Ref. Ares(2024)2476373 - 04/04/2024

HORIZON 2020

HORIZON 2020 RESEARCH AND INNOVATION FRAMEWORK PROGRAMME OF THE EUROPEAN ATOMIC ENERGY COMMUNITY

Nuclear Fission and Radiation Protection 2018 (NFRP-2018-4)

Project acronym:	**SANDA**
Project full title:	**Solving Challenges in Nuclear Data for the Safety of European Nuclear facilities**
Grant Agreement no.:	**H2020 Grant Agreement number: 847552**

Workpackage N°:	***WP5***
Identification N°:	***D5.5***
Type of document:	***Deliverable***
Title:	**Report on assessment of nuclear data needs**
Dissemination Level:	**PU**
Reference:	
Status:	***VERSION 1***
Comments:	

	Name	Partners	Date	Signature
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Abstract

To report specific assessment on nuclear data, the general inputs of this deliverable are multiple:

- Sensitivities and Uncertainties analyses (S/U) without experimental data studies made for [SANDA/Work Package 5/Task 5.1], and
- Target Accuracy Requirement (TAR) exercises.

Nuclear data trends through validation studies (involving so experimental data) and S/U analyses are made for [SANDA/WP5/T5.2].

On a first attempt, one can consider that each application (reactor studies, waste management and others) will give their own needs for improvement for specific involved nuclear data. We will show that this is also dependent on which nuclear data covariance matrices are used for such exercises. This deliverable is then organized according to each application.

[SANDA/WP5/T1/D5.2+other] ESFR, MYRRHA, ALFRED and LWR S/U

Full detailed studies are available in three non-contractual reports stated respectively in Annex A for **ALFRED, ESFR and ASTRID**, in Annex B for **MYRRHA** and in ANNEX C for **LWR/PIE** analyses. Depending on applications here are synthetic Target Accuracy Requirement results:

Table 1. Summary of current ND uncertainties requirements for multiple integral parameters of ALFRED-ASTRID-ESFR cases, keff parameter for MYRRHA case and LWR/PIE plutonium content.

Reaction	Above Threshold Fertile 2.23 10^6 eV - 1.96 10^7 eV	Above Threshold Inelastic 4.98 10^5 eV - 2.23 10^6 eV	Continuum to URR 6.74 10^4 eV - 4.98 10^5 eV	URR 2.03 10^3 eV - 6.74 10^4 eV	RRR 2.26 10^1 eV - 2.03 10^3 eV	EPITHERMAL 5.4 10^{-1} eV - 2.26 10^1 eV	THERMAL 1.0 10^{-5} eV - 5.40 10^{-1} eV	HRPL entry number for the reaction (https://oecd-nea.org/dbdata/hprl/)
^{238}U(n,γ)		2.4%	1.5%	0.4% - 0.6%		0.9%	0.6%	
^{238}U(n,n')	0.9% - 1.3%	0.9% - 1.5%	5.8% - 8.4%					18H (2%)
^{238}U(n,f)	1.6%	1.6%						
^{239}Pu(n,n')		4.4% - 7.0%						
^{239}Pu(n,γ)				0.8% - 1.5% 1.4%	2.2% - 2.6% 3.0%			32H (3%RRR, 3%% URR)
^{239}Pu(n,f)		0.3% - 0.4%	0.2% - 0.3%	0.2% - 0.3%	0.6% - 0.7% 1.8%			Below standards uncertainties
^{240}Pu(n,γ)			5.8%	3.9%			2.2%	
^{240}Pu(n,f)		1.1% - 1.8% 2.3%	2.0% - 6.8% 3.8%	2.3% - 6.8% 5.4%	13.1%			37H (2-3% SFR)
^{241}Pu(n,γ)							3.1%	33H (2-4% VTR+PWR)
^{206}Pb(n,n')	1.1% - 1.6%	1.0% - 1.5%						41H (5% LFR)
^{207}Pb(n,n')		1.0% - 1.5%						42H (5%-LFR)
^{56}Fe(n,n)		-	4.8% - 7.2%	3.9% - 4.1%				
^{56}Fe(n,n')		1.2% - 1.8%						34H (2%-ADMAB)
^{23}Na(n,n)			2.6% - 3.1%	3.9% - 4.0%				
^{23}Na(n,n')	2.0% - 2.4%	1.3% - 2.0%						ID29 (4%)
^{16}O(n,n)P1		5.2% - 6.5%						
^{238}U(n,n)P1		3.2% - 3.6%	3.8% - 4.9%					

It is noteworthy that, whatever is the selected scenario (cost functions choice), the reduction of ^{240}Pu(n,γ) and ^{240}Pu(n,f) cross section uncertainties is highly needed for all fast concepts, especially in the 2keV-2MeV neutron incident energy range. ^{239}Pu requires also a high reduction of its cross section uncertainties in the same energy range.

[SANDA/WP5/T1/D5.3] JHR S/U

[CEA/G. Truchet]

Following [SANDA/WP5/Deliverable 5.3], dedicated to S/U on critical mass for the fresh start-up core and a just-refueled core at 38 GWd/t_{HM}, the total COMAC-V2.1 uncertainties reach 730 and 770 pcm respectively.

To reduce such *a priori* uncertainty, one can extract the following ranked needs for improvement:

- ^{27}Al(n,n'), ^{27}Al(n,γ),
- υ_{tot} from ^{235}U(n_{th},f),
- ^{27}Al(n,n),
- ^{1}H(n,n) + ^{1}H(n,γ)
- ^{235}U(n,γ), PFNS from ^{235}U(n_{th},f) and ^{235}U(n,f) itself,
- And ^{135}Xe(n,γ) for just-refueled core.

Integrated sensitivity vectors can be found into D5.3.

[SANDA/WP5/T1/D5.4] HLW S/U

[KIT/R. Dagan]

“The nuclear data needs stemming […/…] on salt and clay rocks concern not only iron ‘[…] nuclear data should be carefully checked, up to about 1 MeV […]’, but also the main nuclides within the rocks.

- For salt rocks one concentrates mainly on sodium Na23 and chlorine: Cl35, 36 and 37. Where Cl36 is a beta emitter with very long half-life time and can be generated by neutron absorption of Cl35.
- The clay rocks are usually covered by concrete to gain stability of the gallery and here the list is quite long. Beside oxygen one has to look at different isotopes of silicon (Si28,29,30) and Ca. Further impurities are iron Fe, magnesium Mg and potassium K.

The scattering of neutron from the wall galleries to the gallery inner space increase the dose and reduces the allowed time for workers to be in the gallery. The issue of the secondary energy distribution, including energy and scattering angle is hence important.“

[SANDA/WP5/T1/Other] Nuclear data needs for fusion applications

[UKEA/I. Kodeli]

Those specific nuclear data needs can be stressed [UKAEA]:

Neutron induced cross sections:

- several issues were observed in nuclear data relevant for activation and heating calculations, such as W and Os chain,
- long-lived activation products (e.g. Ni, Nb isotopes),
- gas production data (for Fe, C12)

Need for covariance matrices for neutron induced reactions:

- secondary energy/angular distributions (SED/SAD): except for a few isotopes, such as Fe56, SAD covariance data are either missing or unrealistic, SED covariances are only available for PFNS,
- gamma-ray data: no covariances are available.

Annex A

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Grant Agreement no.:	**H2020 Grant Agreement number: 847552**

Workpackage:	***WP5***
Identification N°:	
Type of document:	***Non-contractual report***
Title:	***Target Accuracy Requirements on the MYRRHA k_{eff}***
Dissemination Level:	***PU***
Reference:	***ER-1270 / SCK CEN/55264898***
Status:	***VERSION 1.0***
Actual Delivery date:	***11 May 2023***
Comments:	

	Name	Partner	Date	Signature
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Reference N°	Creation Date	
SCK CEN/55264898	2023-05-10	
Alternative Reference N°	Revision	Version
N/A	1.0	10
ISC	Revision Status	
Public	Approved	

Report on MYRRHA v-1.8 TAR analysis.docx

Authors*
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Review information since previous revision*		
Name	**Outcome**	**Date**
Alexey Stankovskiy	Reviewed	2023-05-09
Pablo Romojaro	Reviewed	2023-05-10

Approval information for current revision*		
Name	**Outcome**	**Date**
Gert Van den Eynde	Approved	2023-05-11

Change log*				
Revision	**Version**	**Status**	**Date**	**Description of change**
1.0	10	Approved	2023-05-10	

**This automatically generated cover page shows references and document information as were available in the Alexandria document management system on 2023-05-11. Please refer to Alexandria for current and complete metadata, or to the document contents and/or author for additional information.*

ISC motivation
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Exploring
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ER-1270

Target Accuracy Requirements on the MYRRHA k_{eff}

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Publication date: 2023-05-11

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Glossary of abbreviations

ADS	Accelerator Driven System
ENDF	Evaluated Nuclear Data File
JEFF	Joint Evaluated Fission and Fusion
JENDL	Japanese Nuclear Data Library
LBE	Lead-Bismuth Eutectic
NEA	Nuclear Energy Agency
OECD	Organization for Economic Co-operation and Development
MYRRHA	Multi-purpose Hybrid Research Reactor for High-tech Applications
TAR	Target Accuracy Requirements
SANDA	Supplying Accurate Nuclear Data for energy and non-energy Applications
SLSQP	Sequential Least Squares Programming
S/U	Sensitivity and Uncertainty
WPEC	Working Party on International Nuclear Data Evaluation Cooperation
SG46	SubGroup46

Abstract

MYRRHA is a flexible experimental facility being designed at the SCK CEN, in Mol, Belgium. Cooled by lead-bismuth, it is conceived to operate both in sub-critical mode, as an accelerator driven system, and in critical mode, as a fast reactor. In order to comply with MYRRHA reactor design requirements, uncertainties due to nuclear data must be quantified. Significant gaps between the uncertainties and the target accuracies have been systematically shown in the past. In this report, first, a Sensitivity and Uncertainty analysis with JEFF-3.3 nuclear data library of the effective neutron multiplication factor k_{eff} of the latest MYRRHA reactor design - v1.8 - is presented. Then, because the target accuracy for k_{eff} of 300 pcm has been surpassed, a Target Accuracy Requirement (TAR) tool is utilized and described, and a TAR evaluation is performed, which allows determining the required accuracy on cross section data to satisfy the requested target accuracy. It is concluded that in order to reach the requested target accuracy, a reduction of the uncertainty in the fission and capture cross sections of ^{240}Pu JEFF-3.3 evaluation is needed in the fast energy range.

Keywords

MYRRHA; Target Accuracy Requirements; Sensitivity; Uncertainty; JEFF-3.3; SANDY.

1. Introduction

The Belgian Nuclear Research Center (SCK CEN) has been developing a flexible experimental facility called the Multi-purpose hYbrid Research Reactor for High-tech Applications (MYRRHA) since 1998. MYRRHA has been designed as an Accelerator Driven System (ADS) cooled by liquid lead-bismuth eutectic (LBE) and powered by a 600 MeV proton accelerator. In addition, the reactor can also operate in critical mode when disconnected from the accelerator. There are many benefits that will come with the development of this facility [1]:

- demonstration of the ADS concept on a smaller, pre-industrial scale;
- research and development of the transmutation of the spent nuclear fuel;
- ensuring the ongoing production of medical radioisotopes;
- improving the reliability and availability of accelerator systems, due to the unique requirements of the ADS application;
- and, offering an accelerator for basic and applied research.

The project is currently in its first phase, which involves the construction of the 100 MeV accelerator [1, 2] and will be continued with the two following phases (construction of the 100-600 MeV accelerator and of the nuclear reactor), which can be carried out in parallel or sequentially, enabling the reduction of risks and the spread of investment costs [1, 2].

To build this innovative and sophisticated technology with an emphasis on safety, several simulation codes are required. Accurate simulations can help to improve understanding and optimize the design and safety margins in any operational conditions. The quantification of uncertainties associated with the computational outcomes is imperative to establish the credibility of the results and make robust decisions based on simulations. In nuclear reactor design, material qualities, manufacturing tolerances, operating circumstances, modeling tools, and nuclear data are often the main causes of uncertainty. Particularly, nuclear data is one of the most significant causes of uncertainty in reactor neutronics simulations [3, 4]. Furthermore, it has already been proved that nuclear systems parameters, like k_{eff}, have significant gaps between their uncertainties and their objective accuracies (or uncertainties) [4-6].

The needs and requirements for nuclear data can be identified through assessments of Target Accuracy Requirements (TAR). Considering that there are nuclear data libraries with updated uncertainty evaluations that have most recently been released (JEFF-3.3 [7], ENDF/B-VIII.0 [8], and JENDL-5 [9]) while new ones are actively being created, such as JEFF-4 [10], and also knowing that uncertainties in the reactor parameters are highly dependent on the assumed initial uncertainty data [6], new target accuracies for nuclear data and reactor design parameters are required [4].

