Date: January 23rd, 2024
Place: “The n_TOF Nuclear Physics Winter School 2024”, Saint-Gervais Mont-Blanc (France)

Lesson 2

A Nuclear Data User Perspective

Sensitivity Analysis (SA)/Uncertainty Quantification (UQ)
and
Target Accuracy Requirements in Reactor Physics

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Content

A nuclear data user perspective in Reactor Physics

☐ **Reactor design and operation are based on “computational simulations”**

- **Validated calculation tools (+ ND) using expensive integral experiments**
  - How well can we calculate neutron fields, reaction rates, nuclide inventories, radioactivity, dose rates, decay heat, …?
  - Do we have a penalty for inaccuracy?

- **Better accuracy gives an increase in safety margins in design and operation**
  - Core reactivity
  - Power distribution
  - Reactivity coefficients
  - Burnup/time to refuel
  - Shielding
  - Spent fuel storage
  - …
- **Reliable predictions with credible uncertainty margins**
  - Then, neutronic calculations require **better nuclear data**
  - **Uncertainties in nuclear data** become the most important contributor to the total uncertainties in neutronic calculations

2. Sensitivity Analysis and Uncertainty Quantification

☐ Sensitivity coefficients (SA)

- The sensitivities of the system’s response to variations in the system's parameters:

$$S_i = \left(\frac{\partial R}{\partial \alpha_i}\right)_{\alpha^0}$$

these sensitivities can be used for:

- ranking sensitivities to evaluate the relative importance to the response
- assessing changes in the response due to parameter variations
- performing uncertainty analysis by using the sandwich formula
- optimization process (e.g. target accuracies for uncertainty reduction)

Therefore, sensitivity analysis requires very precise sensitivity coefficients, and they should be given for:

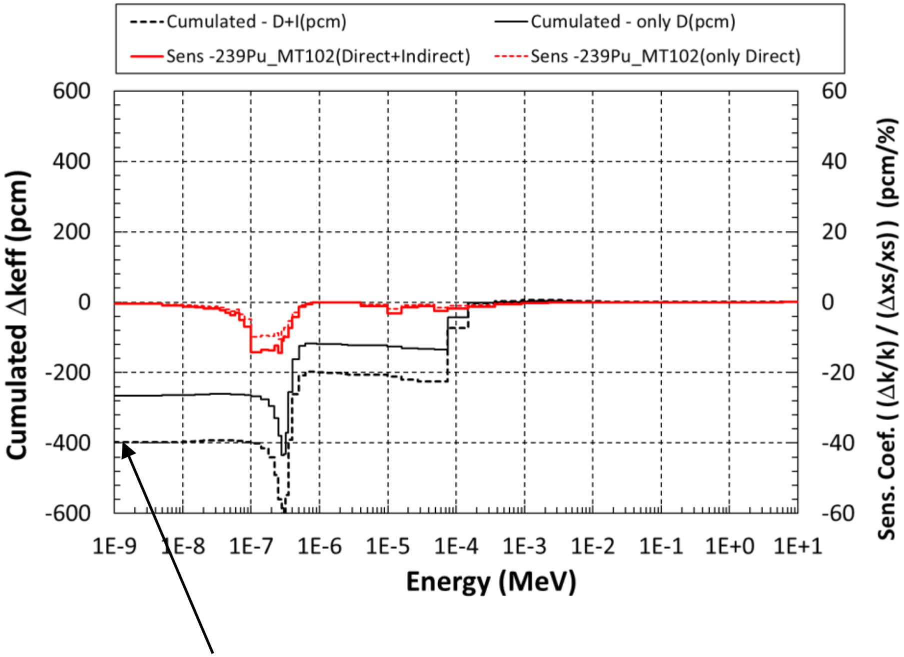
- All materials in the systems with the most relevant isotopes in each material
- The most important reactions (fission, gamma nubar, PFNS,… angular distribution,…)
- Neutron energy, multigroup (238 energy groups, 33 energy groups, etc …) or continuous energy
- For all important responses in the system (keff, reaction rates, isotopic inventory, decay heat, etc…)

Sensitivity Analysis

Figure . ^{239}Pu(n, gamma) sensitivity coefficients **(in red)** in a PWR Fuel Assembly 17x17 - 4.8wt% at 32GWd/MTU.

Relative perturbation **(in black)** in keff between JEFF-3.3 and ENDF/B-VII.1

- "Only Direct" (D) - only changes in cross-sections
- "Direct + Indirect" takes into account changes in the inventory (ΔN)



Total change between JEFF-3.3 and ENDF/B-VII.1: -400 pcm

- ○ Sensitivities predicted by perturbation of nuclear data using FRENDY capabilities
- ○ The cumulated change is the cumulative change from high (g=G) to thermal energy (g=1):

$$\Delta k_{eff}^{i} = \sum_{g=G}^{1} S_g^i \cdot \Delta\sigma_g^i$$

Ref: JEFF Meeting - Depletion Session , Nov 2021 JEFFDOC-2111

Uncertainty Propagation

❑ **Uncertainty Quantification (UQ)** based on S/A - Error propagation

- **Being any response as (first order approach) :**

$$R(\alpha_1, \alpha_2 \ \ldots \alpha_k) = R(\alpha_1^0, \alpha_2^0, \ldots, \alpha_k^0) + \sum_{i_1=1}^{k} \left(\frac{\partial R}{\partial \alpha_{i_1}}\right)_{\alpha^0} \delta\alpha_{i_1}$$

- **The sandwich formula gives:**

$$var[R] = \left[\sum_{i=1}^{k} S_i^2 \, var(\alpha_i) + 2\sum_{i \neq j=1}^{k} S_i S_j \, cov(\alpha_i, \alpha_j)\right] = \mathrm{S} \cdot \mathrm{V}_\alpha \cdot S^T$$

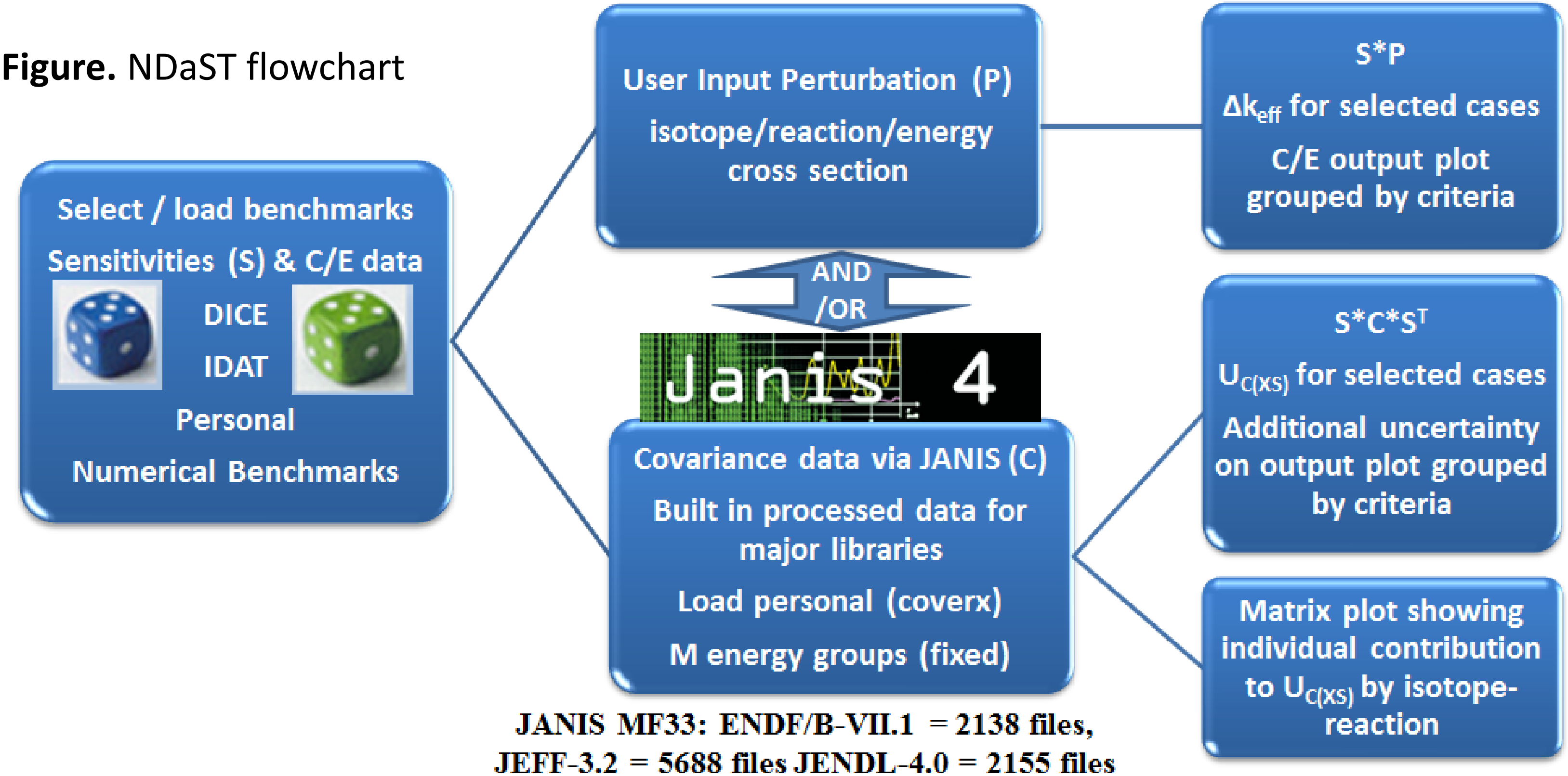
where:

