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WPEC/SG46 Exercise on Target Accuracy Requirement

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Abstract. Recently, a second Target Accuracy Requirements (TAR) exercise is launched in the framework of the WPEC/S46 on "*Efficient and Effective Use of Integral Experiments for Nuclear Data Validation*". The TAR exercise aims at quantifying nuclear data needs, in terms of uncertainty reduction, to meet target accuracies on specific integral parameters. These target accuracies are driven by reactor and fuel cycle design. The goal is to provide the NEA/HPRL with new requirements of "nuclear data uncertainty reduction"

1 Introduction. The legacy work – WPEC/SG26

The first TAR exercise was performed at NEA in the period 2005-2008 within the framework of WPEC/SG26 on "*Uncertainty and target accuracy assessment for innovative systems using recent covariance data evaluations*" [1]. The WPEC/SG26 exercise did provided both crucial entries to the NEA High Priority Request List (HPRL) and guidance for new experiments and data evaluations via the NEA/HPRL [2].

Moreover, it was the triggering factor for a worldwide revival of covariance data evaluations in all major cross section data evaluation projects. A large expert participation contributed to WPEC/SG26 (2005-2008). As a main outcome of this project, a first list of 14 data priorities (i.e. uncertainty reductions) for GEN-IV reactors was established and implemented in the HPRL at NEA.

In 2018, the second TAR exercise has been launched in the framework of the WPEC/S46 on "*Efficient and Effective Use of Integral Experiments for Nuclear Data Validation*" [3]. This second TAR exercise aims to: i) review the status of WPEC/SG26 design target accuracies and their potential evolution in reactor operation and fuel cycle parameters, and ii) quantify updated priority nuclear data needs or uncertainties reduction to meet design (reactor and fuel cycle) integral parameters target accuracies.

2 New TAR Exercise in WPEC/SG46

The second TAR exercise is mainly devoted to update and enlarge the scope of the previous WPEC/SG26 exercise, and to provide updated target accuracies for nuclear data uncertainty reduction. This updated TAR exercise will take advantage of:

- progress of covariance data assessment in different international projects (e.g. WPEC/SG44 [4] on "*Investigation of Covariance Data in General Purpose Nuclear Data Libraries*") and evaluation projects of nuclear data (e.g. JEFF-3.3 [5], ENDF/B-VIII.0 [6], etc…)
- potential nuclear data issues and requirements for systems (reactor and associated fuel cycles) recently emerging as new and innovative concepts of interest for the international community
- expansion of S/U methodologies
- assessment of "correlations" between reactions in the "inverse method" optimization. In WPEC/SG26 TAR exercise, the correlations in nuclear data were neglected, and it was pointed out as one of the major weakness of this work. Current studies have shown that taking into account correlations may require tighter uncertainties on the nuclear data [7, 8].
- credit of the uncertainty reduction of nuclear data for design optimization, margins reduction, optimized reactor operation and innovative fuel cycles feasibility assessment.

The TAR exercise should result as far as possible from reactor and associate fuel cycle designers, reactor physicists involved in data validation using integral experiments and nuclear data physicists. Consequently, design code system developers should also be included in this work.

2.1 Review of TARs

Target Accuracy Requirements (TAR) represent typical industrial targets to be met. For nuclear reactors and nuclear fuel facilities these targets may represent safety acceptance limits on different integral parameters for a safe operation both in normal (e.g. nominal operation, manoeuvres, …) and accidental transients (e.g. Loss-Of-Coolant Accident (LOCA)).

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Different safety design limits may be defined to assess: i) the source term with limits in radiotoxicity, dose, etc… ii) the criticality with safety limits in k_{eff}, iii) the damage of fuel in accidents with safety limits peak power distributions. However, the target accuracies are difficult to specify and are often hidden behind/included in an engineering margin. It is recognized by the community that a thorough analysis of TARs would require best estimate of the uncertainty quantification (BE&UQ) with multi-physics codes and simulations. This BE&UQ analysis would allow assessing all potential uncertainties contributing to the uncertainty of simulations. Thus, BE&UQ could help to investigate if nuclear data uncertainties may or may not be the main contributor to the uncertainty.

For this exercise, the values of TAR should include only the impact of nuclear data uncertainty, assuming recognizing that this is only a part of the total uncertainty. The design-oriented TAR values should be specified for the integral parameters in terms of maximum uncertainties accepted in the design. A robust methodology to estimate the overestimation or underestimation of integral parameters to be the most limiting for them can be found in Ref.[9].

