Italian National Agency for New Technologies,
Energy and Sustainable Economic Development

Progress Towards a Framework for Assessing the Impact of ENDF-6 Evaluations on Nuclear Technologies Using n_TOF Data

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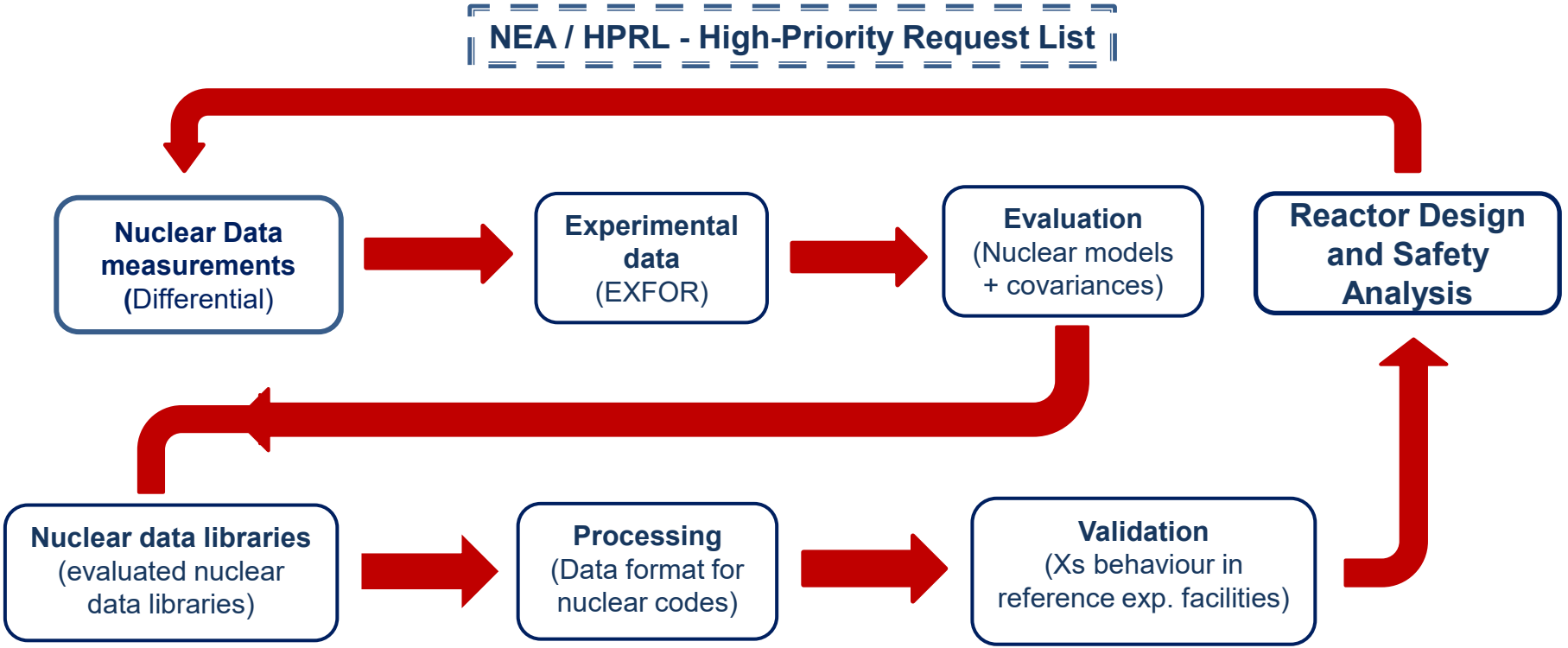
Reference framework