- S (RxK) are the Sensitivity coefficients of the R responses to all system parameters: $\boldsymbol{S} = \begin{bmatrix} \frac{\partial R_1}{\partial \alpha_1} & \cdots & \frac{\partial R_1}{\partial \alpha_k} \\ & \ddots & \\ \frac{\partial R_R}{\partial \alpha_1} & \cdots & \frac{\partial R_R}{\partial \alpha_k} \end{bmatrix}_{\alpha^0}$
- ***V_α*** is the covariance matrix (KxK): $V_\alpha = \left[\begin{bmatrix} var(\alpha_1) & \cdots & cov(\alpha_1, \alpha_K) \\ \vdots & \ddots & \vdots \\ cov(\alpha_K, \alpha_1) & \cdots & var(\alpha_K) \end{bmatrix}\right]$

Uncertainty Propagation

- ❑ **UQ tool based on "Sandwich formula"**

Figure. NDaST flowchart



Select / load benchmarks

Sensitivities (S) & C/E data

DICE

IDAT

Personal

Numerical Benchmarks

User Input Perturbation (P)

isotope/reaction/energy cross section

AND /OR

Covariance data via JANIS (C)

Built in processed data for major libraries

Load personal (coverx)

M energy groups (fixed)

$S*P$

Δk_{eff} for selected cases

C/E output plot grouped by criteria

$S*C*S^T$

$U_{C(XS)}$ for selected cases

Additional uncertainty on output plot grouped by criteria

Matrix plot showing individual contribution to $U_{C(XS)}$ by isotope-reaction

JANIS MF33: ENDF/B-VII.1 = 2138 files, JEFF-3.2 = 5688 files JENDL-4.0 = 2155 files TENDL-2013 = 77811 files

- ❑ (https://www.oecd-nea.org/ndast/webstart/NDaST.jnlp)

Uncertainty Propagation

☐ UQ tool based on “Monte Carlo” techniques

- Provide many samples of nuclear data files, for each sampled nuclear data file simulation is performed

- Methodologies for randomly sampled “σ”
  - **XSUSA [1], NUDUNA [2]**
  - **SANDY (**https://github.com/luca-fiorito-11/sandy**)**
    FRENDY(https://rpg.jaea.go.jp/main/en/program_frendy/**)**
    - Samples of ND files for “a priori” $p_0(\sigma|\sigma_C, V_C)$ evaluated files
    - Based on normal (or log-normal) distributions because no further information on the distribution of the nuclear data are provided in evaluated files
  - **“Total Monte Carlo”(TMC) [3] – (**https://tendl.web.psi.ch/tendl_2021/tendl2021.html)
    - Sampling performed at the level of nuclear parameters in nuclear reaction codes (e.g. TALYS)
    - $p_0(\sigma|\sigma_C, V_C)$ will be normal !?

[3] A.J. Koning, D. Rochman, Ann. Nucl. Energy 35, 2024(2008)

UQ in PWRs: Critical Boron Let down

Core parameter	Design criteria	Acceptance criteria
Critical boron concentration in ARO	$|(C_B)^M_{ARO}-(C_B)^C_{ARO}|$ <50 ppm Boron	$|(C_B)^M_{ARO}-(C_B)^C_{ARO}|$ <100 ppm

Table. Bias (C-E) and Uncertainties in Critical Boron Concentration (in ppm). 1000 MWe PWR-Westinghouse in cycle-5. Calculations performed with SEANAP-98 and SANDY codes. Nuclear Data is JEFF-3.3

Power (%)	Burnup (GWd/tHM)	Predicted values			Uncertainties (in ppm)								
					Pu239			U235			U238		All
		Measured (ppm)	Calculation (ppm)	Bias (ppm)	XS	ν	χ	XS	ν	χ	XS		
50	0.015	1200	1165	-35	18	14	9	27	46	9	24		64
75	0.031	1113	1085	-28	18	15	9	27	46	10	24		64
100	0.134	985	1011	26	19	15	9	27	46	10	25		65
100	1.340	870	896	26	22	16	9	25	47	10	24		66
…	…	…	…	…	..	..	..	..	..	..	..		…
100	7.716	319	321	2	34	23	9	21	38	10	23		65
100	8.823	227	219	-8	35	24	9	21	37	10	23		66
100	10.284	101	79	-22	37	25	9	20	35	10	23		66
100	11.351	4	-29	-33	39	26	9	20	34	10	23		67

Ref.: A. Alonso, E. de la Fuente, O.Cabellos et al. Comparison of JEFF-3.3 and ENDF/B-VIII.0 in PWR simulations. JEFFDOC-1968. April 2019

UQ in other Nuclear Systems

Table. Uncertainty quantification due to nuclear data uncertainties and SG46/TAR values

System	Parameter	ENDF/B-VII.1	ENDF/B-VIII.0	JEFF-3.3	JENDL-5.0	Target
ALFRED	keff (in pcm)	**717**	**826**	**831**	**736**	300/435 pcm
	Coolant-density (in %)	57.0	30.3	42.9	38.9	10%
	Coppler (in %)	9.0	4.6	6.5	5.5	3%
ASTRID	keff (in pcm)	**999**	**855**	**908**	**851**	300 pcm
	Fully voided (in %)	20.2	17.2	16.1	20.2	10%
ESFR	keff (in pcm)	**1147**	**865**	**967**	**899**	300 pcm
	Fully voided (in %)	37.1	31.2	26.7	33.8	10%
	Doppler (in %)	5.6	3.3	4.1	4.0	3%
	Rod worth (in %)	2.4	1.3	1.8	1.7	3%
JSFR-750	keff (in pcm)	**971**	**900**	**920**	**866**	300 pcm
	BRS (in %)	5.5	5.4	5.2	5.1	18% / 27%
	CRW (in %)	2.7	2.7	3.2	2.6	2% /-
	DOP (in %)	3.9	3.1	3.6	4.0	2% / 7%
	Power distribution (in %)	1.7	1.6	1.8	1.5	1% / 2%
	SVR (in %)	4.8	5.3	3.8	4.9	3% / 7%
MYRRHA	keff (in pcm)	**771**	**676**	**588**	**-**	300 pcm
MACRE	keff (in pcm)	**2435**	**-**	**-**	**-**	300 pcm
MOLTEX	keff (in pcm)	**584/836***	**922**	**1090**	**-**	300 pcm
NUSCALE	keff (in pcm)	**748**	**522**	**669**	**397**	300 pcm

ND uncertainty reduction is needed, but mostly for k_{eff} !

❑ UQ performed with sandwich formula ($S \cdot V_{\alpha} \cdot S^{T}$) and using the full ND covariance matrix (V_{α})

* using covariances for ^{35}Cl above 1 MeV from TENDL2021 evaluation

Ref.: O. Cabellos, WONDER 2023

3. What “Target Accuracy Requirement” (TAR) is?

- *“Nuclear facilities provide **safety/operating margins** for their nominal and incidental regimes. For the **Safety Authority**, operators must justify these margins and, in parallel, to seek to reduce them”*

  (Ref: P. Blaise, “Nuclear Data User Perspective: Reactor Physics”, ND2022)

- ***“TAR values are driven by reactor designers and utilities”***

  (Ref: A. Santamarina, “From integral experiments to nuclear data improvement”, ND2007)

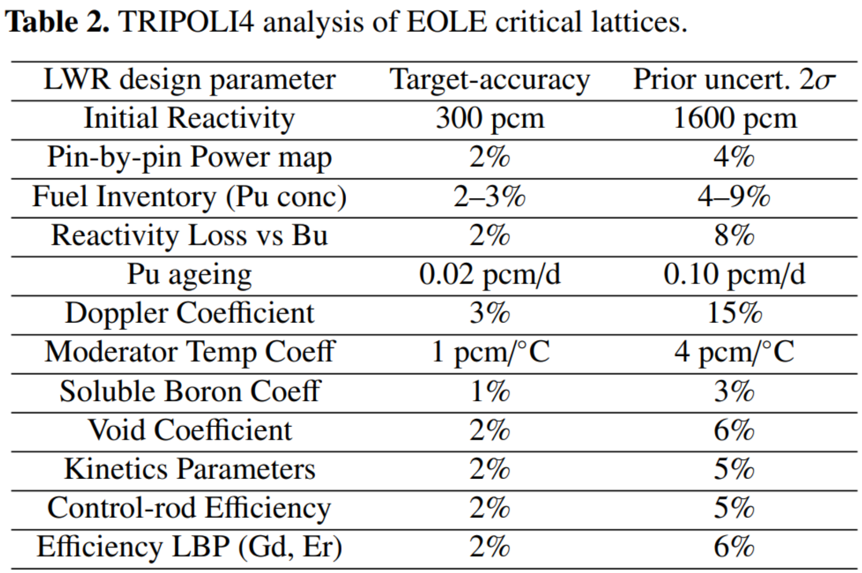


Table 2. TRIPOLI4 analysis of EOLE critical lattices.

