+01	0.34
NB 93M	1.6126E+01	0.85	RA228	5.7514E+00	0.52	PU239	2.4111E+04	0.05
NB 94	1.9986E+04	12.33	AC227	2.1773E+01	0.01	PU240	6.5626E+03	0.08
MO 93	3.9990E+03	20.00	TH229	7.3390E+03	2.18	PU241	1.4329E+01	0.28
TC 99	2.1399E+05	3.74	TH230	7.5386E+04	0.40	PU242	3.7360E+05	0.29
PD107	6.4992E+06	4.61	TH232	1.4050E+10	0.43	AM241	4.3286E+02	0.16
SN126	2.2999E+05	6.09	PA231	3.2765E+04	0.34	AM242M	1.4101E+02	1.42
SB126	3.3938E-02	0.81	U232	6.9809E+01	0.72	AM243	7.3643E+03	0.30
SB126M	3.6315E-05	1.05				CM245	8.4987E+03	2.35
I129	1.6101E+07	4.35				CM246	4.7310E+03	3.17

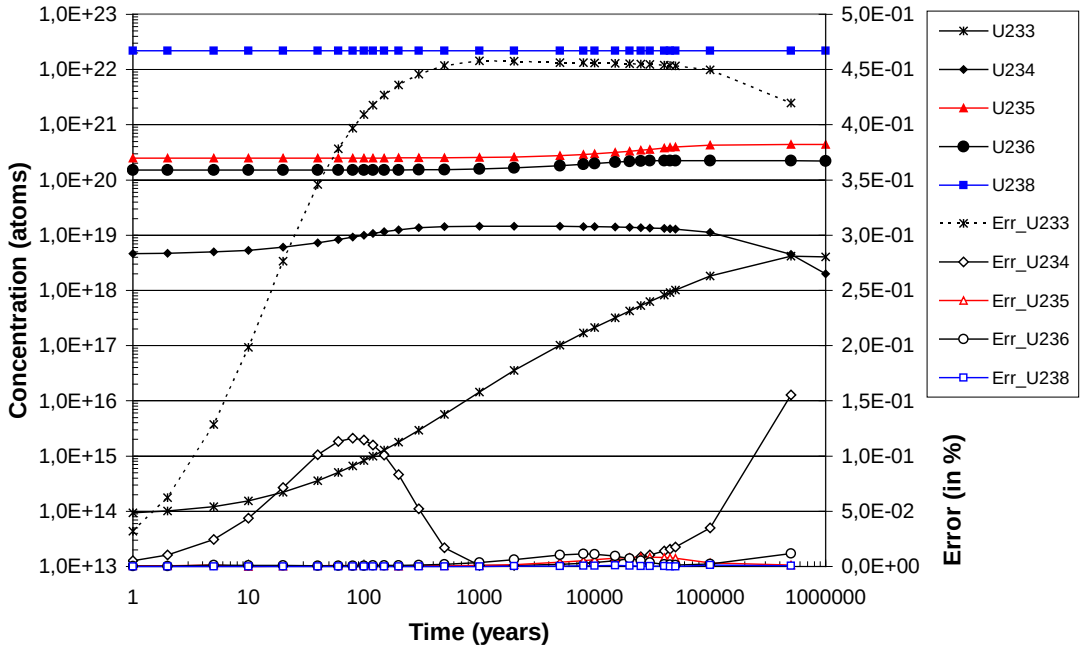
The overall uncertainty analysis by a general Monte Carlo procedure has shown that the most of the errors in the isotopic prediction are not significant (mainly U – see Figure 4 - and Pu). Only a few set of isotopes have shown errors larger than 1% to be taken into account: i) activation/fission products: Ca41, Ni59, Se79, NB93m, Nb94, Mo93, Tc99, Sn126, Sb126, Sb126m, Sm151, Eu151; ii) actinides: Am242m, Cm245, Cm246.

Once the uncertainties in the isotopic inventory due to decay data are evaluated, the next step is to analyse, by using a sensitivity/deterministic methodology, the sensitivity profile of the isotopic inventory to the decay values, identifying the relevant reaction channels and priorizing the data improvement needs. Even if the uncertainty results computed by the sensitivity technique could differ from that computed by MC, it is a suitable tool for analysis.

