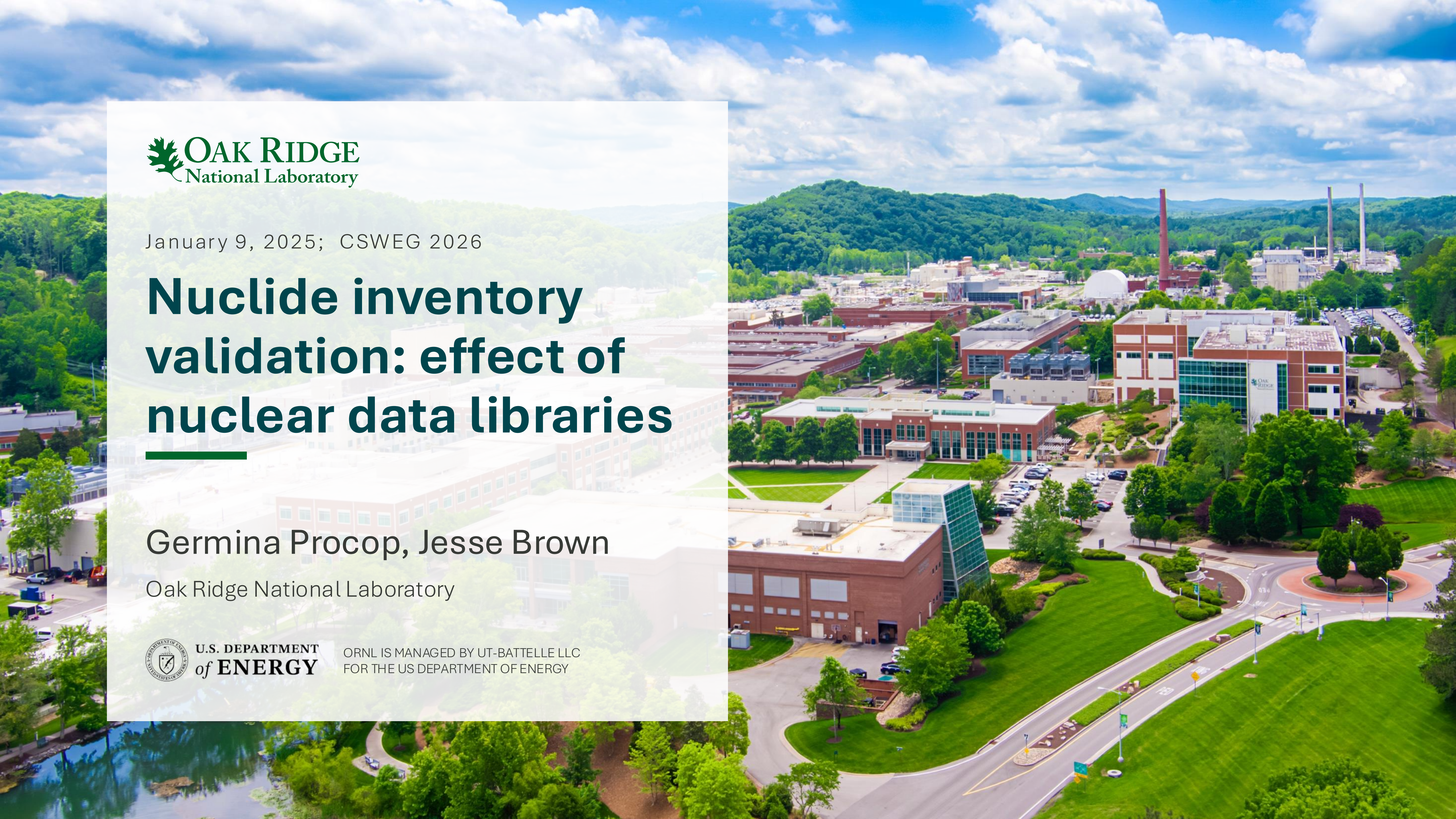

Oak Ridge National Laboratory

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Nuclide inventory validation: effect of nuclear data libraries