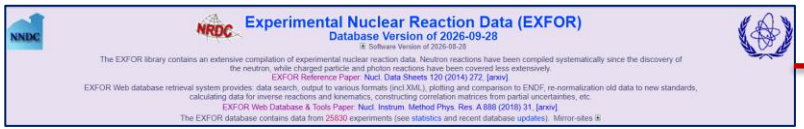


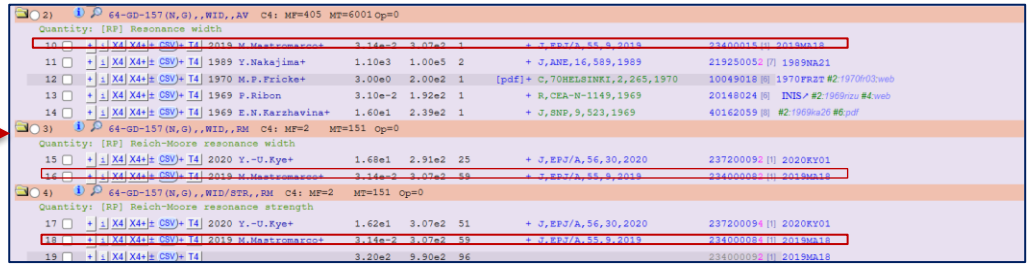
Summary of ENEA activities

- EXFOR: extraction of the Gd resonance parameters in C4 format;
- ENDF/B: replacement of the original resonance parameters with those extracted from EXFOR using a dedicated Python script;
- FORMAT CHECK: physics and formal verification using official utilities to ensure the internal consistency and correct formatting of the new ENDF/B file;
- PROCESSING: processing of the modified evaluation to generate continuous-energy ACE and multigroup libraries for Monte Carlo and deterministic codes;
- NUMERICAL CHECK: verification of the numerical consistency of the processed cross sections with the reference data using Monte Carlo calculations;
- BENCHMARK SELECTION: selection of gadolinium benchmarks from the official ICSBEP and IRPhE databases and preliminary test analysis.

Nuclear data: the EXFOR database

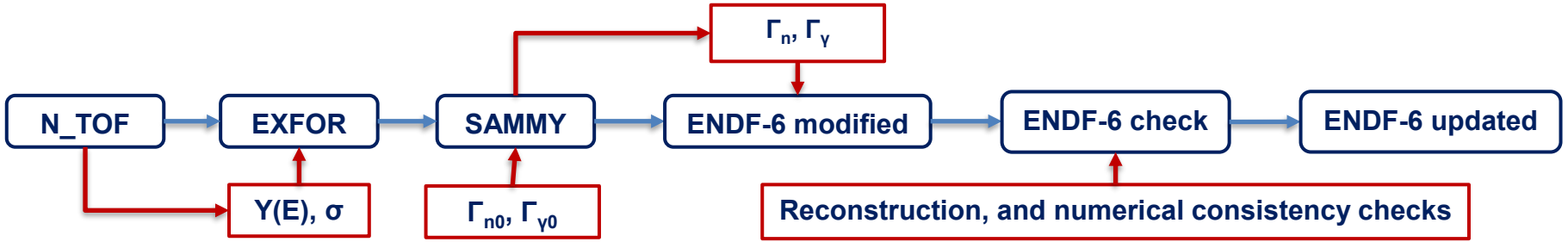
- Several nuclides relevant to nuclear technologies have been measured or are currently being measured at n_TOF and GELINA.
- The goal is to provide high-precision neutron-capture cross sections to address discrepancies among nuclear data libraries, investigate possible new resonances, and improve the predictive capability of the neutron-transport code.
- The analysis of the Gd-155 and Gd-157 measurements has been completed, and the data have been submitted to the EXFOR database.
- Therefore, **the ^{155}Gd and ^{157}Gd measurements were selected as the first test case for the calculation chain under development**.





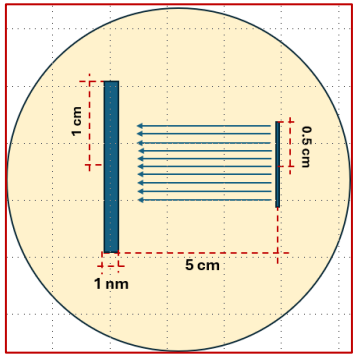
From n_TOF measurements to an ENDF-6 evaluation

- Nuclear data evaluation combines experimental measurements, reaction theory, models, and physical constraints into a consistent description of nuclear reactions.
- The evaluator combines experimental data, models, and constraints to produce a consistent and physically reliable representation.
- The evaluated file may contain resonance parameters, cross sections, angular and energy distributions, decay data, neutron multiplicities, and covariance information.
- These data are stored in the standard ENDF-6 format and can be processed for transport and reactor calculations. In this work, the **focus is on updating the Resolved Resonance Region (RRR)**.