As an example, we studied the decay of a single radionuclide governed by the formula $N(t) = N_0 \cdot e^{-\lambda * t}$, where t is the time, and λ is the decay constant. The simple error propagation analysis can describe the fractional error in N in terms of the fractional error in λ: $\frac{s_N}{N} \approx \lambda t \cdot \frac{s_\lambda}{\lambda}$; where λt is the error amplification factor.

This simple formula shows the importance of the half-live relative error in: Ca41, Ni59, Se79, Nb94, Mo93, Tc99, Sn126, Sm151, Am242m, Cm245, Cm246.
The uncertainty for Nb93m, is due to the beta- decay mode from Zr93. For Sb126 and Sb126m, the main decay is: Sn126(B-)Sb126m(IT)Sb126. And, Eu151 is produced by beta- decay from Sm151. Several isotopes, with important half-live relative errors (Zr93, Pd107, I129,Cs135) have a negligible effect due to their large half-lives (greater that 1.0E+6 years).

FIG 4. Concentrations and rel. error (in %) in the isotopic prediction of $U^{233,234,235,236}$ and U^{238}.



Finally, the results of these uncertainties in the inventory prediction will be assessed in the k_{eff} value of this Benchmark. This assessment requires determining the k_{eff} sensitivities profiles for the main fuel isotope concentrations (see next section), and, it can be seen that these uncertainties are absolutely insignificant.

4.2. Criticality calculations

To take advantage of the previous decay sensitivity analysis, the sensitivity profiles to the isotopic composition have also been calculated. This permits the identification of the most contributing cross sections and the most relevant uncertainties in this problem.

We define the k_{eff} sensitivity profile as the change in k_{eff} due to a relative change in a cross-section in energy group g ($\Delta k/(\Delta\sigma_g/\sigma_g)$) or a relative change in the atomic density for the relevant isotope-i ($\Delta k/(\Delta N_i/N_i)$). These sensitivity profiles are obtained using the perturbation option of MCNP (invoked with the PERT-card with the default option (i.e. method = 1)). The sensitivity profile thus produced by MCNP and the relevant variance/covariance matrices are then used to carry out an uncertainty calculation.

Figure 5 shows the k_{eff} evolution versus cooling time and the k_{eff} sensitivity profiles (1% change in concentration) for the most important fuel isotopes in the Benchmark. For these sensitivity calculations we conclude:

- U235: For the first 1.0E+4 years Δk_{eff} ~ +100 pcm, and increased up to 300 pcm in 1.0E+5 years
- Pu239: For the first 1.0E+4 years Δk_{eff} ~ +150 pcm, thus being negligible or very small for times above 1.0E+5 years

- Pu241: Δk_{eff} ~ +50 pcm up to the first 10 years, negligible at 100 years
- U238: For the first 1.0E+4 years Δk_{eff} ~ -100 pcm, and decreased up to -130 pcm in 1.0E+6 years
- Pu240: For the first 1.0E+4 years Δk_{eff} ~ -50 pcm, and being negligible or very small for times above 1.0E+5 years
- Am 241: Zero at shutdown, maximum Δk_{eff} ~ -50 pcm at 100 years, and negligible above 1.0E+3 years

FIG. 5. The k_{eff} evolution and k_{eff} sensitivity profiles due to a relative change of 1% in the atomic density for the main fuel isotopes at shutdown. Calculations performed for the case of actinide-only burnup-credit nuclides.