LWR design parameter	Target-accuracy	Prior uncert. 2σ
Initial Reactivity	300 pcm	1600 pcm
Pin-by-pin Power map	2%	4%
Fuel Inventory (Pu conc)	2–3%	4–9%
Reactivity Loss vs Bu	2%	8%
Pu ageing	0.02 pcm/d	0.10 pcm/d
Doppler Coefficient	3%	15%
Moderator Temp Coeff	1 pcm/°C	4 pcm/°C
Soluble Boron Coeff	1%	3%
Void Coefficient	2%	6%
Kinetics Parameters	2%	5%
Control-rod Efficiency	2%	5%
Efficiency LBP (Gd, Er)	2%	6%

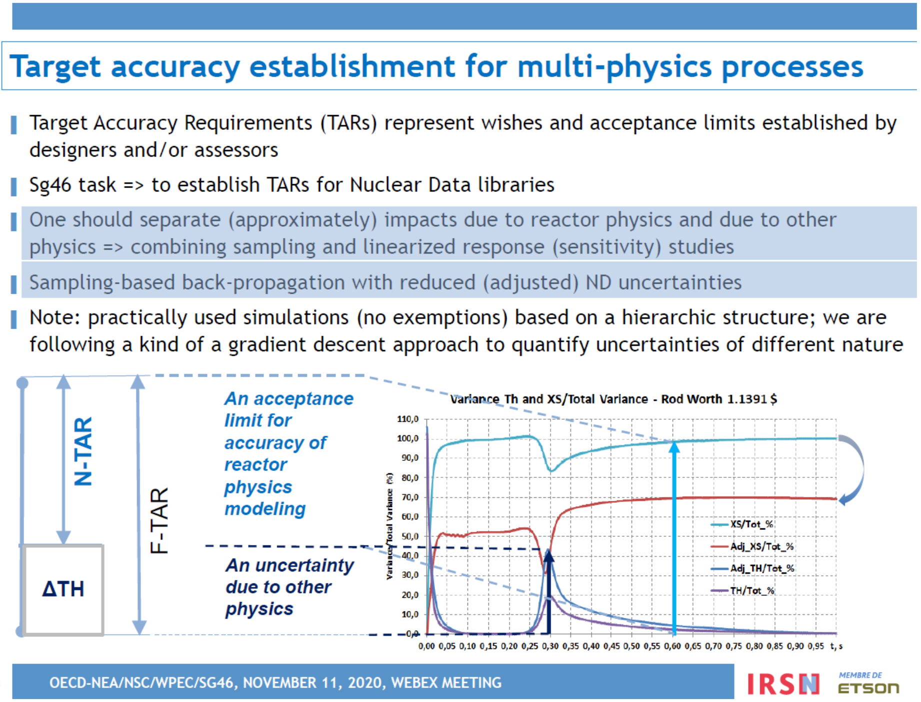
- *“Target-accuracies on LWR parameters are 2–5 times lower than calculation uncertainties linked to nuclear data” (2007)*

Ref: https://nd2007.edpsciences.org/articles/ndata/pdf/2007/01/ndata07723.pdf

Necessity of “Expert Judgment” in TAR values

- The necessity to quantify the biases and uncertainties in a multi-physics approach:

→ **neutronics**, thermal-hydraulics and materials



Target accuracy establishment for multi-physics processes

- Target Accuracy Requirements (TARs) represent wishes and acceptance limits established by designers and/or assessors
- Sg46 task => to establish TARs for Nuclear Data libraries
- One should separate (approximately) impacts due to reactor physics and due to other physics => combining sampling and linearized response (sensitivity) studies
- Sampling-based back-propagation with reduced (adjusted) ND uncertainties
- Note: practically used simulations (no exemptions) based on a hierarchic structure; we are following a kind of a gradient descent approach to quantify uncertainties of different nature

23 OECD-NEA/NSC/WPEC/SG46, NOVEMBER 11, 2020, WEBEX MEETING

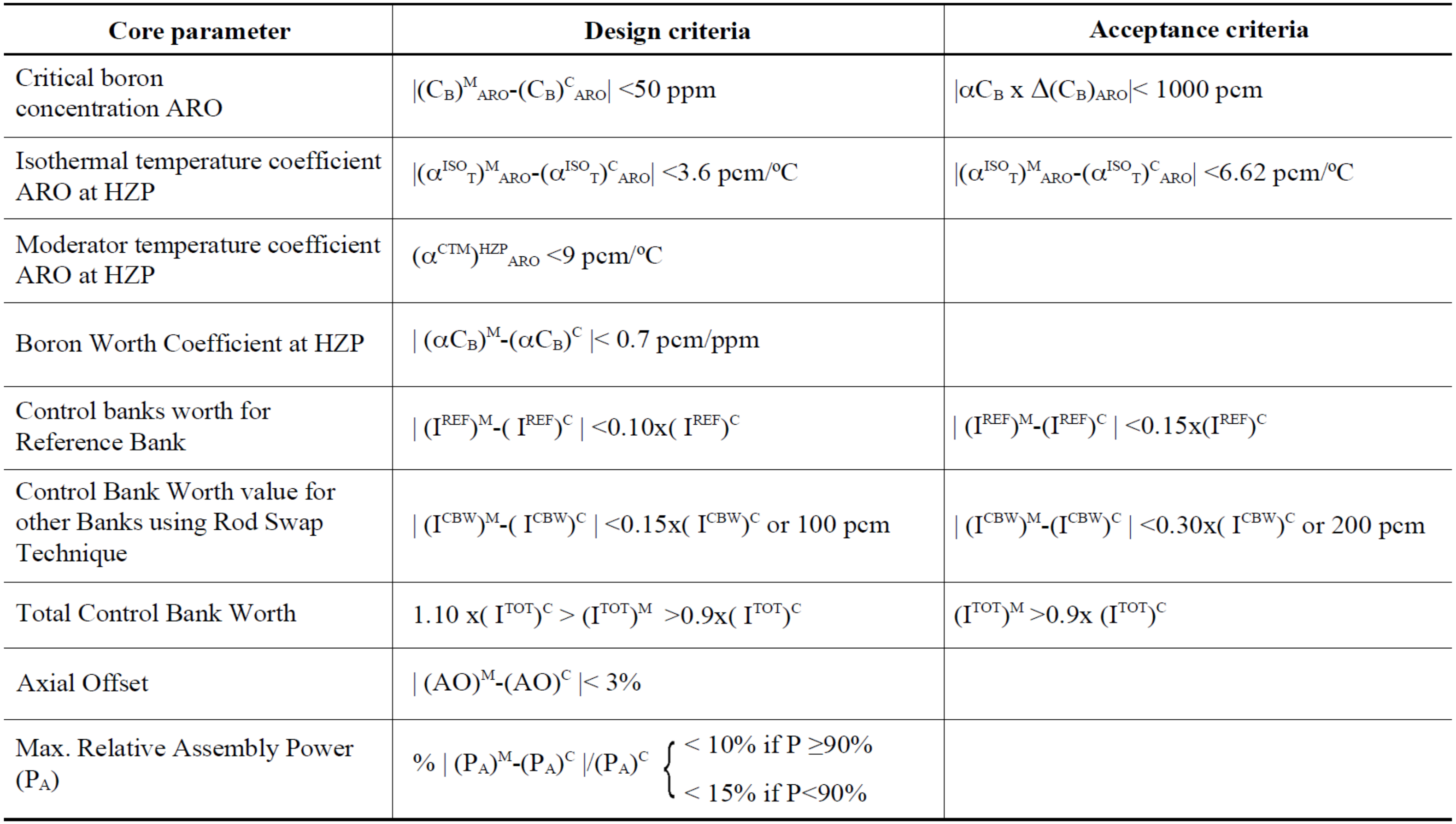
Ref.: *Evgeny Ivanov, WPEC/S46, Nov. 2020*

- *“TAR values should result* ***as far as possible from designers and design code system developers*** *and they are not supposed to replace, although being* ***compatible with e.g. the “Acceptance” criteria for the assessment of the safety case of specific systems,*** *defined, in some cases, by the regulator, in other cases, proposed by the designer and to be approved by the regulator”*

(Ref.: M. Salvatores, January 27, 2020)

Target Accuracy Requirements
An example: For LWRs

- ❑ Design and Acceptance Criteria for Start-up and Operation in PWRs



Core parameter	Design criteria	Acceptance criteria
Critical boron concentration ARO	$\|(C_B)^M_{ARO}-(C_B)^C_{ARO}\| < 50$ ppm	$\|\alpha C_B \times \Delta(C_B)_{ARO}\| < 1000$ pcm
Isothermal temperature coefficient ARO at HZP	$\|(\alpha^{ISO}_T)^M_{ARO}-(\alpha^{ISO}_T)^C_{ARO}\| < 3.6$ pcm/°C	$\|(\alpha^{ISO}_T)^M_{ARO}-(\alpha^{ISO}_T)^C_{ARO}\| < 6.62$ pcm/°C
Moderator temperature coefficient ARO at HZP	$(\alpha^{CTM})^{HZP}_{ARO} < 9$ pcm/°C	
Boron Worth Coefficient at HZP	$\| (\alpha C_B)^M-(\alpha C_B)^C \| < 0.7$ pcm/ppm	
Control banks worth for Reference Bank	$\| (I^{REF})^M-(I^{REF})^C \| < 0.10x(I^{REF})^C$	$\| (I^{REF})^M-(I^{REF})^C \| < 0.15x(I^{REF})^C$
Control Bank Worth value for other Banks using Rod Swap Technique	$\| (I^{CBW})^M-(I^{CBW})^C \| < 0.15x(I^{CBW})^C$ or 100 pcm	$\| (I^{CBW})^M-(I^{CBW})^C \| < 0.30x(I^{CBW})^C$ or 200 pcm
Total Control Bank Worth	$1.10\ x(I^{TOT})^C > (I^{TOT})^M > 0.9x(I^{TOT})^C$	$(I^{TOT})^M > 0.9x\ (I^{TOT})^C$
Axial Offset	$\| (AO)^M-(AO)^C \| < 3\%$	
Max. Relative Assembly Power (P_A)	$\% \| (P_A)^M-(P_A)^C \|/(P_A)^C \begin{cases} < 10\% \text{ if } P \geq 90\% \\ < 15\% \text{ if } P < 90\% \end{cases}$	

Ref.: O.Cabellos et al. Propagation of Nuclear Data Uncertainties for PWR Core Analysis. NUCLEAR ENGINEERING AND TECHNOLOGY, VOL.46 NO.3 JUNE 2014.