Therefore, for this second TAR exercise it has been essential to update and verify the status of WPEC/SG26 design target accuracies and their potential evolution (reactor operation and fuel cycle parameters) since then. A first attempt of this work is to update TAR results for the nuclear systems including the WPEC/SG26 systems (Gen IV, MA burners, and ADS systems) and WPEC/SG33 systems (such as ABR type and JOYO). However, more efforts have been conducted to new reactors concepts (SMR and MSR), sodium-cooled fast reactors and lead-cooled fast reactors, ADS systems.

2.2 Specifications SG46 – TAR Exercise

The specifications for the updated TAR exercise can be found at the WPEC/SG46 official website (https://oecd-nea.org/download/wpec/sg46/). Figure 1 shows the procedure for contributing to this exercise.

SG46 defined a new set of only seven energy groups for sensitivity and uncertainty analysis. Table 1 shows the new energy structure. The definition of the energy limits is based on physical considerations with broad energy bands that cover the region the entire neutron spectrum.

Table 1. Energy group structure for WPEC/SG46

Group	Upper energy (eV)	
1	1.96403 10^7	Above threshold fertile
2	2.23130 10^6	Above threshold inelastic
3	4.97871 10^5	Continuum to URR
4	6.73795 10^4	URR
5	2.03468 10^3	RRR
6	2.26033 10^1	Epithermal
7	5.40000 10^{-1}	Thermal

An example of specific application is the ESFR system [10] where the sensitivity profiles for the ^{239}Pu reactions in the 7-energy groups are shown in Figure 2.

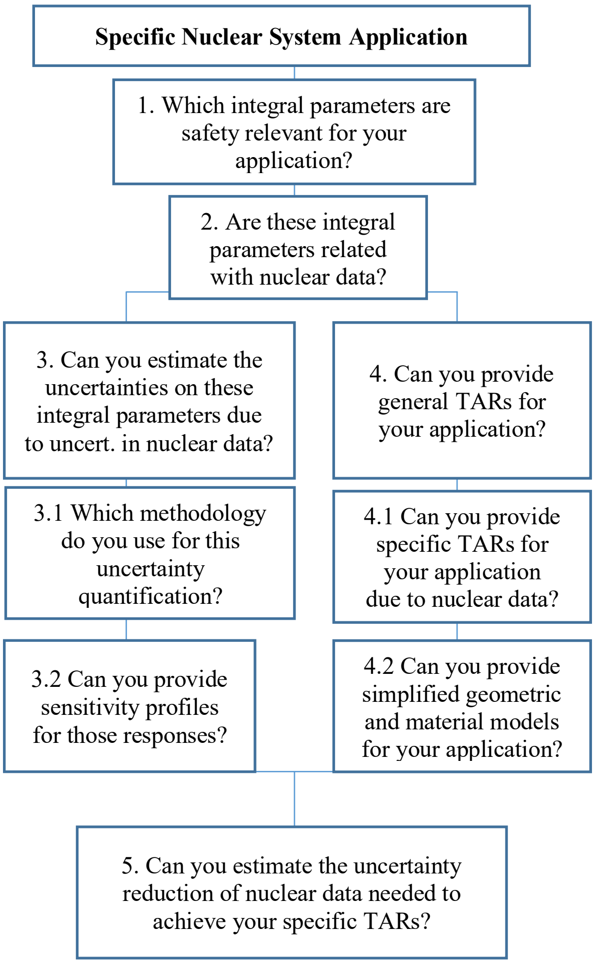

Figure 1. Procedure for any specific application to participate in WPEC/SG46 exercise on TAR

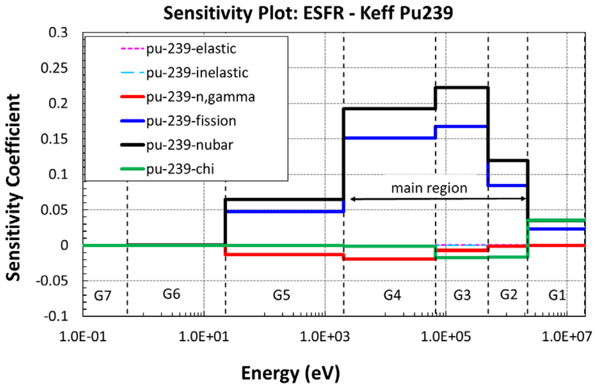

Figure 2. Sensitivity profiles for ^{239}Pu in ESFR system

This SG46/TAR exercise is also useful to test different optimization methodologies compared with the "*traditional*" methodology used in WPEC/SG26. Particularly, one of the main objectives is to assess the importance of correlations in nuclear data.