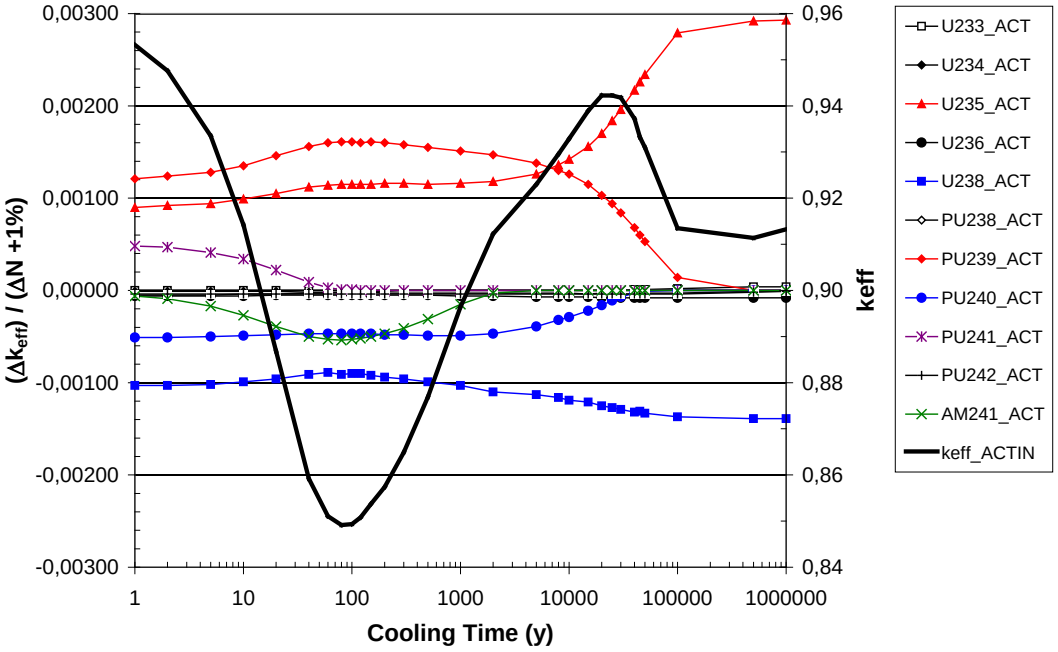
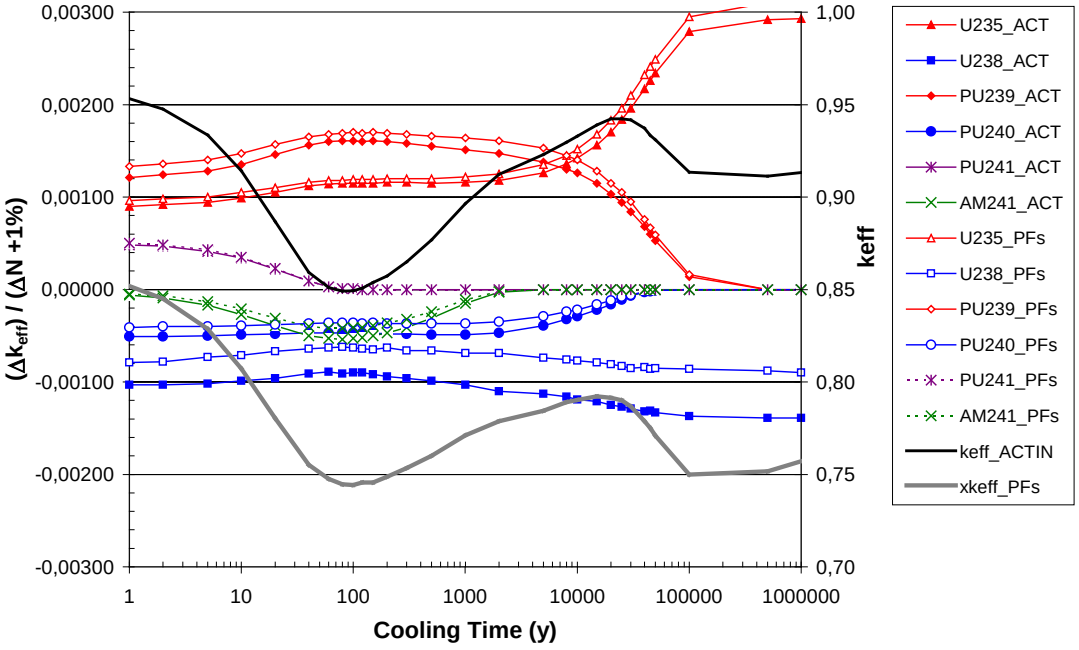


FIG. 6. The k_{eff} evolution and k_{eff} sensitivity profiles for the two calculations performed in the Benchmark: actinide-only (ACT) and actinide+fission products (PFs) burnup-credit nuclides.