The work presented in the following has been developed in the framework of the SANDA (Supplying Accurate Nuclear Data for energy and non-energy Applications) [11] EU Horizon2020 project and the OECD/NEA (Organization for Economic Co-operation and Development /Nuclear Energy Agency) WPEC (Working Party on International Nuclear Data Evaluation Co-operation) SG46 (SubGroup 46) [12], with the objective of improving nuclear data in the JEFF-3.3 library and to stablish target accuracy requirements in advanced reactors. Hence, the report focuses on the TAR analysis of a selected neutronics parameter (k_{eff}), explaining the process and presenting the results obtained with the tool developed at SCK CEN.

2. Sensitivity and uncertainty analyses

There are multiple types of sensitivity analyses, but in the case of nuclear data and reactor physics simulations their goal is to examine the variation of a physical parameter or reactor response when system parameters change (for example, and related to this report, how k_{eff} changes when nuclear data change). Moreover, they enable the identification of the most crucial nuclear data for neutron-induced reactions and the establishment of a hierarchy of importance for the investigated response. On the other hand, uncertainty analyses quantify the reactor's response uncertainty that has been propagated from uncertainties in nuclear data [4].

Even though there have already been analyses done for previous MYRRHA designs [5, 13-16], there is an analysis needed for the new core design (revision v1.8 [10]). In particular, this report focuses on the determination of k_{eff} target accuracy using MYRRHA's v1.8 critical configuration, homogenized at the fuel assembly level [17].

The S/U (Sensitivity and Uncertainty) analyses have been carried out using the JEFF-3.3 evaluated nuclear data library.

The sensitivity calculations have been performed with the Serpent 2 reactor physics Monte Carlo code [18] and the ECCO 33 energy group structure [19].

The results obtained in the sensitivity calculations can be seen in Figure 1, where the sensitivity coefficients to the ten most significant nuclides and reactions for the k_{eff} of MYRRHA are shown.

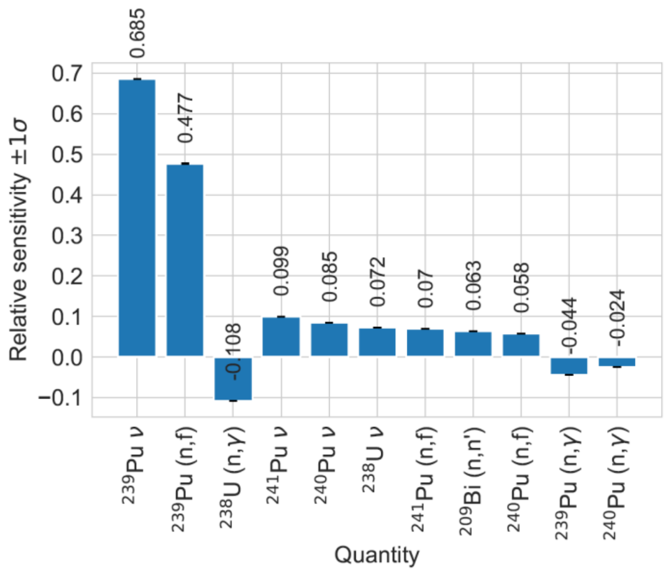

Figure 1. k_{eff} integrated sensitivity coefficients for MYRRHA [4].

Once the sensitivity coefficients have been obtained, the propagation of uncertainties from the nuclear data to the final responses can be performed. The uncertainty quantification was conducted using the OECD/NEA NDaST tool [20], which employs the so called "Sandwich formula".

The **Sandwich Formula** is essential to the propagation of uncertainties and the TAR problem, as it will be seen. It is used to calculate the uncertainty $\Delta \boldsymbol{R}$ of an integral parameter **R**, as follows:

$$\Delta R = \sqrt{S_R^{+} D S_R} \qquad (1)$$

Where:

- ***D*** is the relative covariance matrix with the standard deviations on the diagonal and the covariances on off-diagonal terms
- $\boldsymbol{S_R}$ are the relative sensitivity coefficient arrays

Uncertainties in the average number of emitted neutrons from fission ν and in the average fission spectrum χ have not been propagated, since those covariance were not available in NDaST.

The results from the uncertainty quantification are presented in Table 1. It can be concluded that fission and capture reactions from ^{240}Pu, ^{239}Pu, ^{238}U are the highest contributors to the total uncertainty of k_{eff}.

Table 1. k_{eff} nuclear data uncertainty quantification for MYRRHA. Uncertainties due to Monte Carlo counting statistics are negligible (the maximum value accounting for 0.004% in relative terms), thus they are omitted [4].

Quantity				**$\Delta k_{eff}/k_{eff}$ (%)**
^{240}Pu	(n,f)	^{240}Pu	(n, γ)	-0.614
^{240}Pu	(n,f)	^{240}Pu	(n,f)	0.558
^{239}Pu	(n,f)	^{239}Pu	(n,f)	0.276
^{239}Pu	(n,f)	^{239}Pu	(n, γ)	0.259
^{240}Pu	(n,γ)	^{240}Pu	(n, γ)	0.202
^{238}U	(n, γ)	^{238}U	(n, γ)	0.172
^{238}U	(n,f)	^{238}U	(n, γ)	0.171
^{239}Pu	(n, γ)	^{239}Pu	(n, γ)	0.126
^{238}U	(n,f)	^{238}U	(n,f)	0.113
Total uncertainty of listed				**0.588**

The determination of the k_{eff} target accuracy is a rather complex issue due to the number of factors to take into account, such as reactor criticality, rods' safety margins, safety parameters, etc. The estimated reactivity worth of the safety rods in MYRRHA's critical configuration is ~5000 pcm. The combined uncertainty from all sources, nuclear data among them, should not exceed this value. On the other hand, a possible underestimation of k_{eff} will require loading of additional fuel assemblies in the core periphery to reach the criticality. Following the MYRRHA core rotational symmetry, 3 or 6 fuel assemblies would have to be added. Taking into account that preliminary studies have shown that the reactivity worth of a peripheral fuel assembly is ~50 pcm, a k_{eff} target accuracy of 300 pcm is deemed to be satisfactory in order to minimize the increase in the costs of additional fuel assemblies [4, 5, 21].

3. TAR analysis

3.1. Theory

The TAR analysis is understood, in a simple way, as the inverse problem of the uncertainty evaluation. The following theoretical description is based on the process normally applied for TAR analyses [22] in Generation IV systems.

- First, target accuracies on the design parameters are defined;
- then, the unknown uncertainty data requirements $\boldsymbol{d_i}$ are obtained by solving a minimization problem.

As already explained, to obtain the unknown uncertainty data requirements $\boldsymbol{d_i}$, it is necessary to minimize a function **Q**. This is called the minimization problem**:**

$$Q = \sum \frac{\lambda_i}{d_i^2} = min, \qquad i = 1 \dots I \tag{2}$$

When the variables are not correlated between themselves, the constraints of the problem are defined as the following:

$$\sum_i S_{ni}^2 d_i^2 \leq (R_n^T)^2 \ , \ \ n \ = \ 1 \dots N \tag{3}$$

Where :

- $\boldsymbol{N}$ is the total number of integral design parameters;
- $\boldsymbol{S_{ni}}$ are the sensitivity profiles with the coefficients for the integral parameter;
- $\boldsymbol{R_n}^{\boldsymbol{T}}$ are the target accuracies of the integral parameters;
- $\boldsymbol{\lambda_i}$ are the cost parameters. They are provided by experimentalists and serve as a tool to quantify how much it would cost to minimize the uncertainty of each cross section measurement in real experiments;
- $\boldsymbol{d_i}$ are the variables or the standard deviations of the nuclear data (cross sections) whose target accuracies are to be determined;
- and, $\boldsymbol{I}$ is the number of variables, which has been obtained after selecting the variables that contribute most to the global uncertainty, using the sensitivity analysis.

If the correlations of the variables are taken into account, the constraints equation becomes:

$$\sum_i G_i^n + \sum_{ii'} C_{ii'}^n \ + \sum_i F_i{}^n + P_n \leq (R_n^T)^2 \tag{4}$$

Where:

- $\boldsymbol{G_i^n}$ is the term where the uncertainty related to the standard deviations of the selected variables is located:

$$G_i^n \ = \ S_{ni}^2 d_i^2 \tag{5}$$

  As explained, it is composed by the sensitivity profiles (S_{ni}) and the unkown uncertainties (d_i), which are to be determined. The sensitivity profiles are expressed as vectors:

$$S_{ni} = \left(S_{x,i}\right) = \begin{pmatrix} S_1 \\ \vdots \\ S_j \\ \vdots \\ S_J \end{pmatrix}_{x,i} \tag{6}$$

  Where :

  - $\boldsymbol{J}$ is the total number of components per sensitivity profile, determined by the energy structure;
  - and, $\boldsymbol{x}$ is the reference to a specific cross section type.

The unknown uncertainties or standard deviations conform a diagonal matrix where $\boldsymbol{N}$ marks the size of the matrix, which is directly related to the sensitivity profiles:

$$d_i = \begin{pmatrix} d_{11} & 0 & \cdots & 0 & 0 \\ 0 & \ddots & 0 & \cdots & \vdots \\ 0 & \cdots & d_{jj} & \cdots & 0 \\ \vdots & \cdots & 0 & \ddots & 0 \\ 0 & 0 & \dots & 0 & d_{NN} \end{pmatrix} \tag{7}$$

- $\boldsymbol{C^n_{ii'}}$ includes the correlation terms among the selected variables, not considering the correlation between themselves (i.e., $i \neq i'$), as they are considered in the previous term. It is expressed as follows:

$$C^n_{ii'} = S_{ni} d_i Corr_{ii'} d_{i'} S_{ni'} \tag{8}$$

Where:

- $\boldsymbol{Corr_{ii'}}$ is the correlation value between the variables **i** and **i**', which is basically the covariance divided by the standard deviations of the selected variables. Both **i** and **i'** variables go from 1 to $\boldsymbol{I}$.

$\boldsymbol{G^n_i}$ and $\boldsymbol{C^n_{ii'}}$ may be combined into a single large correlation term, where $\boldsymbol{G^n_i}$ accounts for the covariance matrix's diagonal and the second element $\boldsymbol{C^n_{ii'}}$ accounts for the remaining components. This results in a term that is essentially equal to the "Sandwich Rule," which was previously described [23].

- $\boldsymbol{F^n_i}$ includes the correlation between the unselected and the selected variables:

$$F_i^{\,n} = S_{ni} d_i Corr_{ij} d_j S_{nj} \;,\; j = 1 \dots K \tag{9}$$

Where:

- $\boldsymbol{d_j}$ denotes the standard deviations that are not variables but considered constants.
- and, $\boldsymbol{K}$ the total number of constant terms correlated to variable **i**.

- $\boldsymbol{P_n}$ is the constant residual uncertainty, due to unselected variables, for the integral parameter.

Ultimately, the minimization problem may be formulated as follows, taking into account that the lower limit of bounds is set to zero (to guarantee that it is impossible to obtain a negative uncertainty value) and that the upper limit is determined by the initial uncertainty of the nuclear data:

$$\boldsymbol{Q} = \sum_i \frac{\boldsymbol{\lambda_i}}{\boldsymbol{d_i^2}} \quad \boldsymbol{i = 1, \dots, I}$$

$$\sum_i S_{ni}^2 d_i^2 + \sum_{ii'} S_{ni} d_i Corr_{ii'} d_{i'} S_{ni'} + \sum_i S_{ni} d_i Corr_{ij} d_j S_{nj} + P \leq (R_n^T)^2 \tag{10}$$

$$n = 1, \dots, N \quad j = 1, \dots, K$$

$$0 \leq d_i \leq d_0$$

3.2. Inputs and characteristics of the TAR analysis

- **The parameter** selected to be studied is the k_{eff} with a target accuracy of **300 pcm** [4] due to its importance in the physics of the reactor and the fact that a specific design target accuracy was already established for MYRRHA [4].

- **The nuclear data library** selected, following what has been done in the S/U analyses, is the **JEFF-3.3**.
- **The energy group structure** was chosen following the OECD/NEA SG46 recommendations, which proposes a 7 energy group structure that can be seen in Table 2.

Table 2. Energy grid structure recommended by OECD/NEA WPEC SG46 [24].

Energy group	***Lower energy (eV)***	***Upper energy (eV)***	***Spectrum region***
1	$2.23130 \cdot 10^{6}$	$1.96403 \cdot 10^{7}$	Above threshold fertile
2	$4.97871 \cdot 10^{5}$	$2.23130 \cdot 10^{6}$	Above threshold inelastic
3	$2.03468 \cdot 10^{3}$	$4.97871 \cdot 10^{5}$	Continuum to unresolved resonances
4	$2.03468 \cdot 10^{3}$	$6.73795 \cdot 10^{4}$	Unresolved resonances
5	$2.26033 \cdot 10^{1}$	$2.03468 \cdot 10^{3}$	Resolved resonances
6	$5.40000 \cdot 10^{-1}$	$2.26033 \cdot 10^{1}$	Epithermal
7	$1.40000 \cdot 10^{-5}$	$5.40000 \cdot 10^{-1}$	Thermal

- **The variables selected** for the minimization of uncertainties in the TAR analysis were chosen after the sensitivity analysis that showed the individual contribution to the uncertainty of the parameter (Table 1).