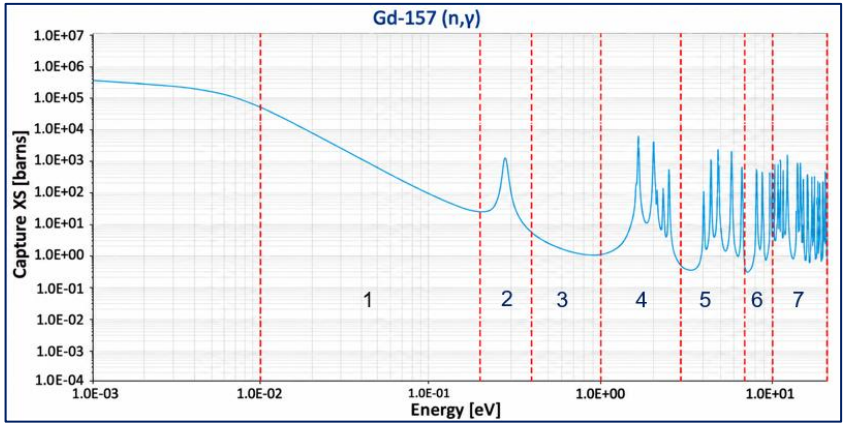


Consistency check of the updated ENDF/B: model

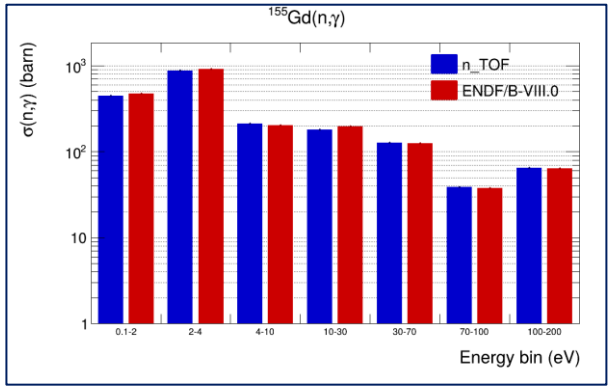
- The RRR gadolinium capture cross sections were updated using new resonance parameters obtained with SAMMY from n_TOF measurements, resulting in an updated ENDF/B evaluation.
- A differential analysis using MCNP was performed to assess the consistency of the updated data with the reference ENDF/B-VIII.0 evaluation.
- Two MCNP-based analyses were performed:
  - Comparison of Gd(n,γ) values over selected energy bins.
  - Comparison of k_{eff} sensitivity over the same energy bins.

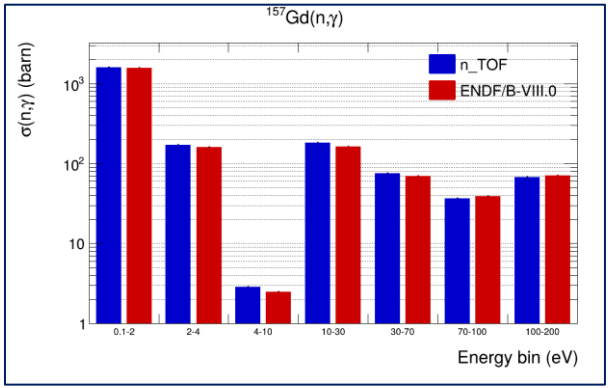


- **Geometry**: 2 × 2 cm² thin Gd-155 or Gd-157 foil, 1 nm thick;
- **Source**: 0.5 × 0.5 cm², 5 cm from the foil; uniform spectrum from 10^{-2} eV to 200 eV;
- **Tally:** microscopic capture cross section derived from (F14/F4 N) tally ratio;
- **Bin:** seven energy bins: 0.1-2, 2-4, 4-10, 10-30, 30-70, 70-100, and 100-200 eV