These sensitivity coefficients can be used for different objectives like uncertainty estimates, design optimisation, determination of target accuracy requirements or adjustment of input parameters. These sensitivities depend on the Benchmark case, Figure 6 illustrates these changes; the sensitivity of U238 is modified by 25 pcm. Here, the uncertainty estimates in k_{eff} due to decay data uncertainties (see section above) is always below 10 pcm.

In order to identify the reactions whose cross section uncertainties have a major impact on the k_{eff}, sensitivity calculations have been performed. It should be recalled that the sensitivity coefficients give the subsequent change in the k_{eff} due to a constant variation (in our case 1%) of the cross-sections in the energy group-g. Consequently, a multigroup-energy structure should be defined; we have implemented the 15-groups used in BOLNA uncertainty cross section data. Figures 7 and 8 give the k_{eff} sensitivity profiles for σ_c^{U238} and σ_{fiss}^{Pu241}, respectively. We conclude that these sensitivities depend on both neutron energy (mainly thermal energy) and cooling time.

Once the sensitivity coefficient matrix for k_{eff} (S_{keff})and the covariance matrix (D) are available, the uncertainty on the k_{eff} value can be evaluated as follows:

$$\Delta k_{eff\,0}^{\;2} = S_{keff}^{+} \cdot D \cdot S_{keff}$$

Figures 9 and 10 show the errors in k_{eff} obtained with the diagonal (no correlations among isotopes, reactions and energy groups) BOLNA covariance matrix at different cooling times ranging from 1 year up to 1.0E+6 years. The maximum error is at shutdown, ~300 pcm. In addition, two major data sources for the overall uncertainties (> 100 pcm) are identified:

- Fission of Pu239 and Pu241
- Capture for U238, Pu239, Pu240 and U235

FIG. 7. Sensitivity coefficient of the k_{eff} for σ_c^{U238} at different cooling times ranging from shutdown up to 1.0E+6 years. Calculations performed for the case of actinide-only burnup-credit nuclides.

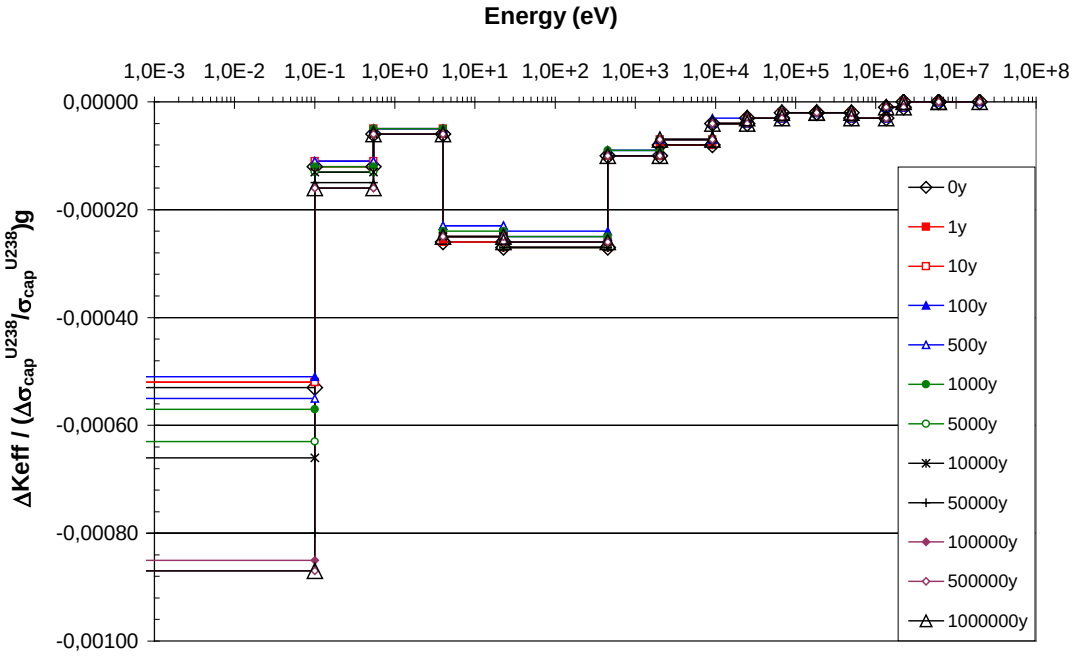


FIG. 8. Sensitivity coefficients of the k_{eff} for σ_{fiss}^{Pu241} at different cooling times ranging from shutdown up to 1.0E+6 years. Calculations performed for the case of actinide-only burnup-credit nuclides.