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Oak Ridge National Laboratory

Goal: Assess the effect of ENDF/B cross section libraries on nuclides relevant to inventory validation for spent nuclear fuel applications

Quantify the effect of the nuclear data library on the C/E nuclide concentration ratio for selected actinides and fission products

Use as basis measured nuclide concentrations from radiochemical assay (RCA) experiments performed at ORNL, for four PWR spent fuel samples with burnups in range 30-70 GWd/MTU

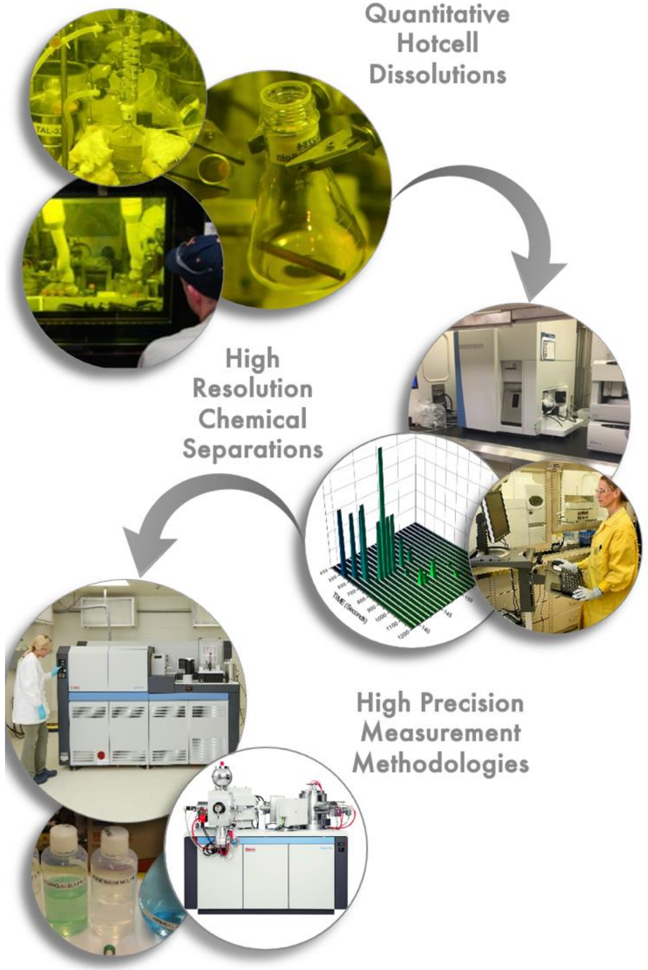
Cross section libraries considered:

ENDF/B-VII.1, ENDF/B-VIII.0, ENDF/B-VIII.1

This is a follow-up on “Germina Ilas and Jesse Brown, Nuclide Inventory Validation: Effect of Nuclear Data Libraries, Proc. of Int. Conf. on the Physics of Reactor (PHYSOR 2024), p. 1122-1130, San Francisco, CA (2024).
https://www.osti.gov/biblio/2397461

Why do we need radiochemical assay (RCA) data ?