Code Developers -
TAR Tables for PWRs

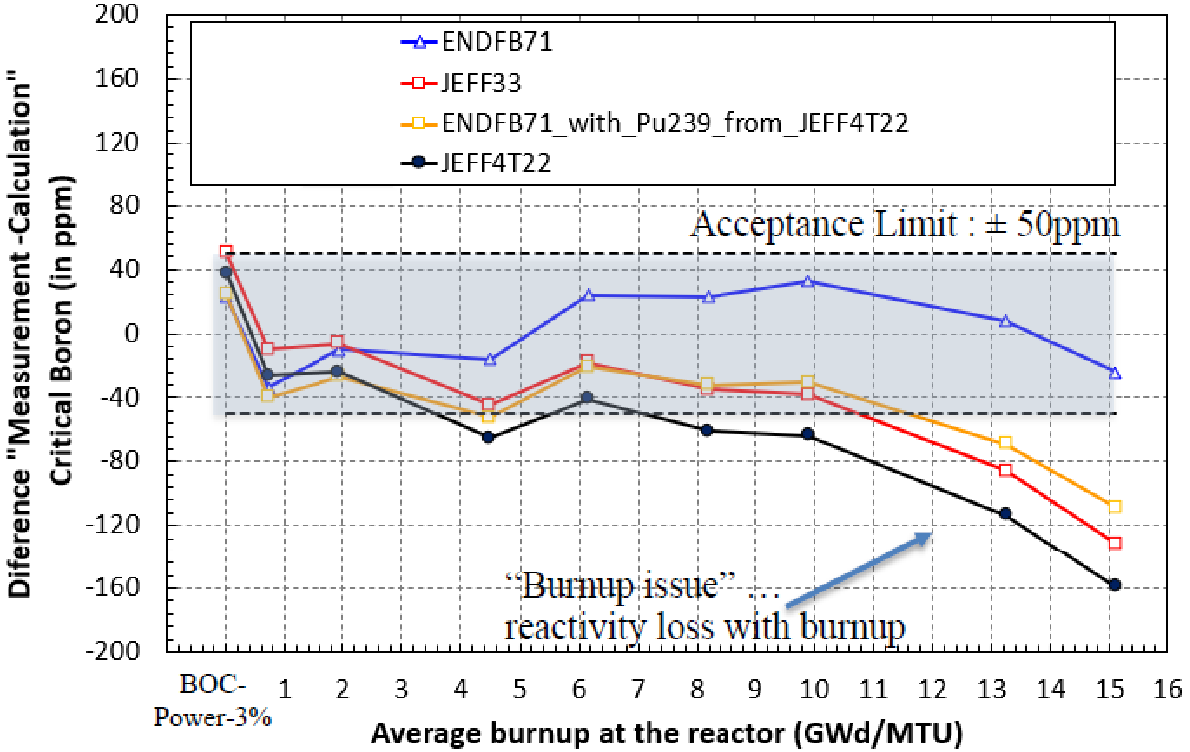
- A High-Fidelity, two cycles, PWR depletion challenge …. **code developers!**

Accuracy criteria		
HZP	boron endpoint concentrations	± 25 ppm
	temperature coefficients	± 1 pcm/K
	rod bank worths	± 5%
HFP	critical boron concentrations predicted with	± 25 ppm
	235U fission axial integrals	± 1.5% rms
	235U fission axial shape with	± 1.0% rms

Ref.: K. Smith, B. Forget. *Challenges in the Development of High-Fidelity LWR Core Neutronics Tools*. MC2013

Modification in reactivity (Critical Boron letdown) versus Critical Boron Measurements

Experimental – measured "Critical Boron concentrations" can be found at:
Ref. IAEA-TEC-DOC 815 "In-Core Fuel Management Code Package Validation for PWRs", 1995
https://inis.iaea.org/collection/NCLCollectionStore/_Public/26/077/26077395.pdf



NNPP – PWR Almaraz I, cycle 1

Ref: https://ceiden.com/wp-content/uploads/2023/06/14_Jose_Miras_INGENIA.pdf

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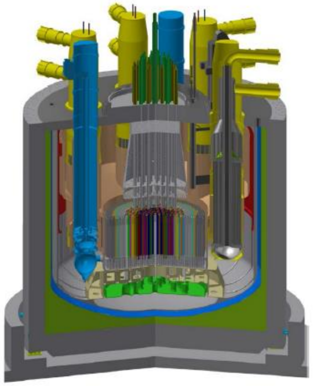
TAR Exercise: ESFR-SMART



- Core Power – commercial size: 3600MWth / **1500 MWe**
- Sodium-cooled fast reactor
- Fuel type: MOX
  - 216 Inner FA, Pu content (%) 17.99wt%
  - 288 Outer FA, , Pu content (%) 17.99wt%
- 24 control rods
- Active fuel region height (inner core): 75 cm

Reference: A. Rineiski et al., ESFR-SMART deliverable D1.1.2

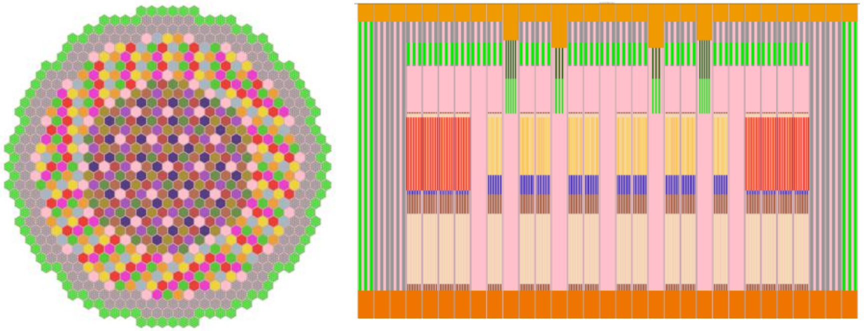
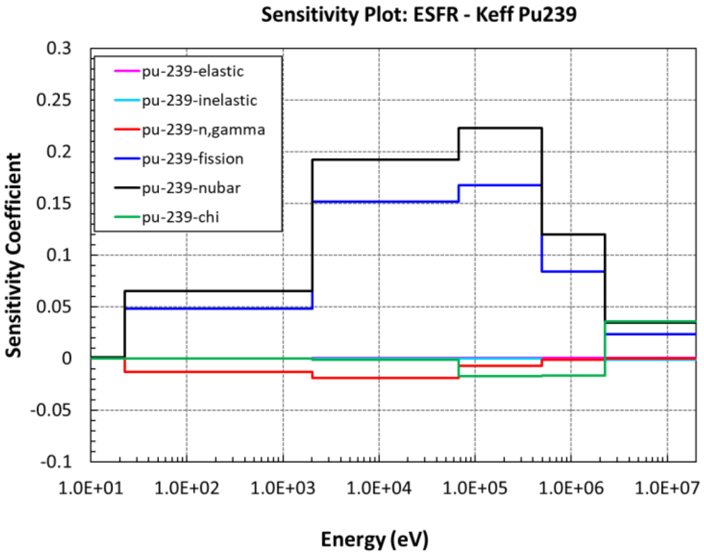


Table. Target accuracy requirement on top-10 most important reactions. **Correlations** in TAR exercise - set A, **JEFF-3.3**: **keff**

Rank #	Reaction	Energy Group	Current (%)	Target (%)	Rel. Unc. Reduction (%)
1	**Pu239 (n,fission)**	Cont->URR	**1.3**	**0.3**	**19.8**
2	**Pu239 (n,fission)**	URR	**1.2**	**0.3**	**18.4**
3	Pu239 (n,fission)	Above >Einel	1.3	0.4	9.6
4	U238 (n,gamma)	URR	1.6	0.5	6.4
5	U238 (n,inelastic)	Above >Einel	4.6	0.8	5.5
6	U238 (n,gamma)	Cont->URR	1.8	0.6	4.9
7	Pu239 (n,gamma)	URR	8.7	1.1	4.9
8	Pu239 (n,fission)	RRR	3.3	0.6	3.9
9	U238 (n,inelastic)	Cont->URR	9.5	1.4	3.4
10	U238 (n,inelastic)	Above >Efertile	3.3	0.9	2.3