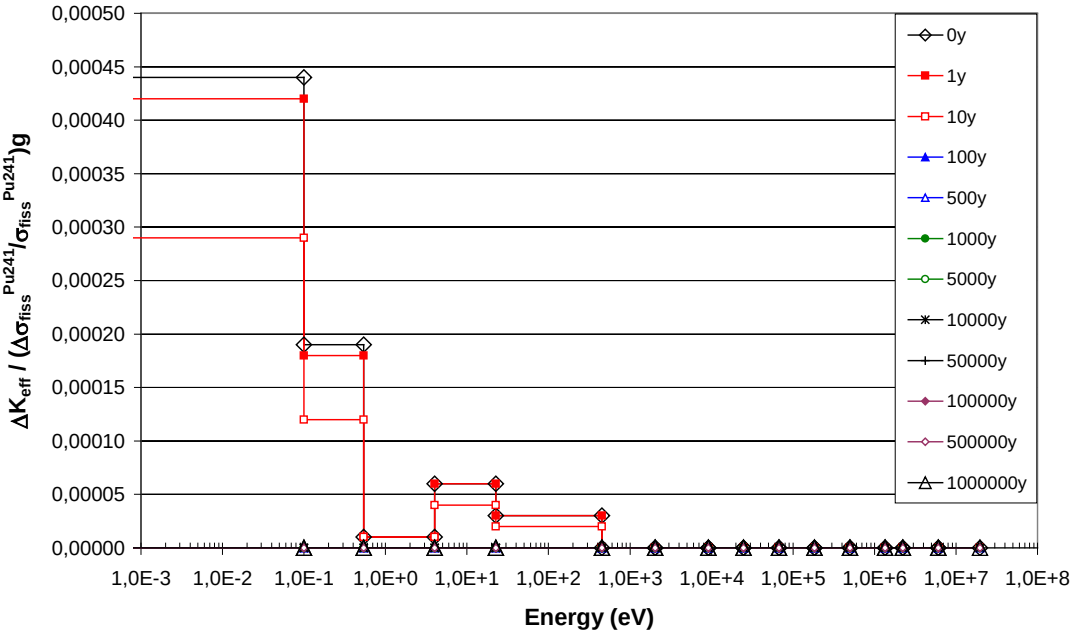


FIG. 9. Errors in k_{eff} using BOLNA diagonal uncertainty by isotope and reaction. Calculations performed for the case of actinide-only burnup-credit nuclides.