  In the end, the total number of chosen variables ***I*** is equal to ten. This was obtained after selecting those variables that globally accounted for at least a 90% of the listed total uncertainty.
- **The cost parameters** $\boldsymbol{\lambda_i}$ have been chosen following the values defined by the Subgroup 26 of the OECD/NEA's WPEC [25]. The WPEC proposes different scenarios for the analysis. The ones that have been used are described in Table 3.
  - **Case A:** The difficulty of measuring the various cross sections or responses is not taken into account in this scenario. It will therefore provide unreal results with measures that are challenging or impossible to get.
  - **Case B:** In this instance, various weight variables are taken into consideration, notably for the inelastic cross sections, which are the hardest to measure experimentally.

Table 3. Cost parameters' value for the different scenarios: Case A and Case B [25].

Isotopes and reactions	***Weight (cost) factors*** ***Case A***	***Case B***
^{235}U, ^{238}U, ^{239}Pu - capture, fission, ν	1	1
Other fuel isotopes – capture, fission, ν	1	2
Non-fuel isotopes – capture	1	1
All isotopes – elastic scattering	1	1
All isotopes – inelastic scattering	1	3

- **The sensitivity file** that has the results of the sensitivity analysis and that has been used as an input in the Python program (described in Section 3.3), contains the information on ^{238}U, ^{239}Pu, ^{240}Pu, ^{241}Pu and ^{209}Bi with the following cross sections: neutron total cross sections (MT1, following ENDF-6 format terminology)), elastic scattering cross section for incident particles (MT2), particle-induced fission (MT18), $\bar{\nu}_T$ average total (prompt plus delayed) number of neutrons released per fission (MT452), $\bar{\nu}_p$ average number of prompt neutrons released per fission event (MT456) and $\bar{\nu}_d$ average number of delayed neutrons released per fission event (MT455).
- **The cross sections** and reactions' uncertainties that have been analyzed are presented in Table 4, following the results of the uncertainty propagation analysis (Table 1):

Table 4. Isotopes and reactions analyzed in this TAR assessment.

Isotope	**Reaction Type**	
^{240}Pu	(n,f)	^{238}U (n,f)
^{239}Pu	(n,f)	(n, γ)
^{238}U	(n,f)	(n, γ)

Other reactions that had significant results in the sensitivity and uncertainty analysis, such as the average number of emitted neutrons from fission, will be evaluated in further TAR assessments.

- **The minimization** of the function has been done using the 'optimize' module from the Scipy library, which is a free and open-source Python programming language library for scientific computing. In particular, with the constrained minimization of multivariate scalar functions, in python called 'minimize'.

  This minimization function provides different algorithms for constrained minimization, such as **"SLSQP"**[26] and **"trust-constr"**[27].
  One of the most important aspects for the minimization function to work properly, is the setting of the correct constraints and bounds. Since the constraints have been already thoroughly explained, it is needed to specify that the **lower bound** has been set to 0.01 and the **upper bound** to the initial relative standard deviation extracted from the data processed by NJOY [28].

3.3. Python tool implementation

One of the objectives of this work was to produce a Python program that automatically performs the TAR analysis employing libraries such as Scipy [29] (for the minimization of the function) or modules like SerpentTools [30] or SANDY [31], a sampling code developed at SCK CEN that can quickly read and process data from ENDF-6 files [32]. Then, the python tool explained in this report will finally be implemented into SANDY, as part of the library being developed by SCK CEN.

This Python tool is meant to have the following advantages:

1. **Accessible**. It is free and available to everyone because it was created in Python and incorporated into SANDY.
2. **Simple**. It is quite simple to use for any user thanks to the programming. It is not necessary to understand how to solve any particular kind of equation or to use additional applications to read and process data. The only inputs required by the software are the sensitivity file, the TAR parameters to be evaluated throughout the analysis, and the nuclear data library that will be utilized.
3. **Quick**. Depending on the number of sensitivity profiles taken into account, the results are displayed in a few seconds or minutes. The NJOY processing (covariance matrices and initial uncertainties) takes the longest amount of time.
4. **Versatile**. Given the way it has been designed, it is possible to alter the cost function values for each energy group as well as each cross section and isotope. Moreover, it is possible to consider one or more reactor parameters at the same time, and also one or several reactors at the same time.
5. It can read any **Serpent sensitivity** output.

3.3.1. Python tool workings

The Python code starts by requesting the following inputs:

- A sensitivity file which comes in **Serpent** format with the already defined **energy group structure** inside it, which is extracted using SerpentTools.
- The nuclear data library: **JEFF-3.3** in this case.
- The method for the minimization problem: A Sequential Least Square Programming (**SLSQP**) approach was chosen to solve the minimization problem since it is ideal for minimizing functions with several variables and a mix of limits, equality, and inequality constraints. It should be good to take into account that although no correlation within nuclear data was considered, some comparable techniques (to conduct a TAR analysis) were used for the ALFRED reactor, which builds confidence on the process followed for this analysis [33].
- The **Target accuracy requirement** for k_{eff} in percentage, which is set to 0.3 %.

The code then works as follows :

The input sensitivity file is treated and processed for the data that is wanted, in this case the sensitivity profiles for the k_{eff}. As a result, there is a DataFrame that contains the important data from the sensitivity input.

Making use of the nuclear data processing code NJOY and the SANDY code, the covariance matrices are extracted, from the requested library, for each nuclide present in the sensitivity input.

Then, the SANDY extracts the necessary information from these matrices, such as the correlation matrix or the standard deviation vector, useful in the TAR. After obtaining all these required data, the constraints function (that will be used in the minimization method) is defined.

Once the objective function and constraints have been defined, the SLSQP procedure is used to determine the best solution. The minimize method will return an optimization result object, which contains information about the optimization process, such as the final solution, the total number of iterations, and any convergence messages.

4. Results

For this report, only limited results are presented, since only the first two terms of the constraints equation have been taken into account. In the future, the performance of the tool will be tested using the full constraints equation and introducing more cross sections and reactions into the analysis.

As it has already been explained, there have been 2 different scenarios for the weight factors (Table 4). Results are presented for Case A and Case B in Figure 2 and Figure 3, respectively.

4.1. Case A

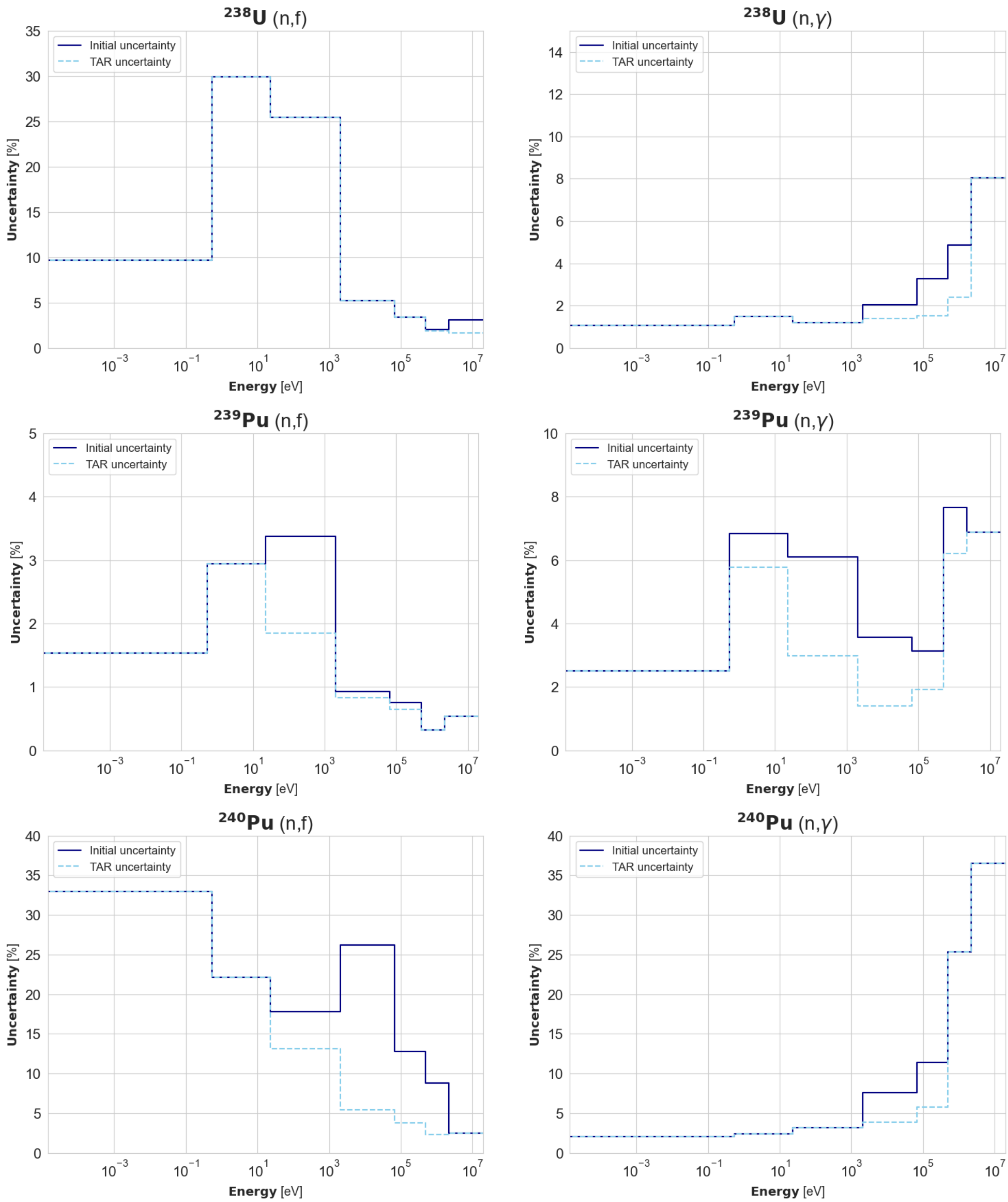

Figure 2. TAR analysis results: Case A.

4.2. Case B

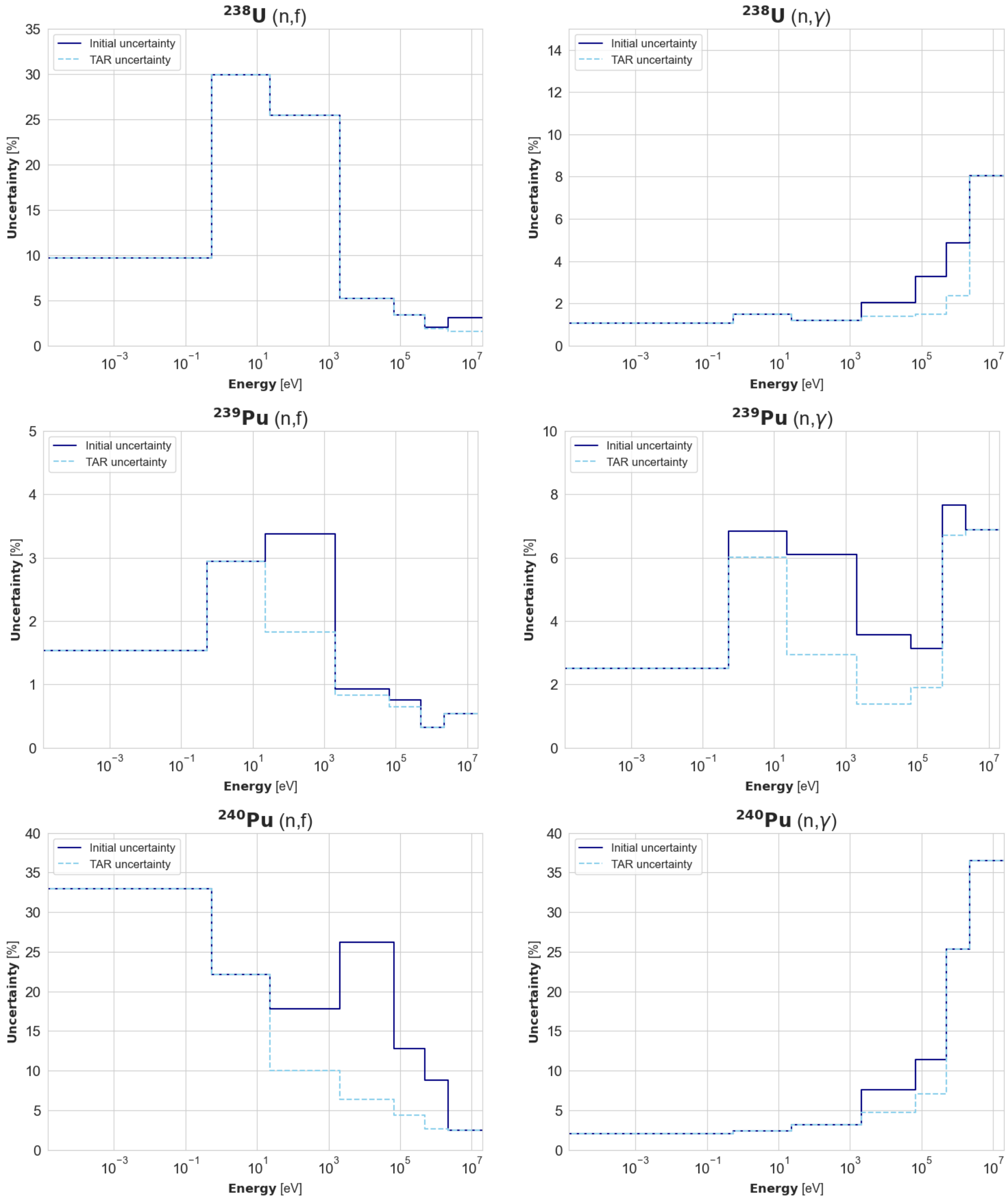

Figure 3. TAR analysis results: Case B.