Figure. Energy-dependent sensitivity keff-profile for ^{239}Pu(n,fission) in ESFR-SMART

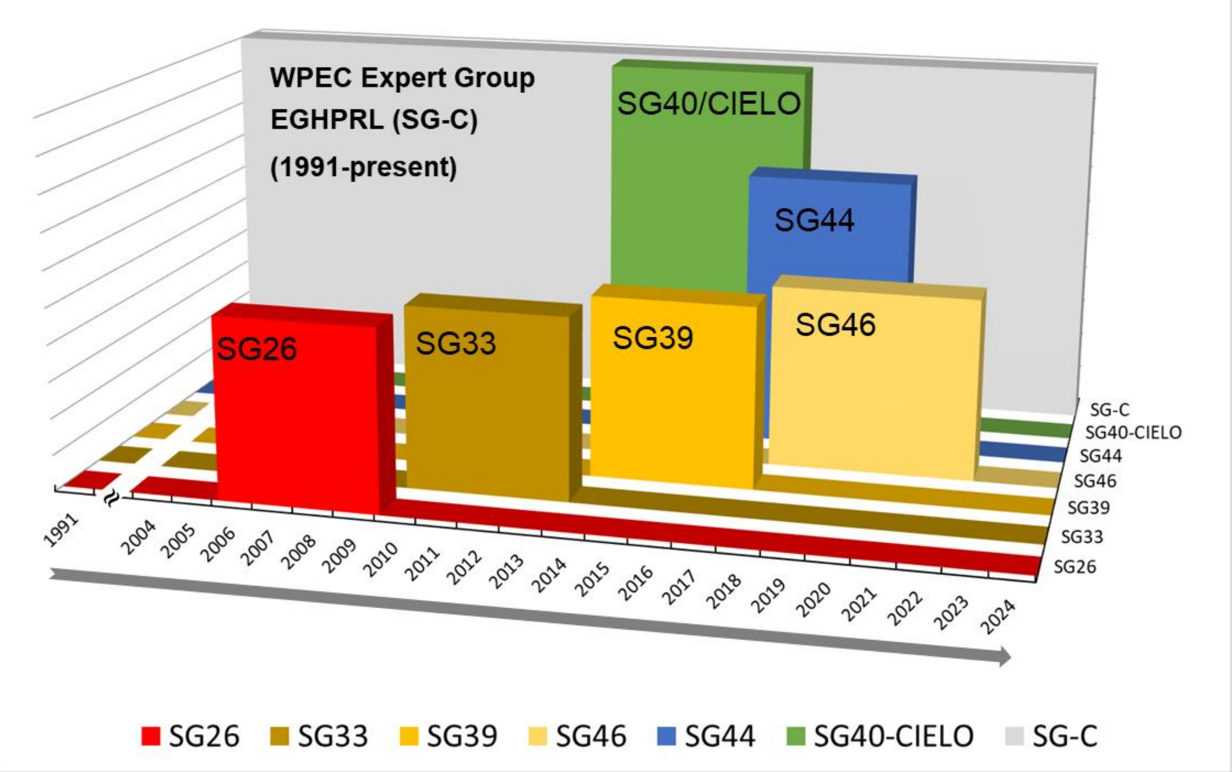


Total keff unc. due to ND with ENDF/B-VIII.0: 865 pcm

TAR ESFR-SMART keff value : 300 pcm

4. The OECD/NEA
Activities on Nuclear Data… The WPEC

- ❑ Overview of **OECD/NEA/NSC/WPEC Sub-groups**
- ❑ SGs on Nuclear Data Adjustment and Target Accuracy Requirements



- Different WPEC/SGs working in ND Adjustment


Vol.26

International Evaluation Co-operation
Volume 26
Uncertainty and Target Accuracy Assessment for Innovative Systems Using Recent Covariance Data Evaluations

Vol.33

International Evaluation Co-operation
Volume 33
Methods and Issues for the Combined Use of Integral Experiments and Covariance Data

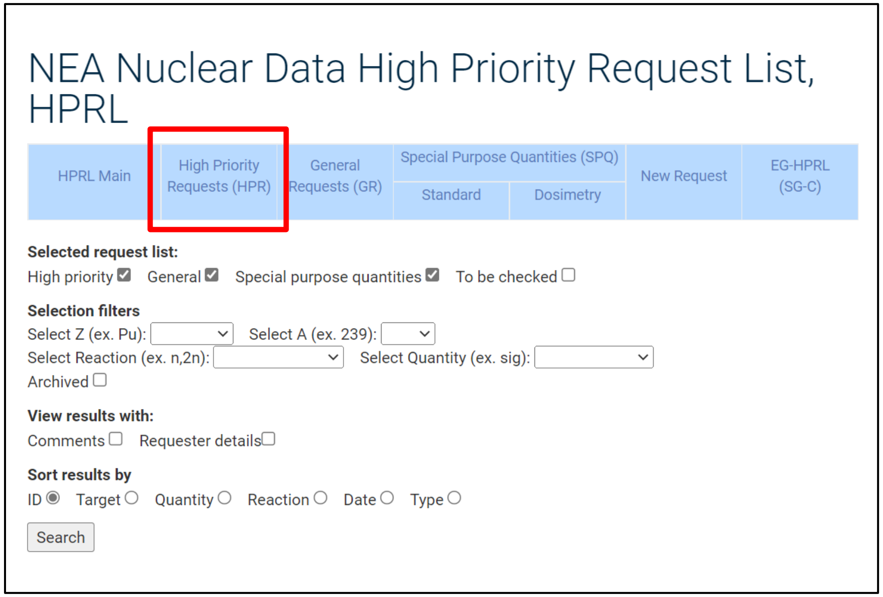
Methods and Approaches to Provide Feedback from Nuclear and Covariance Data Adjustment for Improvement of Nuclear Data Files
Intermediate Report

Vol.39 Part-I

- ❑ In **OECD/NEA - The JEFF Stakeholders** meetings (2017 and 2023)
- ❑ In **US/ENDF - WANDA** - Workshop for Applied Nuclear Data Activities (since 2019)

https://nucleardata.berkeley.edu/wanda/index.html

The NEA/High Priority Request List (HPRL)



NEA Nuclear Data High Priority Request List, HPRL

Selected request list:
High priority ☑ General ☑ Special purpose quantities ☑ To be checked ☐

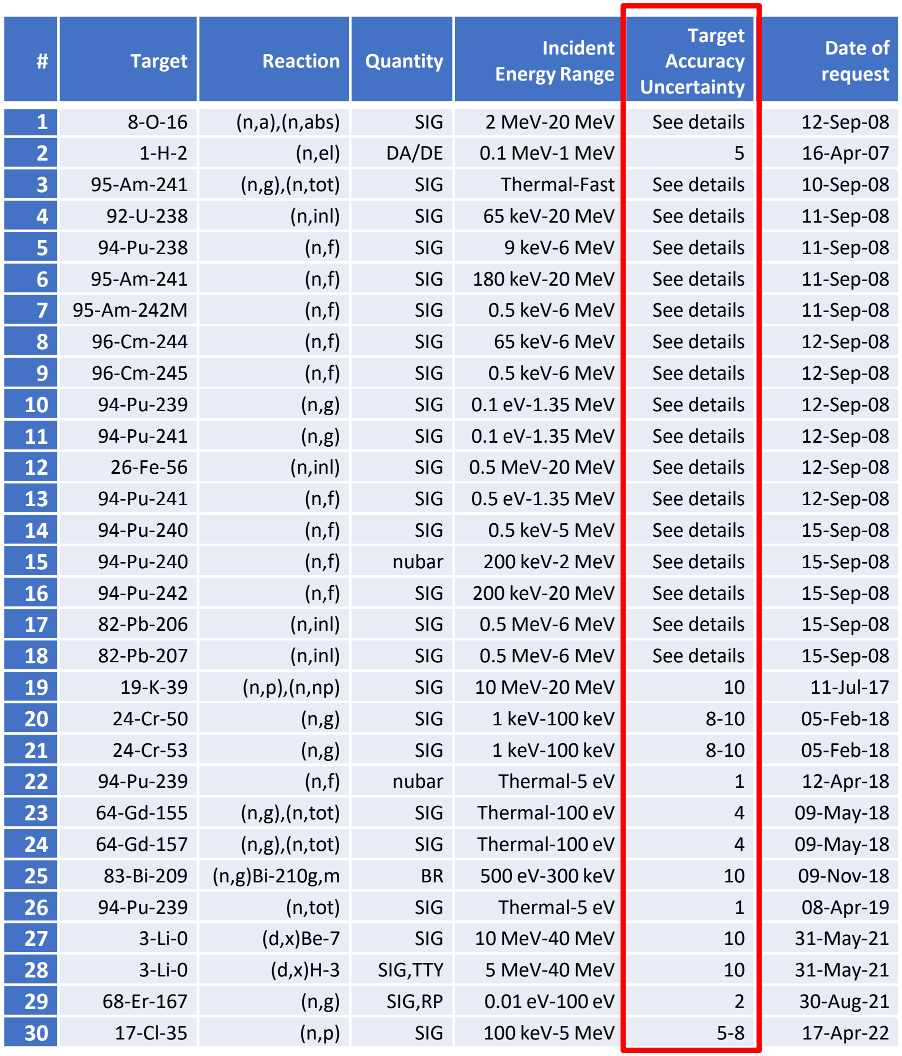
Selection filters
Select Z (ex. Pu):
Select A (ex. 239):
Select Reaction (ex. n,2n):
Select Quantity (ex. sig):
Archived ☐