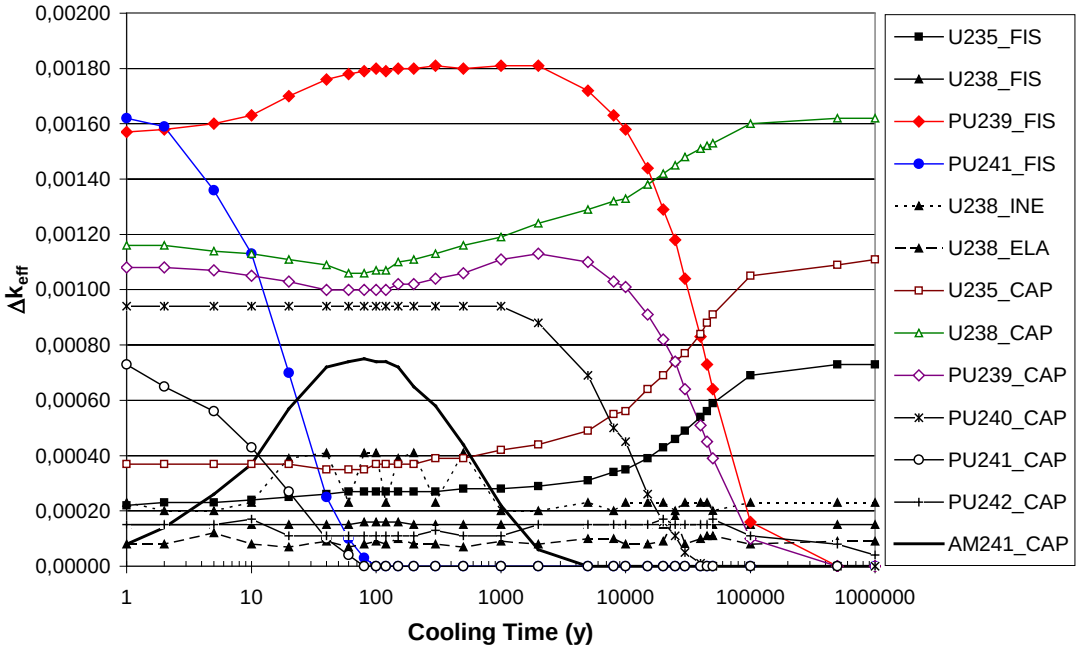
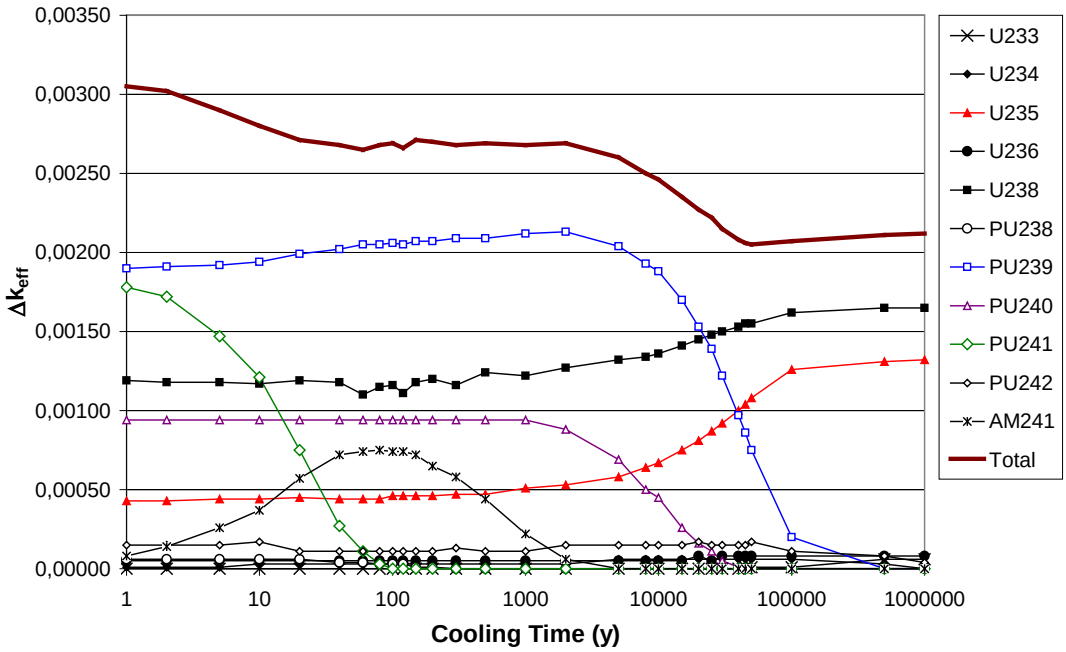


FIG. 10. Errors in k_{eff} using BOLNA diagonal uncertainty by isotope. Calculations performed for the case of actinide-only burnup-credit nuclides.



4.2.1. Uncertainty and target accuracies

As for thermal neutron systems [4], relatively small uncertainties on k_{eff} are observed (see Figure 10) since very small uncertainties are assumed on the low-energy data of U235, U238 and Pu239 and also of the Pu240 capture close to the first resonance. There are however a few significant contributions, e.g. the 241Pu fission.

Regarding target accuracies on the k_{eff} evolution, three Δk_{eff} values were assessed for the target accuracies: 100, 150 and 200 pcm. It was found that generally the uncertainties on k_{eff} decrease with the cooling time. Therefore, cross-sections uncertainties can be reduced so that the k_{eff} along the cooling time fulfill these design target accuracies.