Consistency check of the updated ENDF/B: results

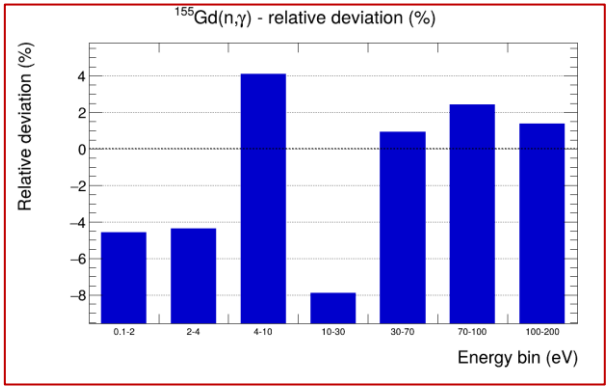


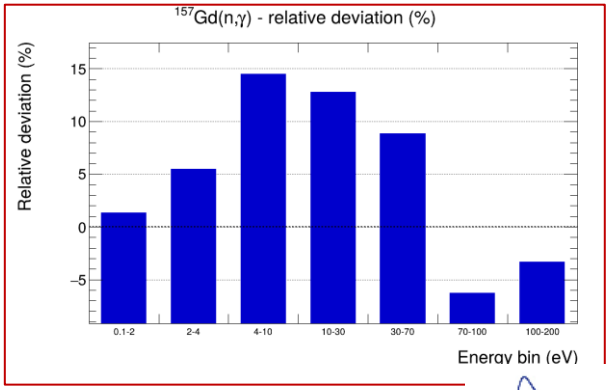


Gd-155: $|R_d| \leq 8\%$ across all energy bins

$$R_d = \frac{\sigma_{n_TOF} - \sigma_{ENDF/B}}{\sigma_{ENDF/B}} \ [\%]$$

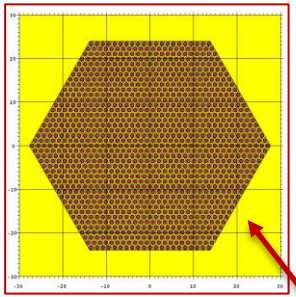
Gd-157: $|R_d| \leq 15\%$ across all energy bins

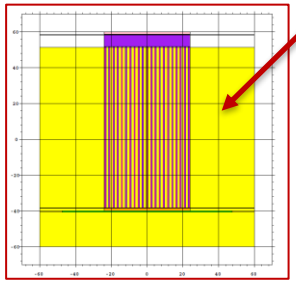




Sensitivity check of the updated ENDF/B: model

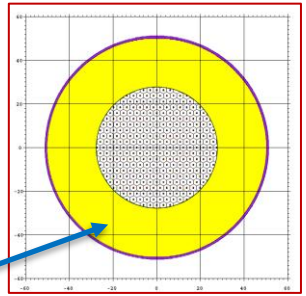
- To further assess the consistency of the updated ENDF/B data, a k_{eff} sensitivity analysis was also performed using MCNP6.
- Two official international benchmark configurations were selected as reference cases:





$Gd(NO_3)_3$ in H_2O

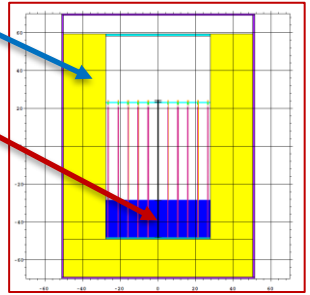
LEU-COMP-THERM-052: experimental critical configuration consisting of a hexagonal (or pseudo-cylindrical) fuel-rod assembly placed inside a parallelepiped tank. The system is moderated and reflected by a gadolinium nitrate solution. The gadolinium concentration was adjusted so that the critical solution height covered most of the fissile columns.



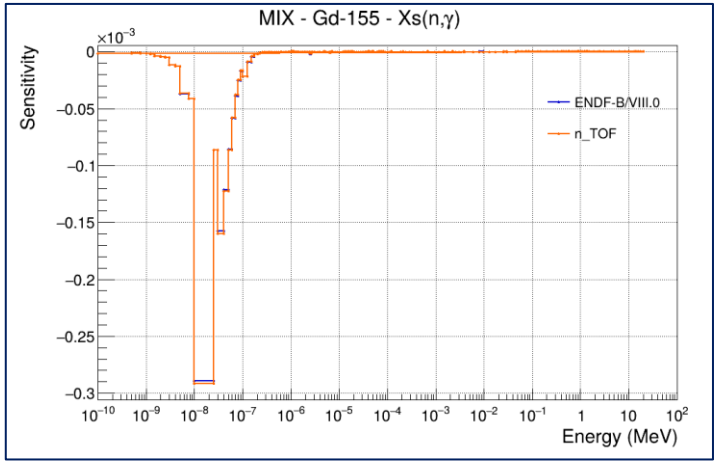
H_2O

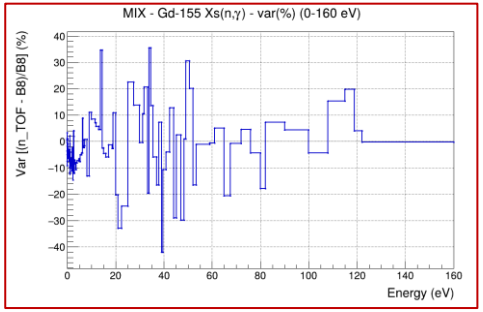
$UO_2(NO_3)_2$, + $Pu(NO_3)_4$ + $Gd(NO_3)_3$ in H_2O

MIX-MISC-THERM-004: experimental critical configuration consisting of triangular-lattice fuel pins contained in a stainless-steel inner vessel, positioned inside a larger water-filled reflector tank. The water level in the reflector tank was set equal to the top of the inner vessel.