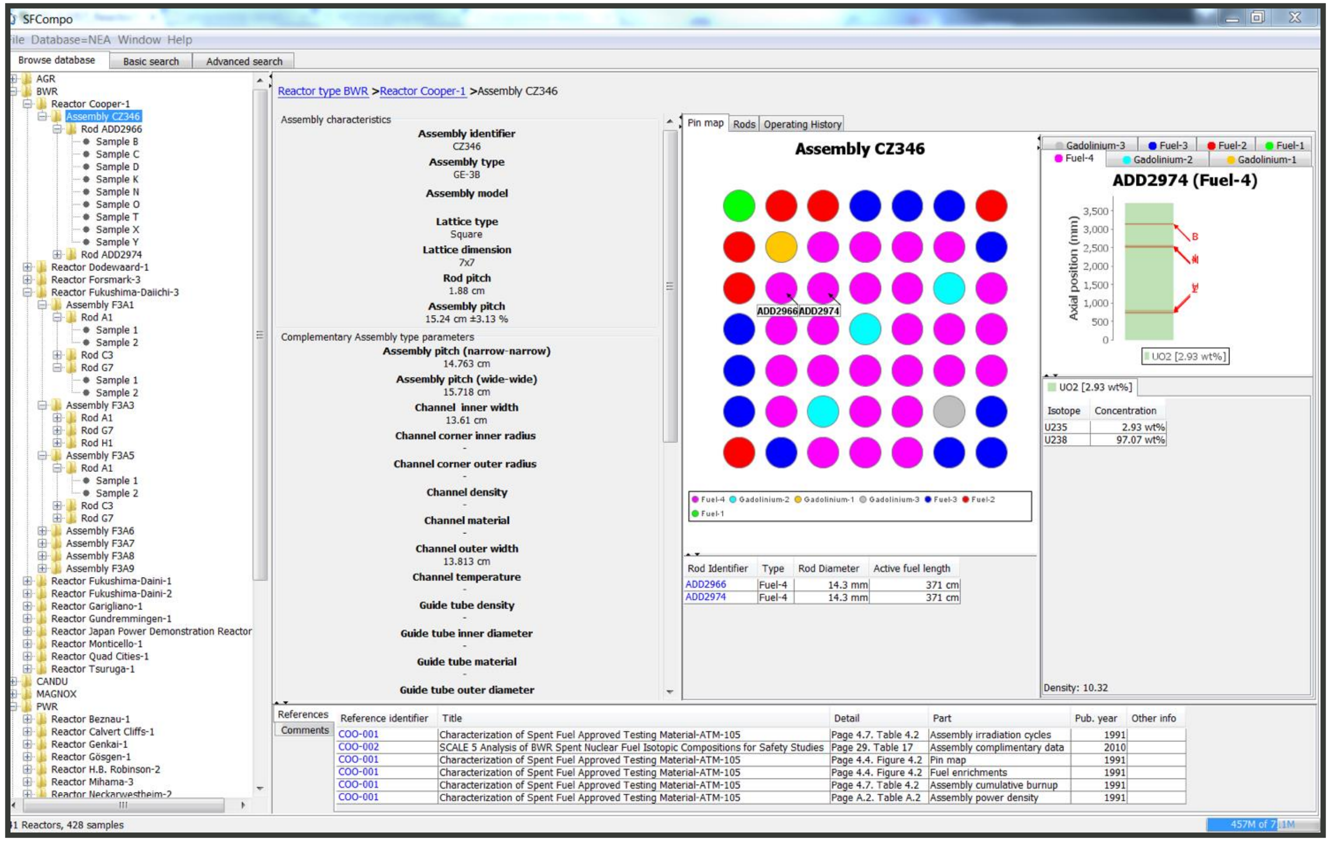
Provide a reliable basis for validating calculated nuclide inventories in irradiated nuclear fuel and other materials	Understand applicability of depletion codes and associated nuclear data in lattice and full-core physics safety-related analyses, and in spent fuel transportation, storage, and disposal applications
Adress challenges in any area where simulating nuclide transmutation and decay in nuclear fuel and other materials during and post irradiation is critical	Impact goes well beyond reactor physics and the nuclear fuel cycle, e.g., isotope production, national security, and nonproliferation applications
Determine bias and uncertainty in calculated nuclide inventories	Adequately cover the changing fuel characteristics space and fill in existing gaps - higher enrichments and burnups, ensure safety and security of soon to be deployed new reactor technologies



What are the current RCA data resources ?