View results with:
Comments ☐ Requester details ☐

Sort results by
ID ● Target ○ Quantity ○ Reaction ○ Date ○ Type ○

Ref. HPRL: https://www.oecd-nea.org/download/wpec/hprl/

Table 3. *High Request List of entries (by June 2022)*

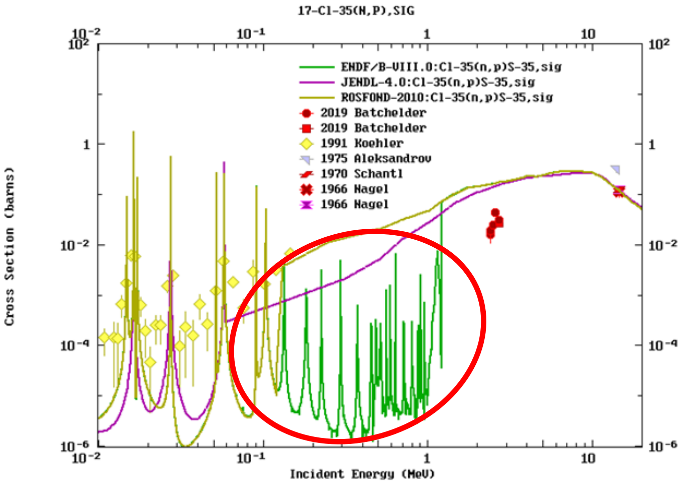


#	Target	Reaction	Quantity	Incident Energy Range	Target Accuracy Uncertainty	Date of request
1	8-O-16	(n,a),(n,abs)	SIG	2 MeV-20 MeV	See details	12-Sep-08
2	1-H-2	(n,el)	DA/DE	0.1 MeV-1 MeV	5	16-Apr-07
3	95-Am-241	(n,g),(n,tot)	SIG	Thermal-Fast	See details	10-Sep-08
4	92-U-238	(n,inl)	SIG	65 keV-20 MeV	See details	11-Sep-08
5	94-Pu-238	(n,f)	SIG	9 keV-6 MeV	See details	11-Sep-08
6	95-Am-241	(n,f)	SIG	180 keV-20 MeV	See details	11-Sep-08
7	95-Am-242M	(n,f)	SIG	0.5 keV-6 MeV	See details	11-Sep-08
8	96-Cm-244	(n,f)	SIG	65 keV-6 MeV	See details	12-Sep-08
9	96-Cm-245	(n,f)	SIG	0.5 keV-6 MeV	See details	12-Sep-08
10	94-Pu-239	(n,g)	SIG	0.1 eV-1.35 MeV	See details	12-Sep-08
11	94-Pu-241	(n,g)	SIG	0.1 eV-1.35 MeV	See details	12-Sep-08
12	26-Fe-56	(n,inl)	SIG	0.5 MeV-20 MeV	See details	12-Sep-08
13	94-Pu-241	(n,f)	SIG	0.5 eV-1.35 MeV	See details	12-Sep-08
14	94-Pu-240	(n,f)	SIG	0.5 keV-5 MeV	See details	15-Sep-08
15	94-Pu-240	(n,f)	nubar	200 keV-2 MeV	See details	15-Sep-08
16	94-Pu-242	(n,f)	SIG	200 keV-20 MeV	See details	15-Sep-08
17	82-Pb-206	(n,inl)	SIG	0.5 MeV-6 MeV	See details	15-Sep-08
18	82-Pb-207	(n,inl)	SIG	0.5 MeV-6 MeV	See details	15-Sep-08
19	19-K-39	(n,p),(n,np)	SIG	10 MeV-20 MeV	10	11-Jul-17
20	24-Cr-50	(n,g)	SIG	1 keV-100 keV	8-10	05-Feb-18
21	24-Cr-53	(n,g)	SIG	1 keV-100 keV	8-10	05-Feb-18
22	94-Pu-239	(n,f)	nubar	Thermal-5 eV	1	12-Apr-18
23	64-Gd-155	(n,g),(n,tot)	SIG	Thermal-100 eV	4	09-May-18
24	64-Gd-157	(n,g),(n,tot)	SIG	Thermal-100 eV	4	09-May-18
25	83-Bi-209	(n,g)Bi-210g,m	BR	500 eV-300 keV	10	09-Nov-18
26	94-Pu-239	(n,tot)	SIG	Thermal-5 eV	1	08-Apr-19
27	3-Li-0	(d,x)Be-7	SIG	10 MeV-40 MeV	10	31-May-21
28	3-Li-0	(d,x)H-3	SIG,TTY	5 MeV-40 MeV	10	31-May-21
29	68-Er-167	(n,g)	SIG,RP	0.01 eV-100 eV	2	30-Aug-21
30	17-Cl-35	(n,p)	SIG	100 keV-5 MeV	5-8	17-Apr-22

- ☐ Target reactions… **uncertainty reduction to achieve TAR values for keff, reactivity coefficients, etc. in nuclear applications!**

An Example Entry in the HPRL: 35Cl(n,p)

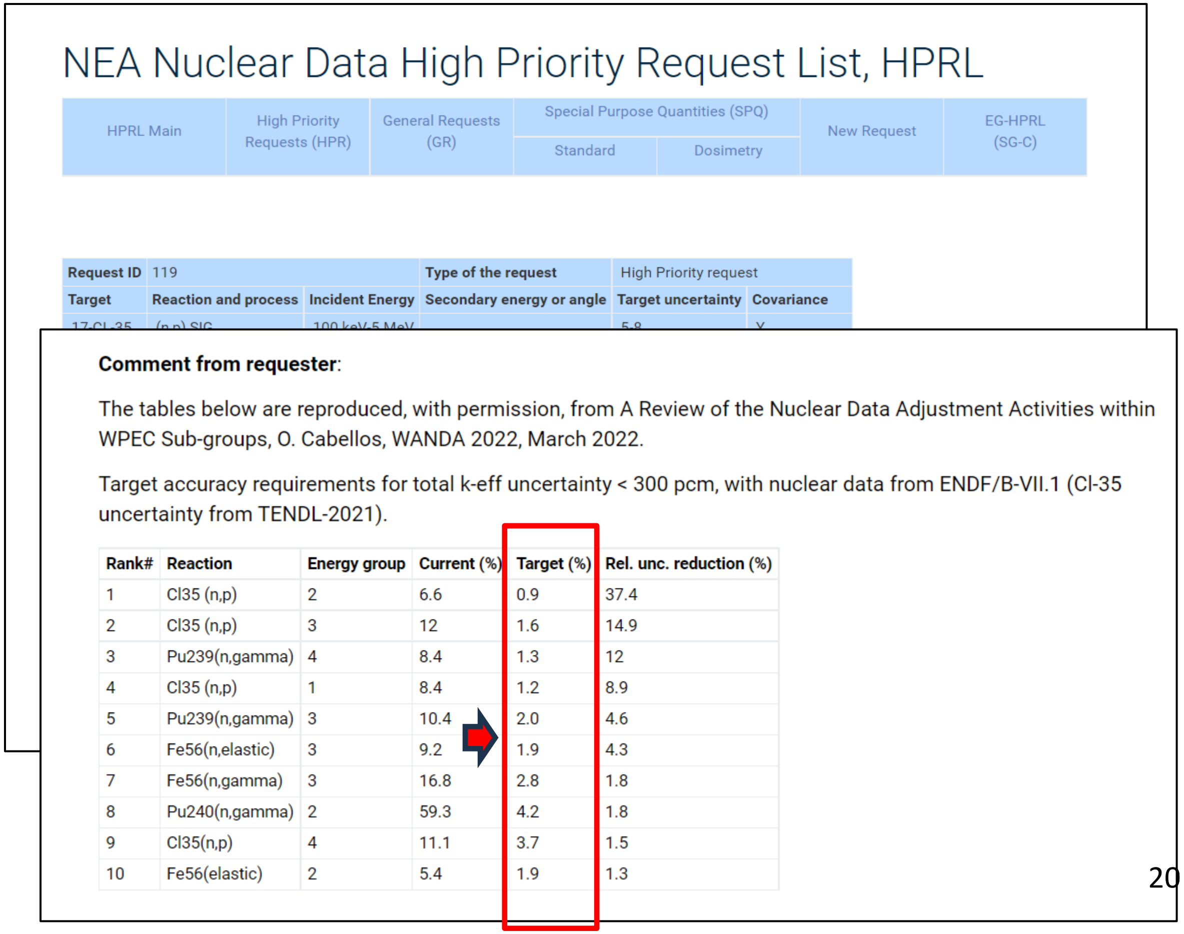
Figure. *The ^{35}Cl(n,p) cross-section: Experimental data versus evaluated data.*



An example:

Nuclear data in Molten Salt Reactors

https://oecd-nea.org/dbdata/hprl/hprlview.pl?ID=540



NEA Nuclear Data High Priority Request List, HPRL

Request ID	119		**Type of the request**	High Priority request	
Target	**Reaction and process**	**Incident Energy**	**Secondary energy or angle**	**Target uncertainty**	**Covariance**
17-CL-35	(n,p) SIG	100 keV-5 MeV		5-8	Y

Comment from requester:

The tables below are reproduced, with permission, from A Review of the Nuclear Data Adjustment Activities within WPEC Sub-groups, O. Cabellos, WANDA 2022, March 2022.