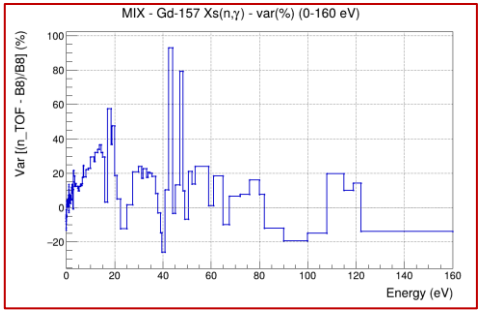
Sensitivity check of the updated ENDF/B: results



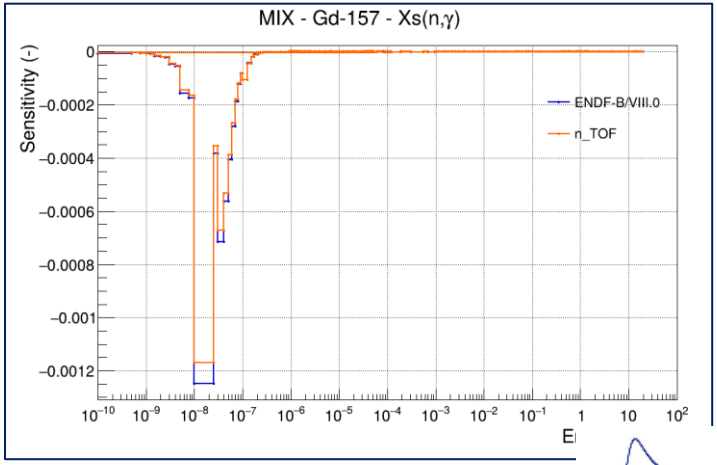


Gd-155: The absolute relative difference in sensitivity is below 40% in all thermal-to-epithermal energy bins.

$$S_i = \frac{dk/k}{d\sigma_i/\sigma_i}$$

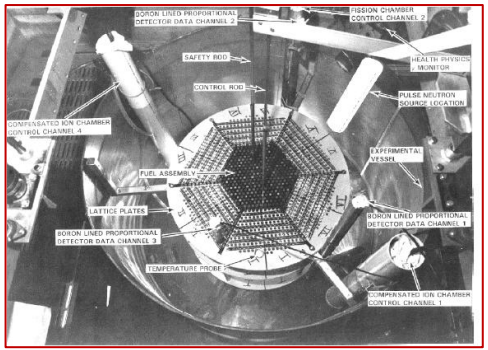


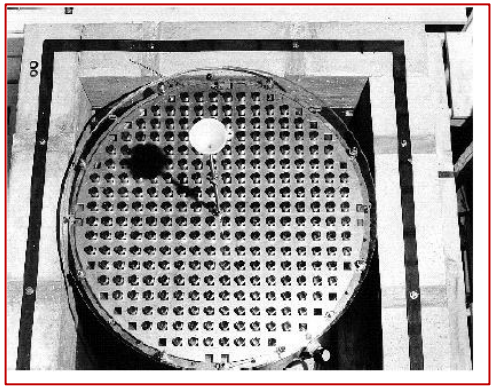
Gd-157: The absolute relative difference in sensitivity is below 100% in all thermal-to-epithermal energy bins



Nuclear data validation: ICSBEP & IRPhE

- **Nuclear data validation:** verify the capability of new XS to improve integral parameter predictions (i.e., k_{eff}) in neutronic code simulations using internationally evaluated experimental benchmarks;
- **ICSBEP and IRPhE**: primary international sources of integral experimental data for reactor physics and criticality safety applications, coordinated and maintained by OECD-NEA.