3 Results and first outcomes

As a first step in the TAR exercise, an uncertainty quantification analysis is carried out. This work helps to evaluate the uncertainty of the relevant reactor design and operation parameters as a function of current covariance nuclear data.

Table 2. Uncertainty quantification due to nuclear data for different reactor systema and integral parameters

Reactor	Quantity	ENDF/B-VII.1	ENDF/B-VIII.0	JEFF-3.3	JENDL-4.0u	Target
ALFRED	k_{eff} (in pcm)	701	865	827	675	435 pcm [9]
	Coolant-density (in %)	57.0	35.0	62.3	64.7	-
	Doppler (in %)	9.4	5.7	6.1	4.9	-
ASTRID	k_{eff} (in pcm)	988	919	894	728	300 pcm
	Full-void (in %)	20.0	21.6	16.5	18.8	-
ESFR	k_{eff} (in pcm)	1199	928	961	774	300 pcm
	Full-void (in %)	10.8	13.2	9.3	10.9	-
	Temp-coef (in %)	4.6	3.7	3.4	3.3	5%
	Control rod worth(in %)	2.1	1.5	1.7	1.4	5%
JSFR	k_{eff} (in pcm)	951	969	903	750	200/300 pcm
	Burnup reactivity swing (in %)	5.0	5.6	5.8	6.1	18%
	Control rod worth (in %)	2.8	2.8	3.0	2.3	2%
	Doppler (in %)	4.1	3.9	3.5	3.0	2%
	Power distribution (in %)	1.6	1.7	1.7	1.3	1%
	Sodium void reactivity (in %)	4.6	5.9	3.9	4.8	3%
NuScale	k_{eff} (in pcm)	777	530	678	536	300 pcm

Table 2 gives a summary of current uncertainties and target accuracies on different integral parameters for four fast systems (ALFRED, ASTRID, ESFR, and JSFR) and one thermal system (SMR/NuScale). In this analysis, four sets of covariance data are used to estimate the uncertainty quantification: ENDF/B-VII.1, ENDF/B-VIII.0, JEFF-3.3 and JENDL-4.0u. In addition, the sensitivity analysis is performed to estimate the top contributors (isotopes-reactions-energy) in the uncertainty quantification.

This calculation gives a first idea if nuclear data uncertainty reduction is needed or not. For all systems, the uncertainty in keff overestimates the target keff-value. In addition, a sensitivity analysis of nuclear reactions can give a first indication on the major contributors to the uncertainties, which will require the most significant uncertainty reduction.

3.1 Methodology for the inverse problem

A traditional methodology used in WPEC/SG26 is based on the "*inverse problem*" which aims 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:

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

where:

- λ_i are the cost parameters. These parameters are used to weight the difficulties to reduce the uncertainty. A first set of λ-values can be set equal to 1 for all reactions (set A). Then, other approaches or sets (B, and C) were defined within the SG26 in order to take into account different cost parameters for reactions, isotopes [1], or even neutron-energy.
- Δx_i are the cross-section uncertainty (i.e. standard deviation) to be minimized.
- I: total number of reactions-energy. Main isotopes (^{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, ...) and energy groups (7).

The **constraints** can be defined as follows**:**

- The TAR constraints defined as R_n^T, the target accuracy on the n-integral parameter:
- $\boldsymbol{\sum_i S_{ni}^2 \cdot (\Delta x_i)^2 + \sum_{ii'} S_{ni} \cdot (\Delta x_i)^2 \cdot corr_{ii'} \cdot (\Delta x_{i'})^2 \cdot S_{ni'}^{+} \le (R_n^T)^2 \,;\, n = 1 \dots N}$ (2)

where:

- N is the total number of integral design parameters
- S_{ni} are the sensitivity coefficients for the integral parameter R_n
- $corr_{ii'}$ are the correlations between energy-reaction cross-section i an i'

It is worth mentioning that the "*inverse problem*" optimization performed in WPEC/SG26 did not take into account such correlation terms. Considering these correlations, tighter uncertainties on the nuclear data are required, because correlations increase in most cases the total uncertainty. See references [3, 4]. In practical cases, the number of "selected" variables can be limited to make the problem feasible. Thus, the number of total reactions-energy (I) is obtained by selecting the variables based on their contribution to the uncertainties; for instance, by selecting only those which globally account 98%.