Target accuracy requirements for total k-eff uncertainty < 300 pcm, with nuclear data from ENDF/B-VII.1 (Cl-35 uncertainty from TENDL-2021).

Rank#	Reaction	Energy group	Current (%)	Target (%)	Rel. unc. reduction (%)
1	Cl35 (n,p)	2	6.6	0.9	37.4
2	Cl35 (n,p)	3	12	1.6	14.9
3	Pu239(n,gamma)	4	8.4	1.3	12
4	Cl35 (n,p)	1	8.4	1.2	8.9
5	Pu239(n,gamma)	3	10.4	2.0	4.6
6	Fe56(n,elastic)	3	9.2	1.9	4.3
7	Fe56(n,gamma)	3	16.8	2.8	1.8
8	Pu240(n,gamma)	2	59.3	4.2	1.8
9	Cl35(n,p)	4	11.1	3.7	1.5
10	Fe56(elastic)	2	5.4	1.9	1.3

Main WPEC/SG46's outcome:
NEEDS in Nuclear Data

- ☐ Spent fuel, criticality, shielding
- ☐ Criticality and depletion: **"Burnup issue"** loss of reactivity at high burnup… transmutation/depletion
  - Pu239, U238, TSL-H2O …
  - **Fission products…** Fission yields + capture cross sections!
- ☐ WPEC/SG46: Advanced Reactors, MSRs, SMRs **(large impact of reflector -> large leakage)**
  - **Necessity of uncertainty reduction in:**

FAST/EPITHERMAL nuclear data	Fuel	Coolant/Structural materials
MSRs (MACRE and MOLTEX)	239Pu(n, γ), 235U(n, γ)	35Cl(n,p)
MYRRHA	240Pu(n,f) & (n,γ),239Pu(n,f) & (n, γ), 238U(n,f) & (n, γ)	
ALFRED	238U(n, n') and (n,γ), 239Pu (n, f) and (n, γ), 240Pu(n, f)	207Pb(n,n'), 206Pb(n,n'), 56 Fe(n, n')
ASTRID	238U(n, n') and (n, γ), 239Pu(n,f) and (n,γ), 240Pu(n,f)	23Na(n,n')
ESFR-SMART	238U(n, n') & (n, γ), 239Pu(n,f), 240Pu(n,f),	23Na(n,n'), 56Fe(n,n')
JSFR-750	238U(n,n') & (n, γ), 239Pu(n,f), 240Pu(n,f) 238U (elasticP1) - 16O(elasticP1)	23Na(n,n)&(n,n'),56Fe(n,n')
THERMAL nuclear data		
SMR/NUSCALE	235U(nubar) and 238U (n,γ)	

- ☐ ND for Thorium Cycle (e.g. U233)
- ☐ Needs in fusion applications
  - IFMIF/DONES and DEMO - Magnetic Fusion Energy (MFE)
  - Inertial Fusion Energy (IFE) … NIF diagnostics

Questions ?

Questions for you?

☐ Why do we need better nuclear data if LWRs are working since 70s?

☐ With different nuclear data we get different results. Then, why do we have different evaluations of Nuclear Data?

☐ General Purpose ND for different Applications? or Adjusting ND for Specific Applications?

References

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4. A. Alonso, E. de la Fuente, O.Cabellos et al. Comparison of JEFF-3.3 and ENDF/B-VIII.0 in PWR simulations. JEFFDOC-1968. April 2019
5. I. Ivanov, “IRSN contributions: from TARs and S/U to V&UQ via DA”, https://oecd-nea.org/download/wpec/sg46/meetings/2020-11/documents/4-Ivanov-IRSN.pdf
6. O. Cabellos, “Target Accuracy Requirements (TAR) Exercise within WPEC/SG46 and Feedback on Nuclear Data Needs”, WONDER 2023
7. O.Cabellos et al. Propagation of Nuclear Data Uncertainties for PWR Core Analysis. NUCLEAR ENGINEERING AND TECHNOLOGY, VOL.46 NO.3 JUNE 2014
8. K. Smith, B. Forget. Challenges in the Development of High-Fidelity LWR Core Neutronics Tools. MC2013
9. O. Cabellos, “UPM contribution to Action 6: Revision of TAR tables”, https://www.oecd-nea.org/download/wpec/sg46/meetings/2019-11/documents/15.1-Cabellos.pdf
10. The OECD/NEA HRPL, https://oecd-nea.org/dbdata/hprl/

Back-up slides ?

Who is involved in TAR Exercise?

Uncertainty reduction of current ND uncertainties: “Δx_i”

- ➢ **TAR Exercise (the “inverse problem”) is not a ND adjustment with integral experiments**
  - ○ XSs and correlations of ND will remain unchanged
  - ○ Relative standard deviations (Δx_i) will be updated, they will be our TARGET values

$$\textbf{To minimize: } \left(\sum_i \frac{\lambda_i}{\Delta x_i^2}\right)$$
$$i = 1, \ldots, K$$

- ❑ **ND Differential measurement experts**
  - ○ Cost parameters assigned to isotopes, reactions, and/or energy group

The objective function is constrained to:

1) $\Delta x_{i0} \geq \Delta x_i \geq 0; i = 1 \ldots K$

- ❑ **ND Processing**
  - ○ AMPX code
  - ○ NJOY code

- ❑ **ND Evaluators**
  - ○ Uncertainties for all MATs/MTs
  - ○ Credible uncertainties

- ❑ **ND Exp/Evaluators**
  - ○ Exp./Eva. lower uncertainties

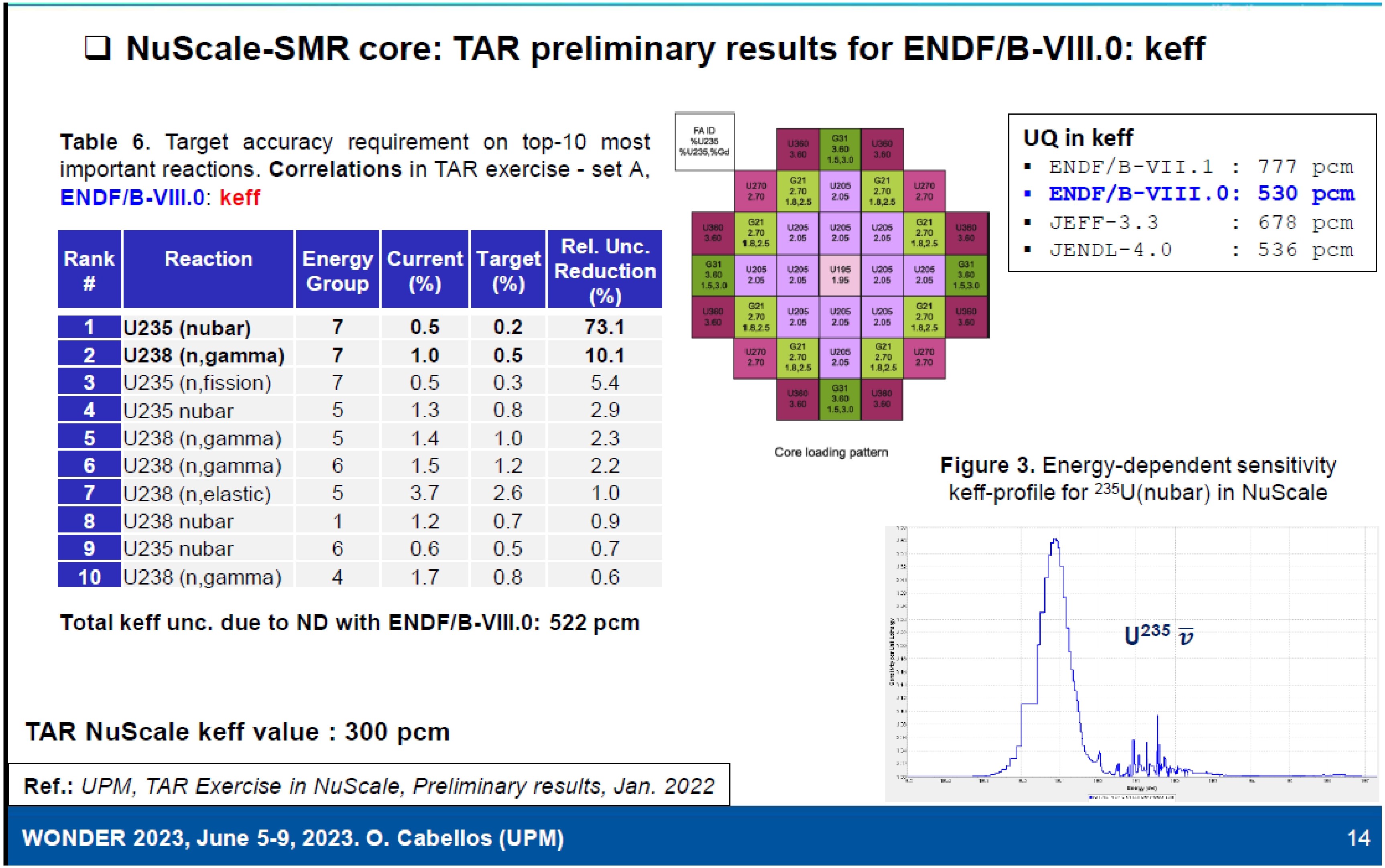
- ❑ **Reactor Designers**
  - ○ Safety margins
  - ○ Licensing