SFCOMPO is the largest international database of open experimental assay data for spent nuclear fuel

- Hosted/maintained by OECD/NEA and managed by the SFCOMPO Technical Review Group
- Contains assay data for **750 samples** from fuel irradiated in **44 reactors** of **8 types**
- SFCOMPO is publicly available and can be downloaded from the NEA website
- Currently under modernization, to migrate to GitLab for improving access, development and QA, providing APIs, enabling better user collaboration.



SFCOMPO graphical user interface

F. Michel-Sendis et al, “SFCOMPO-2.0: An OECD NEA database of spent nuclear fuel isotopic assays, reactor design specifications, and operating data”, Annals of Nuclear Energy, vol. 110 (2017) https://doi.org/10.1016/j.anucene.2017.07.022

Challenges in applying existing RCA experiment data to reliably estimate bias and uncertainty and improve code predictions

Experiments are expensive and require specialized facilities, equipment, instruments, and expertise

To ensure adequate coverage over space of fuel characteristics, we need to make the most of what we have available

Majority of existing data comes from experimental programs prior to 2000s, different than the current state-of-the-art experimental capabilities

How to account for underreported or unknown experimental uncertainties ?

Measured fuel characteristics are not typical of current, modern fuels burnups, design and operation

How to extrapolate knowledge to modern fuel ?

Important modeling data are missing or have large reported uncertainties, important nuclear data may have large or no uncertainties

How to how to address important unknown information ?

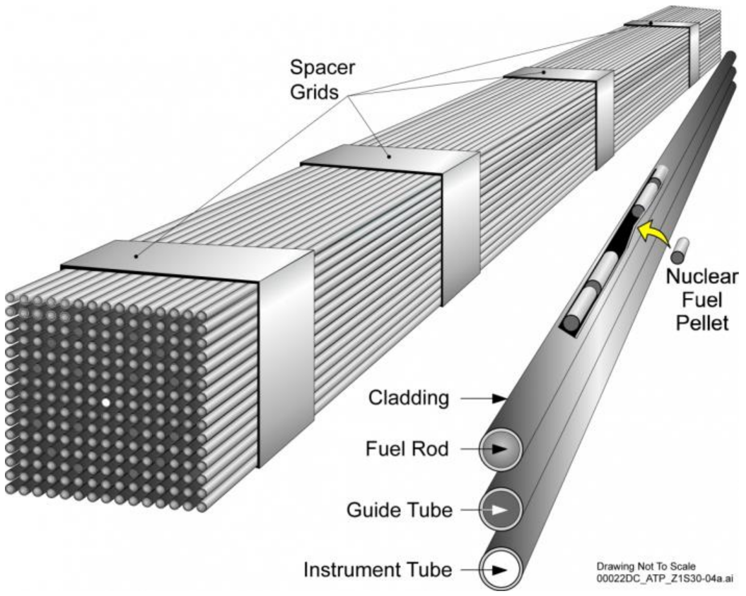
Effect of the nuclear data library on calculated nuclide inventory and validation results was estimated for 4 PWR measured fuel samples

Measurement data for ORNL-measured PWR spent fuel samples in 2020-2021, with available high-precision RCA and adequate fuel design and irradiation history data (less sensitive to limitations in the input data available f or modeling)

Fuel Sample #	Sample ID	Exp. Burnup (GWd/MTU)	Enrichment (wt % ^{235}U)	Cooling time (yr)
1	3A1-F05-150-165	37.5	4.0	27
2	3A1-F05-225-240	43.5	4.0	27
3	3D8-E14-775-796	64.2	4.2	21
4	3D8-E14-1375-1450	64.9	4.2	21