- The precision absolute measurement of cross-section is another constraint which mathematically can be formulated as: $\Delta x_i \geq 0; i = 1 \ldots I$. Although, physically, it may be assumed as a high-precision absolute measurement at the level of L_i. Thus, $\Delta x_i \geq L_i$. For instance, we could assume as a constraint "a high-precision" absolute measurement of around 0.5% for the standards cross-sections.

3.2 Results

SG46/TAR exercise provides uncertainty reduction of nuclear reactions based on different reactor systems and integral parameters. As an example, Figure 2 shows the uncertainty reduction for the ^{238}U(n,n') in the JFSR-750 system for a k$_{eff}$-target of 200pcm for different specifications. Here, different sets of λ-parameters are tested. The set-A is also tested with and without (e.g. SG26 approach) correlation terms in cross-sections in the TAR solver. This impact of correlation terms can be very significant in target accuracy assessment evaluation. In this example, the uncertainty reduction in ^{238}U(n,n') is stringent from 8% to 5%.

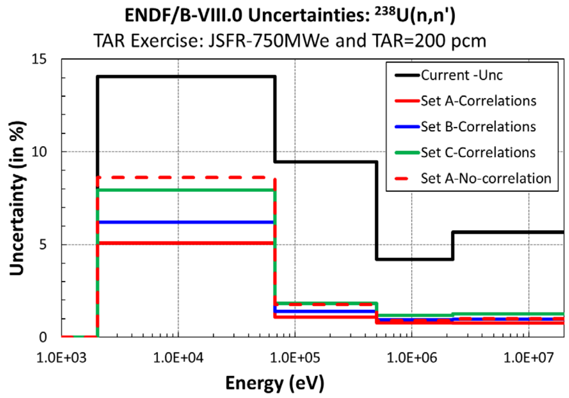

Figure 3. Initial and target uncertainties for the ^{238}U(n,n') in the JSFR-750MWe reactor

Tables 3 and 4 give an example of uncertainty reduction in two different systems, the JSFR-750 fast system and the LWR-NuScale Small Modular Reactor. These tables give a list of top-5 reactions ranked by the relative uncertainty reduction, with the current and target uncertainty reduction. For Table 3, TAR calculation is performed with a low-bound limit of 0.5% to constraint the experimental uncertainty in ^{239}Pu(n,fission) cross sections with the uncertainty in current "standards" libraires.

Table 3. JSFR-750MWe TAR exercise (≤300 pcm in k$_{eff}$): top-5 most important reactions using set C of cost parameters and lower bound uncertainty constraint of 0.5%

#	Reaction	Energy Group	Current (%)	Target (%)	Rel. Unc. Reduction(%)
1	^{239}Pu (n,fission)	3	1.3	0.5	18.0
2	^{239}Pu (n,fission)	4	1.3	0.5	16.6
3	56Fe (n,n')	2	18.9	2.1	11.0
4	^{239}Pu (n,fission)	5	4.6	0.8	6.8
5	^{238}U (n,γ)	4	1.5	0.5	5.5

Table 4. NuScale k$_{eff}$ TAR Exercise (≤300 pcm in k$_{eff}$): top-5 most important reactions using set A of cost parameters

#	Reaction	Energy Group	Current (%)	Target (%)	Rel. Unc. Reduction (%)
1	^{235}U -nubar	7	0.7	0.2	67.8
2	^{238}U (n,γ)	7	1.9	0.5	12.2
3	^{238}U (n,γ)	5	2.2	0.7	6.0
4	^{238}U (n,γ)	6	2.3	0.8	5.3
5	^{235}U (n,γ)	7	1.6	0.6	4.7

4 Conclusion and future work

WPEC/SG46 is working to release the results of this TAR exercise by the end of 2022. This work will serve to assess the effect of nuclear data uncertainty reduction on integral parameters relevant for reactor design; with the goal to provide new requirements of "*nuclear data uncertainty reduction*" within the NEA/HPRL.

An example is the analysis performed using SG46/TAR methodology in MOLTEX reactor design which has served to predict the target accuracy requirement for the ^{35}Cl(n,p) between 100keV and 5 MeV, this values is ~5-8%. Thanks to this work, a new high-priority request entry on ^{35}Cl(n,p) has recently accepted (April 2022) in the NEA/HPRL[11].

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