4.3. Analysis

As it can be noticed in Figure 2 and Figure 3, the uncertainty is not reduced in the thermal energy range. This was expected, since the sensitivities in the thermal energy range are close to zero for fast reactors (such as MYRRHA). Moreover, it also serves as a consistency check and to verify that the minimization tool is working properly, following the expected results.

Detailed information in Table 5 shows that some reactions have a greater reduction of uncertainty than others. For example, ^{240}Pu (n,f) has a significant reduction in the fast energy range (2.035 keV to 67.38 keV) from a 26.2% initial uncertainty to a

5.4% target uncertainty. This is explained as the ^{240}Pu (n,f) is the main contributor to the final uncertainty in k_{eff} and, in addition, it is also the ninth reaction with the biggest integral sensitivity value for k_{eff}. On the other hand, a reaction such as ^{238}U (n,f) that that contributes a little to the final uncertainty in k_{eff} and with a really small sensitivity, will result in small reductions in uncertainty.

In conclusion, the largest uncertainty (and sensitivity) contributors have a greater influence on k_{eff} 's final uncertainty. To achieve the ultimate uncertainty goal, it is therefore more significant to eliminate a larger contributor than a smaller one. The TAR results can be understood taking into account the reactions with the biggest impact in the final uncertainty (^{240}Pu (n,f), ^{239}Pu (n,f), and ^{240}Pu (n, γ)) and the reactions with the biggest sensitivity values. Overall, the ^{240}Pu (fission and capture) requires the biggest reduction in uncertainties.

Table 5. List of isotopes, reactions and energy ranges (E) requiring the major relative reduction of the uncertainty for Case A.

Nuclide	***Reaction***	***E (eV)***			***TAR UNCERTAINTY %***	***INITIAL UNCERTAINTY %***	***DIFFERENCE %***
^{240}Pu	(n,f)	2.04E+03	-	6.74E+04	5.4	26.2	20.8
		6.74E+04	-	4.98E+05	3.8	12.8	9.0
		4.98E+05	-	2.23E+06	2.3	8.8	6.5
	(n,γ)	6.74E+04	-	4.98E+05	5.8	11.4	5.7
	(n,f)	2.26E+01	-	2.04E+03	13.1	17.8	4.7
	(n,γ)	2.04E+03	-	6.74E+04	3.9	7.6	3.6
^{239}Pu	(n,γ)	2.26E+01	-	2.04E+03	3.0	6.1	3.1
^{238}U	(n,γ)	4.98E+05	-	2.23E+06	2.4	4.9	2.5
^{239}Pu	(n,γ)	2.04E+03	-	6.74E+04	1.4	3.6	2.2
^{238}U	(n,γ)	6.74E+04	-	4.98E+05	1.5	3.3	1.7
^{239}Pu	(n,f)	2.26E+01	-	2.04E+03	1.8	3.4	1.5
^{238}U	(n,f)	2.23E+06	-	2.00E+07	1.6	3.1	1.5

5. Conclusions

The preliminary results for the TAR analysis are presented for both scenarios with the SLSQP method of minimization. This is the uncertainty that should be achieved in the selected isotopes and reactions to reach the final k_{eff} uncertainty target. Nevertheless, not all the constraints have been taken into account, so results may vary when a complete analysis is performed. There is no big difference between Case A and Case B. As it has been explained, Case B of the TAR analysis is closer to reality, since it considers the difficulty of improving the measurements in nuclear data. TAR's Case B uncertainty results are a little bit higher in value when compared to Case A, as it was expected.

It is noticeable that there is no uncertainty reduction in the thermal region, this is imposed by the sensitivity profiles of the reactions and these are results obtained using the SLSQP method of minimization.

It can be seen that the main contributors to the final uncertainty of k_{eff}, ^{240}Pu (n,f), ^{239}Pu (n,f), and ^{240}Pu (n, γ), suffer the biggest reductions in uncertainty, while the ones with really low sensitivities and contributions to the final uncertainty, such as ^{238}U (n,f) are less diminished. In order to achieve the required target of uncertainty, it will be necessary to have larger reductions in these reactions with the biggest impact, mainly in ^{240}Pu fission and capture.

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Annex B

UPM report 20240108		
POLITÉCNICA	UPM contribution to Deliverable 5.5 of SANDA project	Date: 08/01/2024
	UPM contribution to D5.5: Report on assessment of nuclear data needs	Pags: 22 Version: 1

SUMMARY

This report contains the UPM contribution to Deliverable 5.5 of the EC SANDA project, Solving Challenges in Nuclear Data for the Safety of European Nuclear facilities (H2020 Grant Agreement number 847552).

MODIFICATIONS TO PREVIOUS VERSION

Written by:	Reviewed by:	Approved by:
Nuria García-Herranz *Oscar Cabellos* *Antonio Jiménez-Carrascosa*	*Oscar Cabellos*	

UPM contribution to D5.5:
Report on assessment of nuclear data needs

Nuria García-Herranz, Oscar Cabellos, Antonio Jiménez Carrascosa

Contents

1. Introduction

In SANDA Deliverable 5.2 [Romojaro, 2022], UPM performed a sensitivity/uncertainty (S/U) analysis for a selected set of integral responses (keff and reactivity effects) for the following innovative reactors: conceptual sodium-cooled fast reactors (ASTRID-like and ESFR) and conceptual lead-cooled fast reactor (ALFRED). The impact of JEFF-3.3 covariance data on the evaluated responses showed that nuclear data-induced uncertainty target accuracies were clearly exceed for some of them (see Table 1 and Table 15 in Deliverable 5.2). A detailed analysis of major contributors allowed to identify the cross-sections in need of improvement. However, nothing was said about the specific energy range to be specifically targeted.

The analysis is extended in this work with an estimation of the energy group-wise uncertainty contribution. That allows to establish a priority list for cross-section uncertainty reduction, with indication of the energy range where the uncertainty should be reduced. Then, a target accuracy requirement (TAR) assessment is performed aiming at finding out the required uncertainty reduction so that the evaluated integral responses can fulfil the target accuracies.

In order to provide potential evaluation priorities, sensitivities in 7 energy groups (energy bands) together with the JEFF-3.3 covariance matrix in 7 energy groups[1] have been chosen to draw conclusions. First, in Section 2, the uncertainties in the quantities of interest due to JEFF-3.3 covariance data are compared to the available target accuracies and critical cross sections are identified. Then, in Sections 3 and 4, the TAR analysis is performed making use of the computed 7-group sensitivities. It is well-known that the impact of nuclear data depends on the specific design choices, even within a given "family" of systems. Then, the analyzed systems were considered individually and jointly to compare the corresponding findings.

In summary, this work aims at making recommendations about the isotope, reaction and energy group with the highest priority for the uncertainty reduction, how much uncertainties should be reduced so that integral parameters can fulfil target accuracies, and what performance gains can be expected as a consequence.

2. Identification of critical cross sections

Table 1 shows a summary of the uncertainty quantification analysis for the analysed reactor integral responses using JEFF-3.3 covariances in both 33 and 7 energy groups. The uncertainty values (in %) have two different terms: the first term corresponds to the uncertainty due to nuclear data, and the second term (±) is the term corresponding to the stochastic calculation of sensitivity profiles.

The total uncertainties are compared to the design target accuracies for fast reactors recently reviewed by the OECD/NEA Working Party on International Nuclear Data Evaluation Co-operation Subgroup 46. At UPM, the same values of target accuracies were chosen for all reactors to maintain uniformity. It can be seen that target accuracies are clearly exceed for the multiplication factor and coolant density, while they are met for Doppler effect and control rod worth. Therefore, results point out that several improvements are still to be addressed concerning the nuclear data need for advanced reactor deployment.

A detailed uncertainty breakdown (in Deliverable 5.2) allowed to identify the main isotopes-reaction pairs contributing to the overall uncertainty. Then, a proposed priority list for future uncertainty reduction when using JEFF-3.3 covariance data is given in **Table 2**, where the uncertainty contribution of each key reaction to the integral response uncertainty is also shown. Even if Doppler and control rod worth uncertainties fulfill target accuracies, main contributors are also included. The list includes 17 quantities along with correlated data for 8 reaction-pairs because of their significant impact on uncertainty estimation.

[1] The 7-energy group structure is the one proposed by M. Salvatores in NEA/WPEC-SG46 and it is included in Appendix 1.

Table 1. Uncertainty quantification results.

Reactor	Response	Target accuracy	Uncertainty [%] 33g Sensitivites 33g JEFF-3.3 COV			Uncertainty [%] 7g Sensitivites 7g JEFF-3.3 COV		
ESFR	**k-eff**	0.3% = 300 pcm	1.04	±	2.5E-04	0.98	±	4.5E-04
	Coolant density	5%	25.69	±	1.2E-01	26.86	±	1.7E-01
	Doppler+300K	5%	4.25	±	5.4E-01	4.16	±	7.6E-01
	Doppler-300K	5%	4.00	±	5.0E-01	3.63	±	6.5E-01
	Control	3%	1.96	±	1.1E-02	1.80	±	2.0E-02
ASTRID	**k-eff**	0.3	0.97	±	2.0E-04	0.92	±	3.6E-04
	Coolant density	5%	15.78	±	5.2E-02	16.19	±	7.7E-02
ALFRED	**k-eff**	0.435% = 435 pcm	0.88	±	1.6E-04	0.84	±	3.0E-04
	Coolant density	5%	6.82	±	2.7E-01	6.42	±	3.6E-01
	Doppler+300K	5%	6.91	±	6.2E-01	6.55	±	7.8E-01
	Doppler-300K	5%	3.57	±	3.3E-01	3.46	±	4.8E-01

Table 2. Priority list for cross-section uncertainty reduction. Uncertainties (in %) in the reactor integral responses due to uncertainties in the specified cross section are given. Cross sections contributing with an uncertainty larger than ~300 pcm in k-eff and ~2% in reactivity effects at least for one reactor and one scenario are selected (main contributors to control rod worth also included).

Reaction	k-eff ESFR	k-eff ASTRID-like	k-eff ALFRED	Doppler ESFR -300K	Doppler ESFR +300K	Doppler ALFRED	Coolant density ESFR	Coolant density ASTRID	Coolant density ALFRED	Control rod worth ESFR
^{240}Pu (n,f)	0.57	0.50	0.55	1.44	1.68		4.61	3.24		1.09
^{238}U (n,n')	0.47	0.39	0.24	1.07	2.75	4.21	8.85	6.07	3.18	
^{238}U (n,γ)	0.29	0.28	0.22				6.10	3.75		
^{239}Pu (n,f)	0.33	0.34	0.32		1.19		19.77	11.46	1.54	
^{239}Pu ν	0.29	0.31	0.32							
^{239}Pu χ	0.32	0.30	0.22	1.21				1.85		
^{239}Pu (n,γ)				1.21	1.35		9.05	6.34		
^{241}Pu (n,f)							5.44	2.65		
^{238}U (n,f)							2.65	2.54		0.52
^{23}Na (n,γ)							6.31	3.70		
^{23}Na (n,n')							4.41	2.09		
^{23}Na elastic							2.64	1.71		
^{56}Fe elastic				1.43			7.25	3.10		0.85
^{56}Fe (n,γ)							2.86	2.16		
^{206}Pb (n,n')						2.12			4.58	
^{207}Pb (n,n')									2.38	
^{208}Pb (n,n')									1.33	
^{238}U (n,n') (n,f)	-0.34	-0.30	-0.20		-1.36		-5.60	-4.46	2.17	-0.49
^{238}U (n,n') elastic					1.74	2.45	-5.23	-3.08		
^{238}U (n,n') (n,γ)						1.76	-4.20	-2.18	1.97	
^{238}U (n,f) (n, γ)							2.53	2.26		
^{238}U (n,f) elastic							2.87	2.02		
^{238}U (n, γ) elastic							2.69			
^{239}Pu (n,f) (n, γ)							-6.93	-4.39		
^{240}Pu (n,f) (n,γ)	-0.41	-0.37	-0.41				3.35	2.42		

A detailed inspection of sensitivity profiles as well as covariance data allowed to estimate the uncertainty contribution of each energy group to the integral response uncertainty, given in Table 3. The major contributors are shaded, indicating the targeted energy groups for which an uncertainty reduction could cause a significant change in the calculated uncertainty. It can be seen that multiplication factor and reactivity effects provide complementary information. Sensitivity profiles denote the relevant energy range for each quantity: while the relevant energy range for keff is mostly centered between 100 keV and 1 MeV, for reactivity coefficients it can be shifted to a softer energy range.