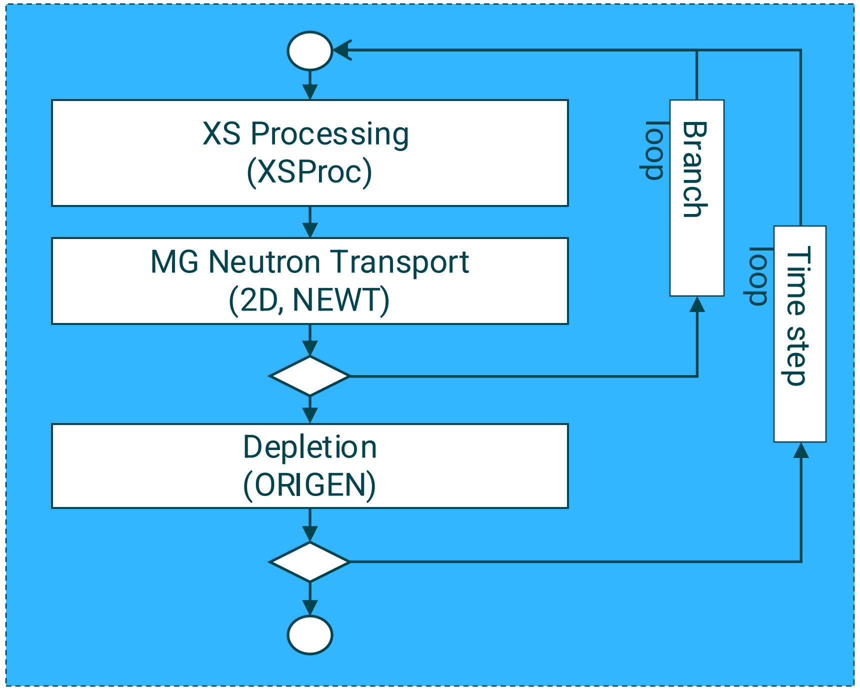
Ref: G. Procop, B. Bevard, J. Giaquinto (2025). Extending the Nuclide Inventory Validation Basis for High-Burnup Fuel with New Radiochemical Assay Data", Nuclear Science and Engineering https://doi.org/10.1080/00295639.2025.2527491

SCALE/TRITON was used for nuclide inventory validation



Fuel design and operation data

- Input (**.inp**)
- Nuclear Data Libraries: 252g ENDF/B-VII.1 XS



- Output (**.out**)
- Few-group XS File (**.t16**)
- ORIGEN Concentration File (**.f71**)
- ORIGEN Library File (**.f33**)