Once these targets are defined, the following step is to minimize an objective function where cross section uncertainties are to be determined. This problem will permit to evaluate the reduction level and establishing priorities when using any uncertainty data library. We define the following objective function to be minimized:

$$\sum_{i=1}^{N} \lambda_i / x_i^2 \ , i=1, ..., N$$

where $x_i = \Delta_{1Gi}$ (uncertainty in one-group of the i reaction), N is the total number of reactions whose cross section uncertainties are to be determined and λ_i represents a cost parameter related with each cross section (in our case, we take a constant value λ_i=1). The objective function is constrained to the following boundary conditions: i) $x_i \geq 0$; ii) the maximum uncertainty in the k_{eff}, in all cooling times, must be lower than the target value.

Table V provides a summary of the main data requirements: i) it is required to improve Pu^{241} σ_{fiss} below ~400 eV, ii) very tight σ_{cap} requirements for Pu^{241}, Pu^{240} and Pu^{239} below ~0.5 eV, iii) in the resonance energy range, U^{238} σ_{cap} from 24.8 to 9.12 keV, and iv) Am^{241} σ_{cap} below ~4 eV is also needed.

Table V. Uncertainty reduction requirements needed to meet Δk_{eff} parameter target accuracies.

			Uncertainty (%)			
			Current Accuracy in BOLNA (%) (diagonal values)	Required Δk_{eff}		
Isotope	Reaction	Energy-range		0.00100	0.00150	0.00200
U235	CAPT	0.54-0.10 eV	1.55	1.43	1.55	1.55
		below 0.10 eV	1.73	0.58	1.29	1.73
U238	CAPT	24.8-9.12 keV	9.43	2.21	2.97	4.13
		9.12-2.03 keV	3.11	1.28	2.14	2.94
		2.03-0.454 keV	2.10	1.10	1.91	2.10
		454.0-22.6 eV	1.71	0.69	1.16	1.60
		22.6-4.0 eV	1.03	0.71	1.03	1.03
		4.0-0.54 eV	2.45	1.69	2.45	2.45
		0.54-0.10 eV	1.66	0.97	1.66	1.66
		below 0.10 eV	1.64	0.44	0.82	1.14
PU239	FISS	0.54-0.10 eV	0.88	0.41	0.63	0.88
		below 0.10 eV	1.11	0.34	0.52	0.74
	CAPT	0.54-0.10 eV	1.36	0.54	0.83	1.14
		below 0.10 eV	1.60	0.55	0.84	1.17
PU240	CAPT	0.54-0.10 eV	3.23	1.80	2.42	3.23
		below 0.10 eV	4.79	0.89	1.36	1.89
PU241	FISS	454.0-22.6 eV	19.38	3.33	3.73	4.91
		22.6-4.0 eV	4.21	2.12	2.63	3.47
		0.54-0.10 eV	2.94	1.00	1.48	1.95
		below 0.10 eV	3.27	0.67	0.97	1.28
	CAPT	0.54-0.10 eV	6.84	1.90	2.44	3.22
		below 0.10 eV	3.59	1.10	1.67	2.20
PU242	CAPT	4.0-0.54 eV	3.78	2.55	3.07	3.78
AM241	CAPT	4.0-0.54 eV	5.54	1.79	2.56	4.38
		below 0.10 eV	1.80	1.01	1.69	1.80

5. Conclusions

Criticality calculations and inventory predictions were performed for the Phase-VII Benchmark using JEFF-3.1.1 nuclear data and computer programs ACAB and MCNP. A set of additional calculations have been carried out using: i) other nuclear decay data libraries (ORIGEN-S and ORIGEN-2.2), ii) a different neutron transport library (ENDFB/VI), and iii) different computing tools (SCALE/KENO-VI). We conclude that decay data libraries have a negligible effect in k_{eff} prediction. By contrary, neutron transport libraries have a very important effect.

Once the sensitivity profiles of composition and multigroup cross-sections have been calculated with MCNP (PERT option), we have performed a global uncertainty assessment. The main conclusions are: i) uncertainties in JEFF-3.1.1 decay data library are negligible in k_{eff} calculations; ii) uncertainties in cross-section data libraries from BOLNA (only variance values) induce a Δk_{eff} ~300-200 pcm. Covariance information of this library could increase these values.

We have corroborated the main data requirements for thermal systems pointed out by the OECD/NEA group of experts [4]. In our uncertainty and target assessment, we have added the Am^{241} σ_{cap} below ~4 eV due to the importance in the reactivity of Am241 at 100 y. of cooling time.

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