The following nuclear data needs in JEFF-3.3 nuclear data library in terms of covariance data can be identified:

- ^{240}Pu fission: key role of group 2 (i.e., 2 MeV – 0.5 MeV), energy region where k-eff sensitivities are the highest for the three reactors and where relative standard deviation in 7g JEFF-3.3 COV is around 8%. Concerning sodium void scenarios, group 5 (i.e., 2 keV – 23 eV) may be also subject of uncertainty reduction. It is also important to note that this cross-section is strongly correlated to ^{240}Pu capture.
- ^{238}U inelastic: group 2 is again the main energy region of interest for the three systems, where a visible reduction is required, being uncertainty in 7g JEFF-3.3 COV around 7.5%. Additionally, for SFRs, group 1 (i.e., 19.6 MeV – 2 MeV), where the JEFF-3.3 uncertainty is around 6%, also plays a notable role. Correlations of this cross section with ^{238}U elastic, capture and fission are also relevant, contributing to an uncertainty in the integral response of at least 2%.
- ^{238}U capture: in this case, accuracy improvements for the three considered systems should be mainly focused in group 4 (i.e., 67 keV – 2 keV), where uncertainty in 7g JEFF-3.3 COV is around 2%. Additionally, for SFRs, the standard deviation of ~7% in group 1 should drop due to its impact on the sodium voiding uncertainty.
- ^{239}Pu fission: multiplication factor is strongly sensitive to this reaction for all the systems, being groups 3, 4 and 5 the main energy regions where accuracy improvements would be required. That is very challenging since both groups 3 and 4 already have a relative standard deviation below 1%; uncertainty of around 3.4% applies for group 5. This cross-section is strongly correlated to ^{239}Pu capture.
- ^{239}Pu nubar: as shown in **Erreur ! Source du renvoi introuvable.**, multiplication factor in the considered systems is mostly sensitive to this reaction. Groups 3 and 4 play a key role (relative standard deviations around 0.47%). . Then, the potential to reduce even more the associated uncertainty may be limited.
- ^{239}Pu χ: multiplication factor in all systems is mostly sensitive to ^{239}Pu χ within the group 1, for which the uncertainty is around 6%, and where a potential improvement would be required.
- ^{239}Pu capture: uncertainty in group 5 (i.e., 2 keV – 23 eV) demands an accuracy improvement due to its impact on the sodium voiding uncertainty, being in JEFF-3.3 equal to 5.6%.
- ^{241}Pu fission: it is also a reaction requested to be improved because of its impact on the sodium void uncertainty. In particular, a reduction of the uncertainty in group 5, from the present value of 4.4%, would be required.
- ^{238}U fission: an uncertainty reduction in group 1, where the relative standard deviation is around 3%, would be desirable to reduce the uncertainty in the sodium voiding of SFRs. Good correlated data with ^{238}U elastic, inelastic and capture are needed because of their impact on the uncertainty estimation.
- ^{23}Na capture: key role of group 3 (i.e., 0.5 MeV – 67 keV), responsible of an uncertainty of almost the 3% in the sodium void uncertainty. A reduction from the current JEFF-3.3 uncertainty of 98% is mandatory.
- ^{23}Na inelastic: this reaction is ranked 7th in the list of largest sensitivities of full sodium void (Table 6). An uncertainty reduction in group 2 (i.e., 2 MeV – 0.5 MeV) would be desirable.

- ^{23}Na elastic: group 4 (i.e., 67 keV – 2 keV) is the most contributing energy range of this reaction to the sodium void uncertainty.
- ^{56}Fe elastic: it requires an accuracy improvement in group 3 (i.e., 0.5 MeV – 67 keV) because of its impact on the sodium voiding uncertainty, being 4.7% its relative standard deviation in 7g JEFF-3.3 COV.
- ^{56}Fe capture: this reaction is also relevant for the sodium voiding uncertainty. In particular, group 5 (i.e., 2 keV – 23 eV) with an uncertainty of 8.6% in 7g JEFF-3.3 COV, would require a reduction.
- ^{206}Pb inelastic: an improvement in group 2 is required to meet target accuracies in Doppler and coolant density effects of LFR. The present uncertainty in 7g JEFF-3.3 COV is around 18% in this energy range.
- ^{207}Pb inelastic: again, an improvement in group 2 would be desirable due to its impact on the the coolant density uncertainty on LFR, being the uncertainty in 7g JEFF-3.3 COV around 12% in this energy range.
- ^{208}Pb inelastic: for this reaction, group 1 plays a role, being the JEFF-3.3 uncertainty around 9.4%.

Table 3. Priority list in 7-energy groups for cross-section uncertainty reduction.

Reaction	Group	k-eff ESFR	k-eff ASTRID-like	k-eff ALFRED	Doppler ESFR +300K	Doppler ALFRED	Coolant density ESFR	Coolant density ASTRID-like	Coolant density ALFRED	Control rod worth ESFR
^{240}Pu (n,f)	1	0.08	0.07	0.06	0.25		1.15	0.69		0.21
	2	0.26	0.24	0.28	0.74		4.71	2.77		0.68
	3	0.10	0.09	0.10	0.30		0.87	0.52		0.18
	4	0.12	0.10	0.11	0.37		0.10	0.14		0.05
	5	0.02	0.01	0.01	0.04		2.06	0.88		0.02
	6	0.00	0.00	0.00	0.00		0.00	0.00		0.00
	7	0.00	0.00	0.00	0.00		0.00	0.00		0.00
	NO CORR	0.31	0.28	0.32	0.92		5.34	3.04		0.73
	TOT	0.57	0.50	0.55	1.68		4.61	3.24		1.09
^{238}U (n,n’)	1	0.17	0.14	0.07	0.25	0.54	3.92	2.58	1.21	
	2	0.24	0.20	0.14	2.34	3.66	4.74	2.77	1.64	
	3	0.08	0.07	0.04	0.13	0.08	0.23	0.90	0.57	
	4	0.00	0.00	0.00	0.19	0.17	0.14	0.15	0.27	
	5	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	
	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	
	7	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	
	NO CORR	0.31	0.25	0.16	2.37	3.70	6.15	3.89	2.13	
	TOT	0.47	0.39	0.24	2.75	4.21	8.85	6.07	3.18	
^{238}U (n,γ)	1	0.01	0.01	0.00			0.11	3.27		
	2	0.08	0.08	0.07			1.98	1.74		
	3	0.12	0.12	0.10			0.90	0.27		
	4	0.22	0.21	0.17			0.69	0.02		
	5	0.05	0.06	0.03			5.18	0.00		
	6	0.00	0.00	0.00			0.01	0.00		
	7	0.00	0.00	0.00			0.00	0.00		
	NO CORR	0.27	0.26	0.21			5.66	3.71		
	TOT	0.29	0.28	0.22			6.11	3.75		
^{239}Pu (n,f)	1	0.01	0.01	0.01			0.17	0.14	0.10	
	2	0.03	0.03	0.04			0.64	0.48	0.02	
	3	0.12	0.12	0.13			1.07	0.93	0.16	
	4	0.15	0.14	0.15			0.30	0.58	0.82	
	5	0.17	0.19	0.13			19.63	11.36	1.12	
	6	0.00	0.00	0.00			0.09	0.04	0.01	
	7	0.00	0.00	0.00			0.00	0.00	0.00	
	NO CORR	0.26	0.27	0.24			19.68	11.43	1.40	
	TOT	0.33	0.34	0.32			19.77	11.46	1.54	

Table 3 (cont.). Priority list in 7-energy groups for cross-section uncertainty reduction.

Reaction	Group	k-eff ESFR	k-eff ASTRID-like	k-eff ALFRED	Doppler ESFR	Doppler ALFRED	Coolant density ESFR	Coolant density ASTRID-like	Coolant density ALFRED	Control rod worth ESFR
^{239}Pu ν	1	0.01	0.01	0.01						
	2	0.05	0.06	0.07						
	3	0.10	0.11	0.11						
	4	0.09	0.09	0.10						
	5	0.03	0.04	0.03						
	6	0.00	0.00	0.00						
	7	0.00	0.00	0.00						
	NO CORR	0.15	0.16	0.17						
	TOT	0.29	0.31	0.32						
^{239}Pu χ	1	0.19	0.18	0.12				1.10		
	2	0.05	0.04	0.02				0.29		
	3	0.08	0.07	0.06				0.43		
	4	0.01	0.01	0.01				0.04		
	5	0.00	0.00	0.00				0.00		
	6	0.00	0.00	0.00				0.00		
	7	0.00	0.00	0.00				0.00		
	NO CORR	0.21	0.20	0.14				1.21		
	TOT	0.32	0.30	0.22				1.85		
^{239}Pu (n,γ)	1						0.00	0.00		
	2						0.16	0.11		
	3						0.14	0.08		
	4						0.05	0.02		
	5						8.96	6.27		
	6						0.10	0.07		
	7						0.00	0.00		
	NO CORR						8.96	6.27		
	TOT						9.05	6.34		
^{241}Pu (n,f)	1						0.04	0.02		
	2						0.15	0.09		
	3						0.15	0.09		
	4						0.06	0.08		
	5						5.49	2.72		
	6						0.04	0.02		
	7						0.00	0.00		
	NO CORR						5.49	2.73		
	TOT						5.44	2.65		

Table 3 (cont.). Priority list in 7-energy groups for cross-section uncertainty reduction.

Reaction	Group	k-eff ESFR	k-eff ASTRID-like	k-eff ALFRED	Doppler ESFR	Doppler ALFRED	Coolant density ESFR	Coolant density ASTRID-like	Coolant density ALFRED	Control rod worth ESFR
^{238}U (n,f)	1						2.26	2.00		
	2						0.64	0.57		
	3						0.00	0.00		
	4						0.00	0.00		
	5						0.02	0.07		
	6						0.00	0.00		
	7						0.00	0.00		
	NO CORR						2.35	2.08		
	TOT						2.65	2.54		
^{23}Na (n,γ)	1						0.16	0.09		
	2						0.94	0.56		
	3						4.67	2.77		
	4						1.49	0.87		
	5						1.01	0.57		
	6						0.07	0.02		
	7						0.01	0.00		
	NO CORR						5.10	3.02		
	TOT						6.31	3.71		
^{23}Na (n,n')	1						2.35	1.05		
	2						2.93	1.44		
	3						0.02	0.02		
	4						0.00	0.00		
	5						0.00	0.00		
	6						0.00	0.00		
	7						0.00	0.00		
	NO CORR						3.76	1.78		
	TOT						4.41	2.09		
^{23}Na elastic	1						0.27	0.29		
	2						1.23	0.13		
	3						2.87	0.24		
	4						1.15	1.20		
	5						0.47	0.67		
	6						0.10	0.02		
	7						0.00	0.00		
	NO CORR						3.37	1.44		
	TOT						2.64	1.71		

Table 3 (cont.). Priority list in 7-energy groups for cross-section uncertainty reduction.

Reaction	Group	k-eff ESFR	k-eff ASTRID-like	k-eff ALFRED	Doppler ESFR	Doppler ALFRED	Coolant density ESFR	Coolant density ASTRID-like	Coolant density ALFRED	Control rod worth ESFR
^{56}Fe elastic	1						0.98	0.59		
	2						3.00	1.64		
	3						4.75	2.06		
	4						3.45	0.97		
	5						0.25	0.10		
	6						0.10	0.04		
	7						0.00	0.00		
	NO CORR						6.67	2.87		
	TOT						7.25	3.10		
^{56}Fe (n,γ)	1						0.03	0.02		
	2						0.39	0.28		
	3						0.27	0.16		
	4						0.05	0.03		
	5						2.92	2.14		
	6						0.02	0.01		
	7						0.00	0.00		
	NO CORR						2.96	2.16		
	TOT						2.86	2.16		
^{206}Pb (n,n')	1					0.18			1.48	
	2					1.95			3.15	
	3					0.00			0.00	
	4					0.00			0.00	
	5					0.00			0.00	
	6					0.00			0.00	
	7					0.00			0.00	
	NO CORR					1.95			3.48	
	TOT					2.12			4.58	
^{207}Pb (n,n')	1								0.60	
	2								1.81	
	3								0.00	
	4								0.00	
	5								0.00	
	6								0.00	
	7								0.00	
	NO CORR								1.91	
	TOT								2.38	

Table 3 (cont.). Priority list in 7-energy groups for cross-section uncertainty reduction.