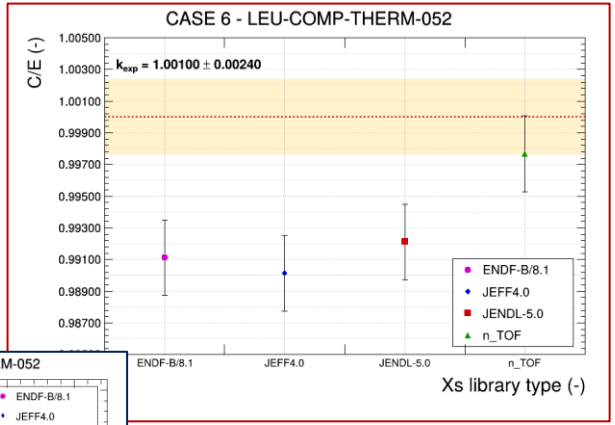
	ICSBEP	IRPhE
Gd-bearing configurations	354	61
Available MCNP input models	301	16
MCNP input availability	85.0%	26.2%

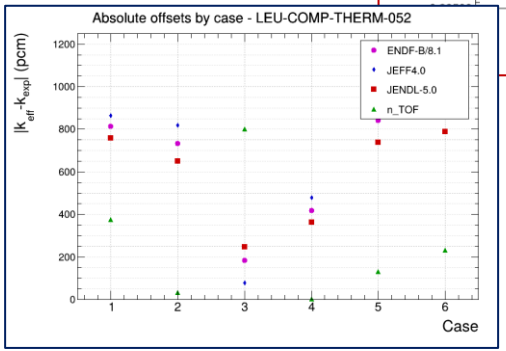
Validation results: LEU-COMP-THERM-052

$$|\overline{\Delta k}| = \frac{10^5}{N}\sum_i |k_{calc,i} - k_{exp,i}| \qquad \frac{X^2}{N} = \frac{1}{N}\sum_{i=1}^{N}\frac{(k_{calc,i} - k_{exp,i})^2}{\sigma^2_{exp,i} + \sigma^2_{MCNP,i}} \qquad |k_{calc,i} - k_{exp,i}| \leq 2\sqrt{\sigma^2_{exp,i} + \sigma^2_{MCNP,i}}$$

Gd-155/157 XS	$\lvert\overline{\Delta k}\rvert$ ± SD	X^2/N	within 2σ
ENDF/VIII.1	647 ± 282	9.85	1/6
JEFF-4.0	694 ± 350	11.80	1/6
JENDL-5.0	591 ± 229	8.03	2/6
n_TOF	262 ± 297	2.71	5/6

- **n_TOF Gd XS reduces the mean absolute offset by ~ 56% (ref. JENDL-5.0) and brings 5/6 config. within 2σ.**
- **n_TOF Gd XS gives the lowest mean |Δk| and the lowest indicative X^2/N**



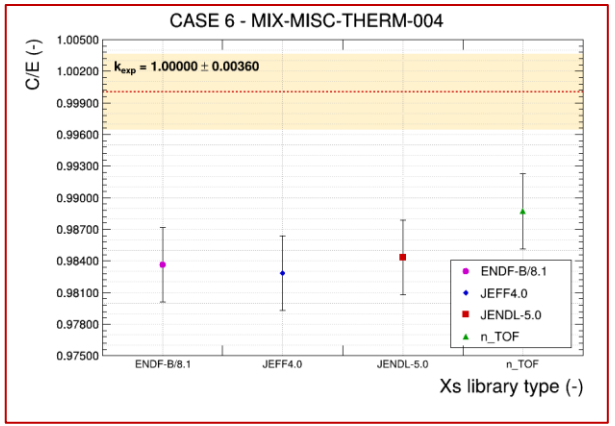


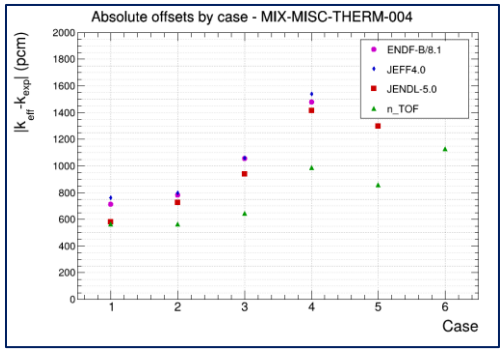
- **CASE 3 remains the main positive outlier and dominates the increase in residual dispersion.**