2) $\sum_i S_{ni}^2 \cdot \Delta x_i^2 + \sum_{ii'} \boldsymbol{S}_{ni} \cdot \Delta \boldsymbol{x}_i \cdot \boldsymbol{corr}_{ii'} \cdot \Delta \boldsymbol{x}_{i'}\, \boldsymbol{S}_{ni}^{+} \leq (R_n^T)^2; n = 1 \ldots N$

- ❑ **TAR Solving**
  - ○ Assumptions
  - ○ Inverse method + other ML/AI

- ❑ **Reactor Physicists**
  - ○ Reactor Model
  - ○ Sensitivity Profiles

Example TAR Exercise: NUSCALE



❑ NuScale-SMR core: TAR preliminary results for ENDF/B-VIII.0: keff

Table 6. Target accuracy requirement on top-10 most important reactions. **Correlations** in TAR exercise - set A, **ENDF/B-VIII.0**: **keff**

Rank #	Reaction	Energy Group	Current (%)	Target (%)	Rel. Unc. Reduction (%)
1	**U235 (nubar)**	**7**	**0.5**	**0.2**	**73.1**
2	**U238 (n,gamma)**	**7**	**1.0**	**0.5**	**10.1**
3	U235 (n,fission)	7	0.5	0.3	5.4
4	U235 nubar	5	1.3	0.8	2.9
5	U238 (n,gamma)	5	1.4	1.0	2.3
6	U238 (n,gamma)	6	1.5	1.2	2.2
7	U238 (n,elastic)	5	3.7	2.6	1.0
8	U238 nubar	1	1.2	0.7	0.9
9	U235 nubar	6	0.6	0.5	0.7
10	U238 (n,gamma)	4	1.7	0.8	0.6

Total keff unc. due to ND with ENDF/B-VIII.0: 522 pcm

FA ID
%U235
%U235,%Gd

		U360 3.60	G31 3.60 1.5,3.0	U360 3.60		
	U270 2.70	G21 2.70 1.8,2.5	U205 2.05	G21 2.70 1.8,2.5	U270 2.70	
U360 3.60	G21 2.70 1.8,2.5	U205 2.05	U205 2.05	U205 2.05	G21 2.70 1.8,2.5	U360 3.60
G31 3.60 1.5,3.0	U205 2.05	U205 2.05	U195 1.95	U205 2.05	U205 2.05	G31 3.60 1.5,3.0
U360 3.60	G21 2.70 1.8,2.5	U205 2.05	U205 2.05	U205 2.05	G21 2.70 1.8,2.5	U360 3.60
	U270 2.70	G21 2.70 1.8,2.5	U205 2.05	G21 2.70 1.8,2.5	U270 2.70	
		U360 3.60	G31 3.60 1.5,3.0	U360 3.60		

Core loading pattern

UQ in keff

- `ENDF/B-VII.1  : 777 pcm`
- **`ENDF/B-VIII.0: 530 pcm`**
- `JEFF-3.3      : 678 pcm`
- `JENDL-4.0     : 536 pcm`

Figure 3. Energy-dependent sensitivity keff-profile for ^{235}U(nubar) in NuScale

TAR NuScale keff value : 300 pcm

Ref.: *UPM, TAR Exercise in NuScale, Preliminary results, Jan. 2022*

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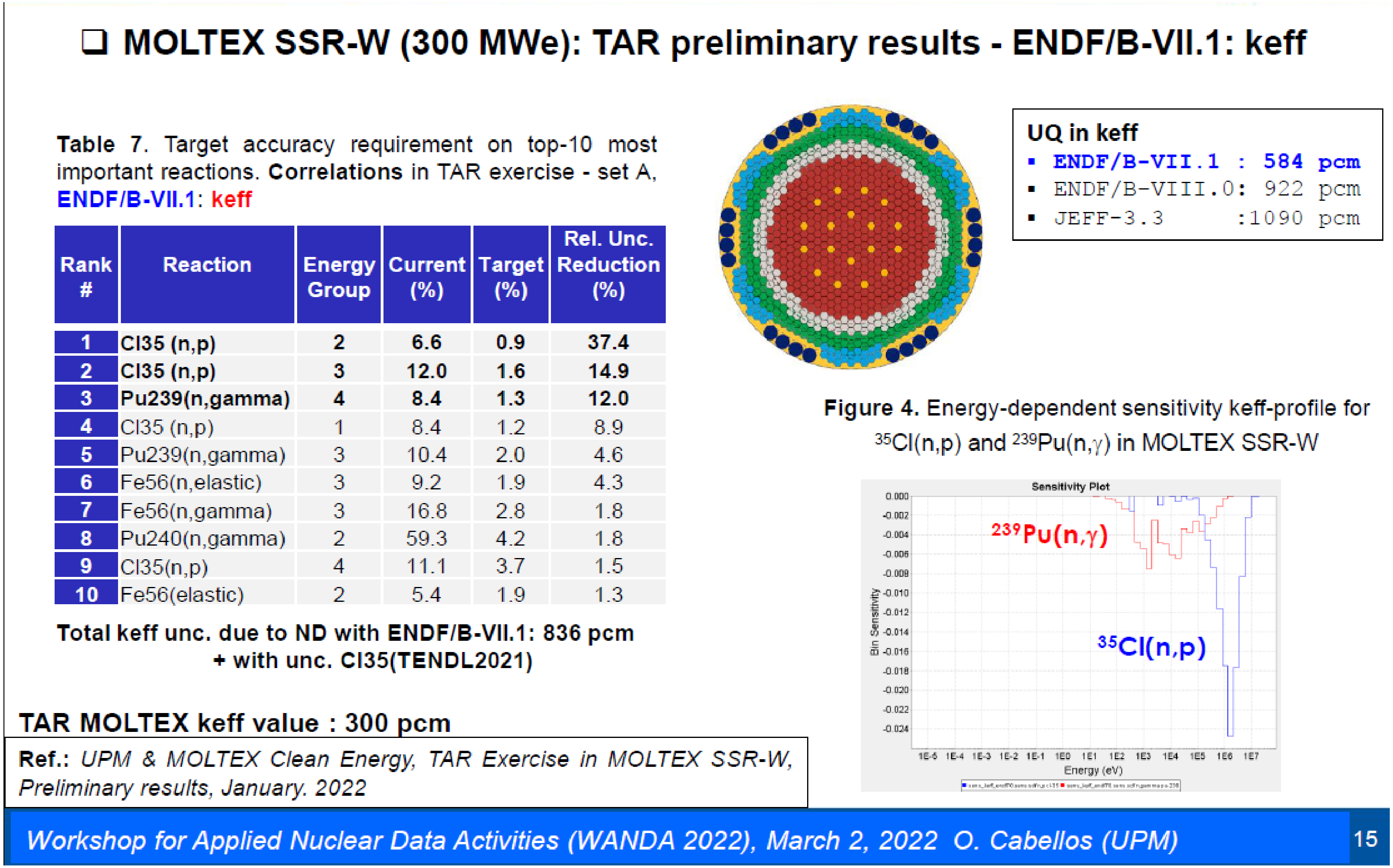
Example TAR Exercise: MOLTEX



❑ MOLTEX SSR-W (300 MWe): TAR preliminary results - ENDF/B-VII.1: keff

Table 7. Target accuracy requirement on top-10 most important reactions. **Correlations** in TAR exercise - set A, **ENDF/B-VII.1**: **keff**

Rank #	Reaction	Energy Group	Current (%)	Target (%)	Rel. Unc. Reduction (%)
1	**Cl35 (n,p)**	**2**	**6.6**	**0.9**	**37.4**
2	**Cl35 (n,p)**	**3**	**12.0**	**1.6**	**14.9**
3	**Pu239(n,gamma)**	**4**	**8.4**	**1.3**	**12.0**
4	Cl35 (n,p)	1	8.4	1.2	8.9
5	Pu239(n,gamma)	3	10.4	2.0	4.6
6	Fe56(n,elastic)	3	9.2	1.9	4.3
7	Fe56(n,gamma)	3	16.8	2.8	1.8
8	Pu240(n,gamma)	2	59.3	4.2	1.8
9	Cl35(n,p)	4	11.1	3.7	1.5
10	Fe56(elastic)	2	5.4	1.9	1.3

Total keff unc. due to ND with ENDF/B-VII.1: 836 pcm
+ with unc. Cl35(TENDL2021)

UQ in keff

- **ENDF/B-VII.1 : 584 pcm**
- ENDF/B-VIII.0: 922 pcm
- JEFF-3.3 :1090 pcm

Figure 4. Energy-dependent sensitivity keff-profile for ^{35}Cl(n,p) and ^{239}Pu(n,γ) in MOLTEX SSR-W

TAR MOLTEX keff value : 300 pcm

Ref.: *UPM & MOLTEX Clean Energy, TAR Exercise in MOLTEX SSR-W, Preliminary results, January. 2022*

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