Reaction	k-eff ESFR	k-eff ASTRID-like	k-eff ALFRED	Doppler ESFR	Doppler ALFRED	Coolant density ESFR	Coolant density ASTRID-like	Coolant density ALFRED	Control rod worth ESFR
^{208}Pb (n,n’)								1	1.33 2	0.00 3	0.00 4	0.00 5	0.00 6	0.00 7	0.00 NO CORR	1.33 TOT	1.33	
^{238}U (n,n’) (n,f)	-0.34	-0.30	-0.20	-1.36			-4.46	2.17	
^{238}U (n,n’) elastic				1.74	2.45		-3.08		
^{238}U (n,n’) (n,γ)					1.76		-2.18	1.97	
^{238}U (n,f) (n, γ)							2.26		
^{238}U (n,f) elastic							2.02		
^{239}Pu (n,f) (n, γ)							-4.39		
^{240}Pu (n,f) (n,γ)	-0.41	-0.37	-0.41				2.42		

3. Target Accuracy Assessment: Methodology

A TAR exercise has been carried out to identify the required uncertainty reduction in JEFF-3.3 covariance data so that the integral responses can fulfil the target accuracies. The JEFF-3.3 covariance matrix in 7 energy groups processed with NJOY2016.69 code has been used.

The methodology is based on the "inverse problem" which objective is to calculate the uncertainties of nuclear data minimizing an "objective function" with some constraints.

The "objective function" to be minimized can be defined as follows:

$$\boldsymbol{Min}\left(\sum_i \frac{\lambda_i}{(\Delta x_i)^2}\right), \boldsymbol{i} = \mathbf{1}, \dots, \boldsymbol{I} \qquad \text{(Eq. 1)}$$

where:

λ_i : cost parameter related with the cost of each cross-section to be measured with high-precision absolute measurement

Δx_i : cross-section uncertainty (i.e. standard deviation) to be minimized

I : total number of reactions-energy

- Isotopes/Materials: ^{52}Cr, ^{56}Fe, ^{58}Ni, ^{235}U, ^{238}U, ^{239}Pu…. + coolant, …others
- Reactions: σ_{cap}, σ_{fiss}, ν, σ_{el}, σ_{inel}, PFNS and elastic-μ, ...
- Energy groups: 7

The constraints can be defined as follows:

- Cross-section uncertainty constraints: Mathematically, $\Delta x_i \geq 0; i = 1 \dots I$, that is, a positive standard deviation is required
- TAR constraints. If we define R_n^T as the target accuracy on the N-integral parameters, then:

$$\sum_i \boldsymbol{S_{ni}^2} \cdot (\Delta \boldsymbol{x_i})^2 + \sum_{ii'} \boldsymbol{S_{ni}} \cdot (\Delta \boldsymbol{x_i})^2 \cdot \boldsymbol{corr_{ii'}} \cdot (\Delta \boldsymbol{x_{i'}})^2 \cdot \boldsymbol{S_{ni'}^+} \leq (\boldsymbol{R_n^T})^2 \qquad ; \boldsymbol{n} = \mathbf{1} \dots \boldsymbol{N} \qquad \text{(Eq. 2)}$$

where:

S_{ni} : Sensitivity coefficient for the integral parameter R_n
$corr_{ii'}$: Correlation between energy-reaction cross-section i an i'

Note that in the optimization problem in Eq. 2, the full set of cross-sections should strictly be taken into account since no additional terms corresponding to the contribution to the uncertainty of unselected cross-sections are included. Note also that correlations are considered unlike the optimization performed in WPEC/SG26, in which correlations were not taken into account. Considering correlations impose tighter uncertainties on the nuclear data, as correlations increase in most cases the total uncertainty (see [Palmiotti, 2011a, 2011b]). An analysis of the limitations of the proposed methodology can be found in [Cabellos, 2023].

3.1. Solver and constraints used

TAR calculations have been performed using the solver DONLP2 (Spelluci P., 19982) based on a SQP (sequential quadratic programming) method.

The objective function has been constrained in practice to the following boundary conditions:

- $\Delta x_{i0} \geq \Delta x_i \geq \Delta x_{i\,lim}; i = 1 \ldots K$ where Δx_{i0} is the initial/current uncertainty value and $\Delta x_{i\,lim}$ is the minimum physical uncertainty achievable (it may be assumed that a higher precision absolute measurement is not feasible). $\Delta x_{i\,lim}$ has been set to 0.2% in this TAR exercise. However, for certain reactions, a higher value should be considered.
- If $\Delta x_{i0} \geq 100\% \Rightarrow \Delta x_{i0} = 100\%$
- If $\Delta x_{i0} = 0\% \quad \Rightarrow \Delta x_{i0} = 10\%$

To prevent very low uncertainty values resulting from the TAR exercise, an additional constraint could be imposed on certain crucial reactions, restricting their minimum uncertainties to the lowest values in current standards[3]. Table 4 shows the values that could be used as an additional constraint for fission cross section of main isotopes.

Table 4. Collapsed standards uncertainties (in %) of ^{235}U, ^{238}U and ^{239}Pu (n,fission)

Group #	Lower Energy (eV)	Upper Energy (eV)	235U (n,fission)	238U (n,fission)	239Pu (n,fission)
1	$2.23130\ 10^{6}$	$1.96403\ 10^{7}$	0.45	0.50	0.50
2	$4.97871\ 10^{5}$	$2.23130\ 10^{6}$	0.43	0.59	0.48
3	$6.73795\ 10^{4}$	$4.97871\ 10^{5}$	0.45	0.76	0.51
4	$2.03468\ 10^{3}$	$6.73795\ 10^{4}$	0.45	-	0.52
5	$2.26033\ 10^{1}$	$2.03468\ 10^{3}$	0.48	-	0.55
6	$5.40000\ 10^{-1}$	$2.26033\ 10^{1}$	0.42	-	0.20
7	$1.40000\ 10^{-5}$	$5.40000\ 10^{-1}$	0.20	-	0.20

3.2. Sets of values for cost parameters

Table 5 shows the values for cost parameters (λ_i) related to each type of cross–section and/or nuclear data used in this work. These set of values could be also energy dependent; however in this study, the same values for the full energy range have been assumed. Note that Set A corresponds to using λ =1 for all reactions, while Set B and C can apply different cost parameters for different cross sections and isotopes.

Table 5. Sets of values for the cost parameters ("λ_i")

	cost parameters ("λ_i")		
Isotopes and reactions	Set A	Set B	Set C
^{235}U, ^{238}U and ^{239}Pu – capture, fission, nubar(ν)	1	1	1
Other fuel isotopes – capture, fission, nubar(ν)	1	2	2
Non-fuel isotopes – capture	1	1	1

[2] Reference: P. Spellucci, "An SQP method for general nonlinear programs using only equality constrained subproblems". Math. Program. 82, 413–448 (1998)

[3] 2017 IAEA Neutron data standards

All isotopes – elastic scattering	1	1	1
All isotopes – inelastic scattering	1	3	10

3.3. Cases

Two TAR exercises have been performed: one with correlations (as recommended in WPEC-SG46) and one without correlations (as performed in WPEC-SG26). Concerning the exercise with correlations (SG46), two cases were analyzed:

- Firstly, a full set of parameters were considered: 14 MATs/9MTs/7g = 882 variables
    - MATS=b-10, o-16, na-23, cr-52, fe-56, ni-58, pb-206, pb-207, pb-208, u-235, u-238, pu-239, pu-240, pu-241
    - MTs= (n,elastic), (n,inelastic), (n,gamma), (n,p), (n,alpha), (n,elastic-P1), (n,fission), nubar, chi
- Secondly, a reduced set of parameters, accounting for around 98% of the total uncertainty, was selected.

In both scenarios, equivalent results were obtained with the optimization solver, demonstrating that the selection of the most relevant parameters enables obtaining reliable outcomes while mitigating convergence issues in solving the optimization problem.

4. TAR results

4.1. Individual TAR results

A summary of results for the TAR exercise *per system and integral response* is shown in Tables 6 to 8. It can be seen that:

- The cost parameters (the same value for the full energy range) impact largely on the required uncertainty reduction to satisfy the TAR constraints, suggesting that if different cost parameters were chosen for different energy groups, results would be modified.
- The consideration of correlations greatly affects the required reduction, generally imposing stricter requirements than when no correlations are considered.
- Examining integral responses other than k-eff allows us to determine the necessary uncertainty reduction in cross sections that are no so significant in k-eff analysis. Examining the Doppler effect following a temperature increase and decrease enables establishing the target accuracy in different cross sections or energy groups.

Table 6. Summary of TAR exercise per integral response in ALFRED system

JEFF-3.3					SG26 -No correlations				SG46 - with correlations		
Keff					A	B	C		A	B	C
Reaction			EG	Current (%)	Target (%)	Target (%)	Target (%)		Target (%)	Target (%)	Target (%)
pu-240	-	fission	2	8.4	1.2	1.4	1.4		1.1	1.3	1.8
pu-240	-	fission	4	25.4	3.5	4.0	3.9		2.3	2.7	4.3
pu-240	-	fission	3	14.9	2.8	3.2	3.1		2.0	2.3	6.8
u-238	-	n,gamma	4	2.0	0.8	0.8	0.7		0.5	0.5	0.6
Coolant density reactivity					A	B	C		A	B	C
Reaction			EG	Current (%)	Target (%)	Target (%)	Target (%)		Target (%)	Target (%)	Target (%)
pb-206	-	inelastic	2	18.1	1.2	1.4	1.7		1.0	1.2	1.5
pb-206	-	inelastic	1	9.1	1.3	1.6	2.0		1.1	1.3	1.6
pb-207	-	inelastic	2	12.2	1.3	1.6	1.9		1.1	1.4	1.7
Doppler reactivity					A	B	C		A	B	C

Reaction			EG	Current (%)	Target (%)	Target (%)	Target (%)		Target (%)	Target (%)	Target (%)
u-238	-	inelastic	2	7.4	2.2	2.4	2.9		1.5	1.8	2.2
pb-206	-	inelastic	2	18.1	4.0	5.2	5.9		3.0	4.4	5.1

Table 7. Summary of TAR exercise per integral response in ASTRID system

JEFF-3.3					SG26 -No correlations				SG46 - with correlations		
keff					A	B	C		A	B	C
Reaction			EG	Current (%)	Target (%)	Target (%)	Target (%)		Target (%)	Target (%)	Target (%)
u-238	-	n,gamma	4	2.0	0.7	0.7	0.6		0.4	0.4	0.4
pu-240	-	fission	2	8.4	1.3	1.5	1.5		1.1	1.3	1.3
u-238	-	inelastic	2	7.4	1.3	1.7	2.2		1.0	1.2	1.6
Full void reactivity					A	B	C		A	B	C
Reaction			EG	Current (%)	Target (%)	Target (%)	Target (%)		Target (%)	Target (%)	Target (%)
pu-239	-	fission	5	3.4	1.3	1.4	1.3		1.4	1.3	1.3
pu-239	-	n,gamma	5	5.6	2.3	2.3	2.2		2.6	2.3	2.2

Table 8. Summary of TAR exercise per integral response in ESFR-SMART

JEFF-3.3					SG26 -No correlations				SG46 - with correlations		
keff					A	B	C		A	B	C
Reaction			EG	Current (%)	Target (%)	Target (%)	Target (%)		Target (%)	Target (%)	Target (%)
u-238	-	n,gamma	4	2.0	0.7	0.6	0.6		0.4	0.4	0.4
pu-240	-	fission	2	8.4	1.3	1.4	1.4		1.1	1.3	1.2
u-238	-	inelastic	2	7.4	1.2	1.5	2.0		0.9	1.1	1.4
Full void reactivity					A	B	C		A	B	C
Reaction			EG	Current (%)	Target (%)	Target (%)	Target (%)		Target (%)	Target (%)	Target (%)
pu-239	-	fission	5	3.4	0.7	0.6	0.6		0.8	0.7	0.7
Doppler reactivity (up)					A	B	C		A	B	C
Reaction			EG	Current (%)	Target (%)	Target (%)	Target (%)		Target (%)	Target (%)	Target (%)
u-238	-	inelastic	2	7.4	3.5	4.1	4.8		3.2	3.6	4.5
Doppler reactivity (down)					A	B	C		A	B	C
Reaction			EG	Current (%)	Target (%)	Target (%)	Target (%)		Target (%)	Target (%)	Target (%)
fe-56	-	elastic	4	6.0	4.0	4.6	4.9		3.9	4.1	3.9
u-238	-	inelastic	3	9.1	5.5	9.0	-		5.8	7.0	8.4

A summary of results for the TAR exercise *per reaction* is shown in Table 9, with the most limiting case shaded in the table.