Validation results: MIX-MISC-THERM-004

$$|\overline{\Delta k}| = \frac{10^5}{N}\sum_i |k_{calc,i} - k_{exp,i}| \qquad \frac{X^2}{N} = \frac{1}{N}\sum_{i=1}^{N}\frac{(k_{calc,i} - k_{exp,i})^2}{\sigma_{exp,i}^2 + \sigma_{MCNP,i}^2} \qquad |k_{calc,i} - k_{exp,i}| \leq 2\sqrt{\sigma_{exp,i}^2 + \sigma_{MCNP,i}^2}$$

Gd-155/157 XS	$\lvert\overline{\Delta k}\rvert$ ± SD	X^2/N	within 2σ
ENDF/VIII.1	1176 ± 383	13.29	0/6
JEFF-4.0	1220 ± 401	14.27	0/6
JENDL-5.0	1088 ± 398	11.49	1/6
n_TOF	791 ± 237	5.99	1/6

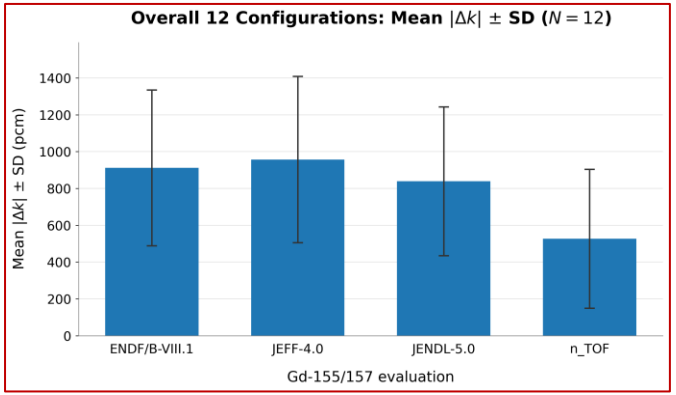


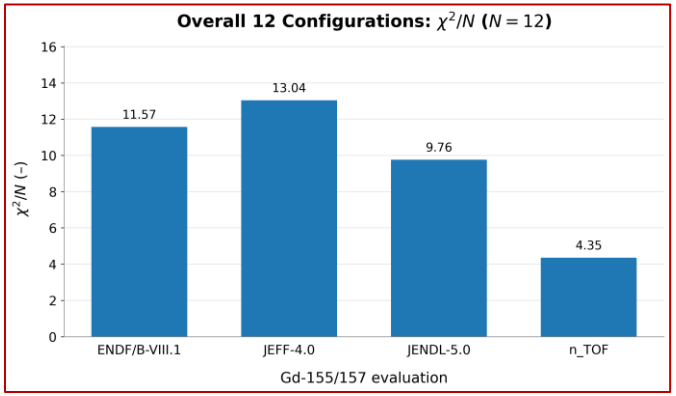


- **n_TOF Gd XS reduces the mean absolute offset by ~ 72% (ref. JENDL-5.0) and brings 1/6 config. within 2σ.**
- **n_TOF Gd XS gives the lowest mean |Δk| and the lowest indicative X^2/N**

Overall validation results: 12 configurations

Gd-155/157 XS	$\lvert\overline{\Delta k}\rvert$ ± SD	X^2/N	within 2σ
ENDF/VIII.1	912 ± 423	11.57	1/12
JEFF-4.0	957 ± 452	13.04	1/12
JENDL-5.0	839 ± 404	9.76	3/12
n_TOF	527 ± 377	4.35	6/12





- **n_TOF Gd XS gives the lowest mean |Δk| and the lowest indicative X^2/N across the full 12-case set.**
- **n_TOF Gd XS reduces the mean absolute offset by ~ 37% (ref. JENDL-5.0) and brings 6/12 config. within 2σ.**

Conclusion

- ENEA is developing the expertise required to establish a **complete calculation chain from EXFOR experimental data to evaluated ENDF nuclear data** and validation analysis.
- The **capability to update existing ENDF evaluations with new RRR data from n_TOF experiments and to process the resulting files for MC codes** has been established.
- A **validation campaign based on official international criticality benchmarks** has been initiated to assess the impact of the new Gd evaluations on k_{eff} predictions.
- **Preliminary results**, based on a limited number of benchmark configurations, **indicate that the new n_TOF Gd data improve the overall agreement with experiments**, reducing both the mean absolute k_{eff} deviation and the indicative X^2/N.

Thank you for your attention!

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