Table 9. Summary of TAR exercise per reaction

JEFF-3.3						Using correlations			Individual integral response considered
						A	B	C	
Reaction			EG	Current (%)		Target (%)	Target (%)	Target (%)	
u-238	-	inelastic	2	7.4		1.5	1.8	2.2	ALFRED – Doppler reactivity
						1.0	1.2	1.6	ASTRID - keff
						0.9	1.1	1.4	ESFR - keff
						3.2	3.6	4.5	ESFR – Doppler reactivity
u-238	-	inelastic	3	9.1		5.8	7.0	8.4	ESFR – Doppler reactivity
u-238	-	n,gamma	4	2.0		0.5	0.5	0.6	ALFRED -keff
						0.4	0.4	0.4	ASTRID -keff
						0.4	0.4	0.4	ESFR - keff
pu-239	-	fission	5	3.4		1.4	1.3	1.3	ASTRID – Full void reactivity
						0.8	0.7	0.7	ESFR – Full void reactivity
pu-239	-	n,gamma	5	5.6		2.6	2.3	2.2	ASTRID – Full void reactivity
pu-240	-	fission	2	8.4		1.1	1.3	1.8	ALFRED -keff
						1.1	1.3	1.3	ASTRID - keff
						1.1	1.3	1.2	ESFR -keff
pu-240	-	fission	3	14.9		2.0	2.3	6.8	ALFRED -keff
pu-240	-	fission	4	25.4		2.3	2.7	4.3	ALFRED -keff
pb-206	-	inelastic	1	9.1		1.1	1.3	1.6	ALFRED – coolant density reactivity
pb-206	-	inelastic	2	18.1		1.0	1.2	1.5	ALFRED – coolant density reactivity
						3.0	4.4	5.1	ALFRED – Doppler reactivity
pb-207	-	inelastic	2	12.2		1.1	1.4	1.7	ALFRED – coolant density reactivity
fe-56	-	elastic	4	6.0		3.9	4.1	3.9	ESFR - Doppler reactivity

4.2. Joint TAR results

A joint optimization, taking into account jointly different systems or different integral responses of one system has been performed and results compared to the ones provided by the individual optimization problems.

Table 10. Joint ALFRED-ASTRID-ESFR TAR exercise for k-eff. Top reactions

JEFF-3.3					SG26 -No correlations				SG46 - with correlations		
keff					A	B	C		A	B	C
Reaction			EG	Current (%)	Target (%)	Target (%)	Target (%)		Target (%)	Target (%)	Target (%)
pu-240	-	fission	2	8.4	1.2	1.0	1.4		1.1	1.2	1.2
pu-240	-	fission	4	25.4	3.1	3.6	3.5		2.2	2.5	2.4
u-238	-	n,gamma	4	2.0	0.7	0.7	0.6		0.4	0.4	0.4
pu-240	-	fission	3	14.9	2.5	3.0	2.9		1.9	2.2	2.1
pu-239	-	fission	4	1.0	0.5	0.5	0.5		0.3	0.3	0.3
u-238	-	inelastic	2	7.4	1.3	1.7	2.0		1.0	1.2	1.5
pu-240	-	n,gamma	4	7.2	1.8	1.4	2.2		1.5	1.8	1.7
pu-239	-	chi	1	5.5	1.2	1.2	1.1		0.7	0.3	0.7
pu-240	-	fission	1	6.3	2.0	2.2	2.3		1.5	1.7	1.6
pu-239	-	n,gamma	4	3.1	1.5	1.4	1.4		0.6	0.6	0.6

Table 11. Joint ALFRED-ASTRID-ESFR TAR exercise for k-eff: main contributions per system

JEFF-3.3					SG26 - No correlations				SG46 - with correlations		
ALFRED - keff					A	B	C		A	B	C
Reaction			EG	Current (%)	Target (%)	Target (%)	Target (%)		Target (%)	Target (%)	Target (%)
pu-240	-	fission	2	8.4	1.2	1.4	1.4		1.1	1.3	1.8
pu-240	-	fission	4	25.4	3.5	4.0	3.9		2.3	2.7	4.3
pu-240	-	fission	3	14.9	2.8	3.2	3.1		2.0	2.3	6.8
u-238	-	n,gamma	4	2.0	0.8	0.8	0.7		0.5	0.5	0.6

JEFF-3.3					SG26 - No correlations				SG46 - with correlations		
ASTRID - keff					A	B	C		A	B	C
Reaction			EG	Current (%)	Target (%)	Target (%)	Target (%)		Target (%)	Target (%)	Target (%)
u-238	-	n,gamma	4	2.0	0.7	0.7	0.6		0.4	0.4	0.4
pu-240	-	fission	2	8.4	1.3	1.5	1.5		1.1	1.3	1.3
u-238	-	inelastic	2	7.4	1.3	1.7	2.2		1.0	1.2	1.6
pu-240	-	fission	4	25.4	3.6	4.1	4.0		2.3	2.7	2.7
pu-240	-	fission	3	14.9	2.9	3.3	3.2		2.0	2.4	2.3

JEFF-3.3					SG26 - No correlations				SG46 - with correlations		
ESFR/SMART - keff					A	B	C		A	B	C
Reaction			EG	Current (%)	Target (%)	Target (%)	Target (%)		Target (%)	Target (%)	Target (%)
u-238	-	n,gamma	4	2.0	0.7	0.6	0.6		0.4	0.4	0.4
pu-240	-	fission	2	8.4	1.3	1.4	1.4		1.1	1.3	1.2
u-238	-	inelastic	2	7.4	1.2	1.5	2.0		0.9	1.1	1.4
pu-240	-	fission	4	25.4	3.4	3.6	3.5		2.1	2.5	2.4
pu-240	-	fission	3	14.9	2.8	3.1	3.0		1.9	2.2	2.2

Table 12. Joint keff + SVR + Doppler TAR exercise for ESFR

JEFF-3.3					SG26 - No correlations				SG46 - with correlations		
keff + reactivity coefficients					A	B	C		A	B	C
Reaction			EG	Current (%)	Target (%)	Target (%)	Target (%)		Target (%)	Target (%)	Target (%)
pu-240	-	fission	2	8.4	1.3	1.4	1.4		1.1	1.2	1.2
u-238	-	n,gamma	4	2.0	0.7	0.7	0.6		0.4	0.4	0.4
u-238	-	inelastic	2	7.4	1.2	1.5	2.0		0.9	1.1	1.4
u-238	-	inelastic	1	5.7	1.3	1.6	2.1		1.0	1.2	1.5
pu-239	-	chi	1	5.5	1.2	1.2	1.1		0.7	0.7	0.7
pu-240	-	fission	4	25.4	3.3	3.6	3.6		2.2	2.5	2.5
pu-240	-	fission	3	14.9	2.8	3.1	3.0		1.9	2.2	2.2
pu-240	-	fission	1	6.3	2.0	2.3	2.2		1.5	1.7	1.6
u-238	-	inelastic	3	9.1	2.5	3.1	4.0		1.3	1.7	2.2
pu-239	-	fission	4	1.0	0.6	0.5	0.5		0.4	0.3	0.3
pu-239	-	fission	5	3.4	0.8	0.7	0.7		0.7	0.7	0.7
fe-56	-	elastic	4	6.0	2.7	2.5	2.4		3.6	3.4	3.3

Table 13. Top contributions per system

JEFF-3.3					SG26 - No correlations				SG46 - with correlations		
keff					A	B	C		A	B	C
Reaction			EG	Current (%)	Target (%)	Target (%)	Target (%)		Target (%)	Target (%)	Target (%)
u-238	-	n,gamma	4	2.0	0.7	0.6	0.6		0.4	0.4	0.4
pu-240	-	fission	2	8.4	1.3	1.4	1.4		1.1	1.3	1.2
u-238	-	inelastic	2	7.4	1.2	1.5	2.0		0.9	1.1	1.4
Full void reactivity					A	B	C		A	B	C
Reaction			EG	Current (%)	Target (%)	Target (%)	Target (%)		Target (%)	Target (%)	Target (%)
pu-239	-	fission	5	3.4	0.7	0.6	0.6		0.8	0.7	0.7
Doppler reactivity (up)					A	B	C		A	B	C
Reaction			EG	Current (%)	Target (%)	Target (%)	Target (%)		Target (%)	Target (%)	Target (%)
u-238	-	inelastic	2	7.4	3.5	4.1	4.8		3.2	3.6	4.5
Doppler reactivity (down)					A	B	C		A	B	C
Reaction			EG	Current (%)	Target (%)	Target (%)	Target (%)		Target (%)	Target (%)	Target (%)
fe-56	-	elastic	4	6.0	4.0	4.6	4.9		3.9	4.1	3.9
u-238	-	inelastic	3	9.1	5.5	9.0	-		5.8	7.0	8.4

4.3. Conclusions TAR Exercise

Table 14. Summary and conclusion of current ND uncertainties and uncertainty reduction requirements

	Above Threshold Fertile 2.23 10^6 eV - 1.96 10^7 eV	Above Threshold Inelastic 4.98 10^5 eV - 2.23 10^6 eV	Continuum to URR 6.74 10^4 eV - 4.98 10^5 eV	URR 2.03 10^3 eV - 6.74 10^4 eV	RRR 2.26 10^1 eV - 2.03 10^3 eV	EPITHERMAL 5.4 10^{-1} eV - 2.26 10^1 eV	THERMAL 1.0 10^{-5} eV - 5.40 10^{-1} eV	HRPL entry number for the reaction (https://oecd-nea.org/dbdata/hprl/)
Reaction	IG=1	IG=2	IG=3	IG=4	IG=5	IG=6	IG=7	
U-238 (n, gamma)	-	-	-	0.4% - 0.6%	-	0.9%	0.6%	
U-238 (n, inelastic)	0.9% - 1.3%	0.9% - 1.5%	5.8% - 8.4%	-	-	-	-	18H (2%)
Pu-239 (n, inelastic)	-	4.4% - 7.0%	-	-	-	-	-	
Pu-239 (n, gamma)	-	-	-	0.8% - 1.5%	2.2% - 2.6%	-	-	32H (3%RRR, 3%% URR)
Pu-239 (n, fission)	-	**0.3% - 0.4%***	**0.2% - 0.3%***	**0.2% - 0.3%***	0.6% - 0.7%	-	-	*Below standards uncertainties
Pu-240 (n, fission)	-	1.1% - 1.8%	2.0% - 6.8%	2.3% - 6.8%	-	-	-	37H (2-3% SFR)
Pb-206 (n, inelastic)	1.1% - 1.6%	1.0% - 1.5%	-	-	-	-	-	41H (5% LFR)
Pb-207 (n, inelastic)	-	1.0% - 1.5%	-	-	-	-	-	42H (5%-LFR)
Fe-56 (n, elastic)	-	-	4.8% - 7.2%	3.9% - 4.1%	-	-	-	
Fe-56 (n, inelastic)	-	1.2% - 1.8%	-	-	-	-	-	34H (2%-ADMAB)
Na-23 (n, elastic)			2.6% - 3.1%	3.9% - 4.0%				
Na-23 (n, inelastic)	2.0% - 2.4%	1.3% - 2.0%	-	-	-	-	-	ID29 (4%)
O-16 (n, elasticP1)	-	5.2% - 6.5%	-	-	-	-	-	
U-238 (n, elasticP1)	-	3.2% - 3.6%	3.8% - 4.9%	-	-	-	-	

5. Conclusions: comparison to HPRL

A priority list covering the uncertainty reduction requirements needed to meet integral parameters target accuracies for ALFRED, ASTRID and ESFR was presented. These needs mostly focused on ^{238}U, ^{239}Pu, ^{240}Pu and ^{241}Pu cross sections as well as few structural and coolant nuclides such as ^{56}Fe, ^{23}Na and ^{206}Pb, ^{207}Pb, ^{208}Pb. The study pointed out the importance of considering different integral parameters since they might provide complementary information in terms of energy ranges to be targeted.

Then, a TAR exercise aiming at quantifying nuclear data needs (in terms of uncertainty reduction) to meet target accuracies on specific integral parameters was performed, using JEFF-3.3 covariance data. Results showed:

- There is a large impact of the non-linear optimization solver to predict the uncertainty reduction. There is then a necessity of a robust methodology to define TAR values in order to establish well defined priorities and quantitative goals, for all the systems of potential interest. This methodology should give a clear indication of which are the key integral parameters of interest for the different reactor cores and, possibly, for the fuel cycle.
- Taking into account correlation terms, TAR assessment produces very stringent requirements in nuclear data (evolution from SG26 to SG46 methodology). On the other hand, individual or joint TAR assessments produce similar results.

Finally, the TAR exercise is able to provide the justification for the uncertainty reduction which is required to feed new entries on nuclear data needs in NEA/HPRL. Concerning the analyzed advanced reactors, the work identified a total of 11 potential new or updated entries to feed HPRL.

- Updated entries in HPRL with tighter uncertainty reduction are:
    - U-238 (n, inelastic): ALFRED - Coolant density reactivity / ESFR -keff
    - Pu-239 (n, gamma): ALFRED -keff
    - Pu-240 (n, fission): ESFR -keff
    - Pb-206 (n, inelastic): ALFRED – coolant density reactivity
    - Pb-207 (n, inelastic): ALFRED – coolant density reactivity
    - Fe-56 (n, inelastic): ALFRED – coolant density reactivity + JSFR - keff
    - Na-23 (n, inelastic): ESFR - Full void reactivity
- New entries in HPRL:
    - Pu-239 (n,inelastic) : ALFRED – Doppler reactivity
    - Fe-56 (n,elastic) : ESFR – Doppler reactivity
    - Na-23 (n,elastic) in JSFR -SVR
- One reaction is identified as very challenging since the required uncertainty reduction exceeds the standards evaluation (given in Table 4):
    - Pu-239 (n, fission) requires around 0.2-0.3% to meet the target accuracies in ALFRED - keff / ESFR – Full void reactivity
    - An attempt was made to include the standards uncertainty constraints specified in Table 4 into the TAR problem. It was shown that, in this scenario, the solver predicts a substantial reduction in other cross-section uncertainties to constrain the Pu-239 (n,fission) uncertainty to 0.5%.

It is worth to note that this work indicates a reduction in the uncertainty of general-purpose nuclear data libraries in accordance with the constraints imposed in this exercise for the analyzed applications or designs. However, if this exercise were to be repeated using information from integral experiments (ICSBEP or IRPHEP) with great similarity to the applications, it would be foreseeable that the reduction of these uncertainties may not be as strong, as this reduction would be dictated by the similarity of these integral experiments. We propose to carry out this analysis in the proposal APRENDE (Addressing PRiorities of Evaluated Nuclear Data in Europe).

6. Acknowledgements

SCALE6.3 beta version has been provided by Oak Ridge National Laboratory. The ESFR model has been obtained through the HORIZON2020 EU ESFR-SMART project (number 754501), while ASTRID-like and ALFRED models through the 7th FP EU ESNII plus project (number 605172).

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Appendix 1. Seven energy groups structure

The seven energy group structure results from an inspection of the energy structure of the main reactions and accounts as far as possible for some physical features of the cross-section energy shapes that could also be associated to specific experimental techniques:

- The first energy group (band) includes most of the plateau in energy of threshold fission reactions and high energy inelastic continuum
- The second band includes most discrete levels inelastic processes
- The third band includes reactions above the unresolved resonance energy range
- The fourth band represents the transition energy range between unresolved and resolved resonance ranges
- The fifth band covers the resolved resonance range
- The sixth band covers the energy range of the large actinide resonances
- The seventh band covers most of the thermal energy range

Seven energy groups structure (eV)

Group	Upper Energy
1	$1.96403\ 10^{7}$
2	$2.23130\ 10^{6}$
3	$4.97871\ 10^{5}$
4	$6.73795\ 10^{4}$
5	$2.03468\ 10^{3}$
6	$2.26033\ 10^{1}$
7	$5.40000\ 10^{-1}$

Annex C

[SANDA/WP5/T1/Other] LWR/UOx loss of reactivity versus burnup

[CEA, A. Rizzo & D. Bernard]

A new study is made here to try to give some insights to JEFF-4.0tx libraries, namely for depletion studies, since the reactivity modification from JEFF-3.1.1 and the latest JEFF-4.0t2 is reaching about -1000 pcm for a 50 GWd/t_{HM} LWR/UOx spent fuel. This new study concerns the uncertainty of such a reactivity loss between 40 GWd/t_{HM} and fresh fuel through pin cell direct sensitivity calculations (owing to a deterministic discretization of the Boltzmann/Bateman equations) and the use of various 26 energy-group covariance matrices: (see Table 2 for sensitivity values and Table 3 for uncertainty values)

Table 2. Sensitivities of LWR/UOx 40GWd/t_{HM} reactivity loss to major nuclear data [pcm/%]:

Incident Energy Group	^{239}Pu		^{241}Pu	
	(n,γ)	(n,f)	(n,γ)	(n,f)
1 (4.966 – 19.64 MeV)	-0.02	-0.76	0.02	-0.09
2 (2.223 – 4.966 MeV)	-0.23	-2.09	-0.07	-0.53
3 (1.337 – 2.223 MeV)	-0.07	-1.95	-0.02	-0.28
4 (0.494 – 1.337 MeV)	0.18	-2.91	0.34	-0.83
5 (195.0 – 494.0 keV)	0.25	-1.49	0.39	-0.18
6 (67.4 – 195.0 keV)	0.48	-1.15	-0.07	-0.34
7 (25.0 – 67.4 keV)	0.46	-0.96	-0.18	-0.28
8 (9.118 – 25.0 keV)	0.50	-0.73	0.11	-0.25
9 (1.910 – 9.118 keV)	1.84	-1.54	0.30	-0.71
10 (410.8 eV – 1.91 keV)	3.92	-4.04	0.53	-1.51
11 (52.67 – 410.8 eV)	16.20	-20.05	2.34	-5.37
12 (4.000 – 52.67 eV)	34.35	-34.35	14.84	-24.87
13 (1.250 – 4.000 eV)	1.19	-4.02	0.46	-2.20
14 (1.148 – 1.250 eV)	0.16	-0.46	-0.02	-0.23
15 (1.104 – 1.148 eV)	0.30	0.11	-0.23	-0.34
16 (1.009 – 1.104 eV)	-0.05	-0.32	0.09	-0.18
17 (0.964 – 1.009 eV)	-0.16	-0.37	-0.21	-0.14
18 (880.0 – 964.0 eV)	0.16	**-1.06**	-0.21	-0.55
19 (625.0 – 880 meV)	**2.55**	**-5.19**	0.23	**-1.51**
20 (353.0 – 625.0 meV)	**45.38**	**-54.26**	**3.74**	**-3.72**
21 (231.2 – 353.0 meV)	**203.00**	**-205.04**	**24.32**	**-25.49**
22 (138.0 – 231.2 meV)	**135.09**	**-145.27**	**32.65**	**-45.08**
23 (76.5 – 138.0 meV)	**93.49**	**-126.21**	**24.57**	**-41.00**
24 (34.4 – 76.5 meV)	**72.84**	**-119.39**	**24.16**	**-39.16**
25 (10.5 – 34.4 meV)	**35.79**	**-66.12**	**16.20**	**-22.90**
26 (1.00 – 10.5 meV)	**7.98**	**-14.36**	**4.15**	**-5.55**
SUM	**655.59**	**-813.96**	**148.44**	**-223.30**

Table 3. Main contributors to 40 GWd/t_{HM} LWR/UOx reactivity loss uncertainty [pcm]@1σ

COMAC-V2.1		JEFF-4.0t1		ENDF/B-VIII.0	
^{239}Pu(n,γ)	**381**	**^{241}Pu(n,γ)**	**469**	**^{239}Pu(n,γ)**	**848**
^{238}U(n,γ)	**193**	**^{239}Pu(n,γ)**	**381**	^{239}Pu(n,f)	386
χ(^{241}Pu)	**177**	**ν(^{239}Pu)**	**286**	ν(^{235}U)	215
^{239}Pu(n,f)	**171**	**ν(^{235}U)**	**263**	^{238}U(n,γ)	200
χ(^{239}Pu)	169	χ(^{239}Pu)	214	ν(^{239}Pu)	191
ν(^{235}U)	137	^{16}O(n,n)	205	χ(^{239}Pu)	117
^{241}Pu(n,f)	105	^{238}U(n,γ)	193	^{241}Pu(n,f)	105
^{241}Pu(n,γ)	103	χ(^{241}Pu)	177	^{241}Pu(n,γ)	103
ν(^{241}Pu)	99	^{239}Pu(n,f)	171	^{1}H(n,n)	95
^{242}Pu(n,γ)	85	^{241}Pu(n,f)	138	^{242}Pu(n,γ)	85
^{238}U(n,f)	83	^{235}U(n,f)	120	^{235}U(n,f)	72
^{1}H(n,n)	81	^{150}Sm(n,γ)	107	ν(^{238}U)	53
^{147}Pm(n,γ)	77	ν(^{241}Pu)	99	^{238}U(n,f)	43
^{235}U(n,f)	63	^{1}H(n,n)	95	χ(^{235}U)	43
^{235}U(n,γ)	58	χ(^{235}U)	90	^{236}U(n,γ)	41
…	…	…	…	…	…
TOTAL	617	TOTAL	901	TOTAL	1036

In the table, the quadratic sum of bold values represents 80% of the overall uncertainty for each given library.

Depending on covariances libraries, total uncertainties are reaching from ±600 to ±1000 pcm, *i.e.* it is more or less consistent @1σ with the JEFF-4.0t2 to JEFF-3.1.1 difference of reactivity loss calculations. The main contributors to the overall uncertainty are $^{239+241}$Pu neutron induced cross sections, ν_{tot} and PFNS but their ranking differs from a covariance matrix to another one.

Correlation analysis:
The weight of the correlations is estimated by comparing full matrices propagation and partially diagonal matrices propagation (inter- and intra-reaction correlations for a given isotope are reduced to zero). This gives respectively 50% of the overall uncertainty (±495 and ±505 pcm for JEFF-4.0t1 and ENDF/B-VIII.0 libraries). Now if we cancel inter-reaction correlations only (reducing covariances to a block diagonal matrix), we find the same results as presented in the table 3. To summarize, except if inter-reaction correlations are sparse or low, the intra-reaction correlations are responsible for half of the overall uncertainty. These intra-reaction correlations come from two parts: on one hand, they originate from the nuclear reaction model used (R-Matrix for instance) and are therefore model-dependent (the phenomenological R-Matrix formalism linking energy ranges from one resonance to another one via amplitude elements, the neutron wave number and the fixed channel radius). On the other hand, correlations come from experimental data itself. For instance, the "normalization" value (total amount of targeted atoms in ToF measurements) correlates all concerned incident energies. Thus, a way to improve half of the total uncertainty is to perform better nuclear reaction models, *e.g.*, decrease the number of degrees of freedom into nuclear physics and to perform better experimental targets.

Uncertainty analysis:

As $^{238}U(n,\gamma)$ uncertainty is rather low, it seems that there is no improvement that can be further expected (maybe we already reached the lower value of uncertainty of Γ_γ by Time-Of-Flight technique measurements). Nevertheless, ^{239}Pu and ^{241}Pu covariances are rather different comparing ENDF/B-VIII.0 and JEFF-4.0t1. Indeed,

- the $^{239}Pu(n,\gamma)$ uncertainty seems a bit pessimistic for ENDF/B-VIII.0: ±4 to ±4.5% for the left wing of the first resonance, to be compared with a reduced yet still important reactivity-loss using JEFF-4.0t1 of ±2.5% thanks to integral (but analytic) measurement feedbacks (MINERVE/CERES oscillation measurements).
- the $^{241}Pu(n,\gamma)$ uncertainty seems very optimistic and thus unrealistic for such a fissile nucleus for ENDF/B-VIII.0: ±2% for the first resonance, to be compared with a more realistic (yet maybe slightly pessimistic) one for JEFF-4.0t1: ±10%, but surprisingly without negative correlation between capture and fission.

To conclude, JEFF-4.0t1 presents reduced uncertainties for ^{239}Pu and (compared to ENDF/B-VIII.0) a more realistic one for ^{241}Pu but surprisingly without correlation between capture and fission for the latter. Beyond new analyses on the major ^{239}Pu, the ^{241}Pu actinide could lead to a better understanding of a significant portion (1/3rd to one half?) of the drift of the reactivity loss with burnup as observed with recent JEFF-4.0tX libraries. More specifically, a decrease of the ^{241}Pu resonant capture cross section combined to a slight increase of its fission cross section (with its estimated -0.4 anticorrelated coefficient to capture cross section, *i.e.* through transmission measurements full analyses) will together go into the right direction to reduce the reactivity loss versus burnup. Unfortunately, applying χ^2 minimization to C/E of LWR/PIE analyses for plutonium amount shows the opposite for $^{241}Pu(n,\gamma)$ cross section.

Finally, as discussed in [SANDA/WP5/T5.2], here are the two clear trends owing to C/E validation:

- JEFF-4.0t1/$^{241}Pu(n_{[0.1\text{-}0.54]eV},\gamma)$ ~ (+1.0±3.1)% (the *a priori* uncertainty was ±5.0%),
- JEFF-4.0t1/$^{240}Pu(n_{[0.1\text{-}0.54]eV},\gamma)$ ~ (+0.3±2.2)% (the *a priori* uncertainty was ±3.0%).

These *posterior* uncertainties (reported in Table 1 in body text of the main document) have to be understood as Target Accuracy Requirements to reach experimental uncertainties of LWR/PIE analyses.