TRITON flowchart MG mode

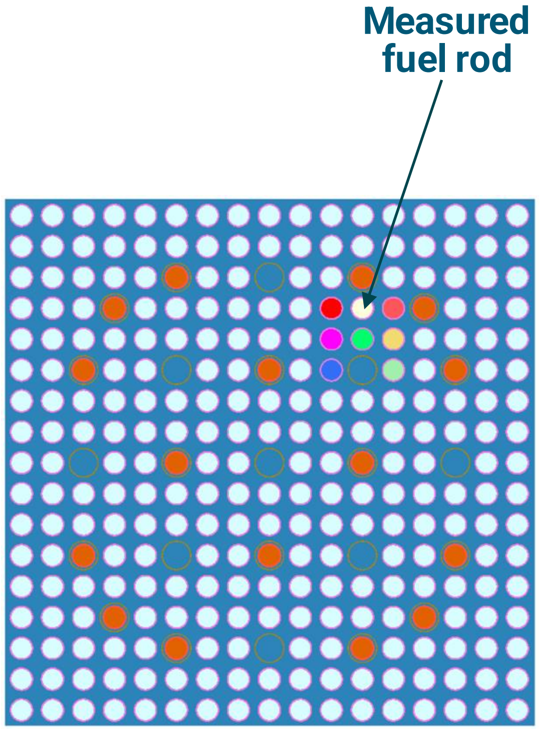
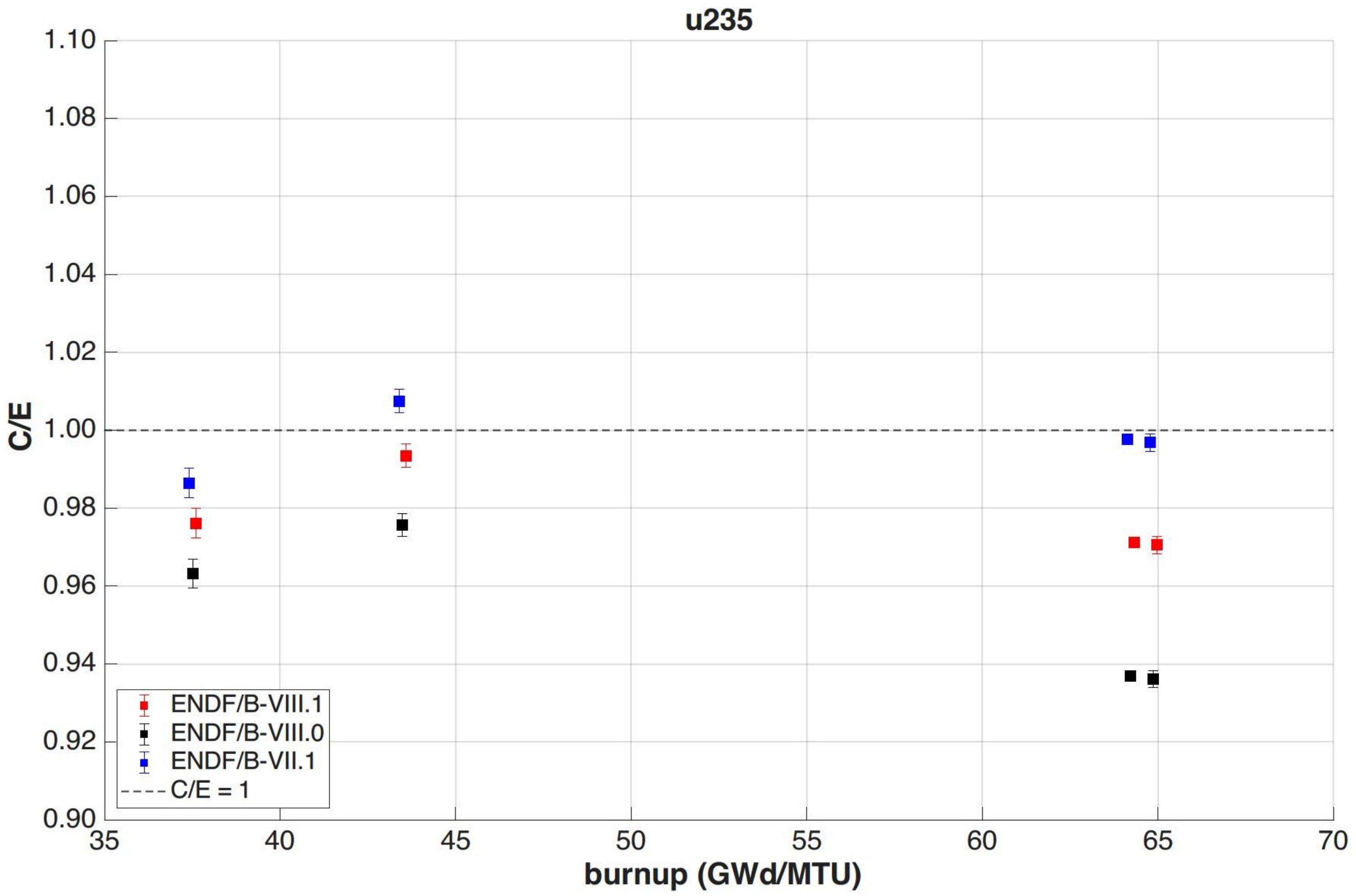


Illustration of a
2D TRITON model

Ref. for flowchart: Oak Ridge National Laboratory. n.d. "Depletion Calculations with." SCALE 6.3. Accessed Jan 2,2026. https://www.ornl.gov/content/scale-63.

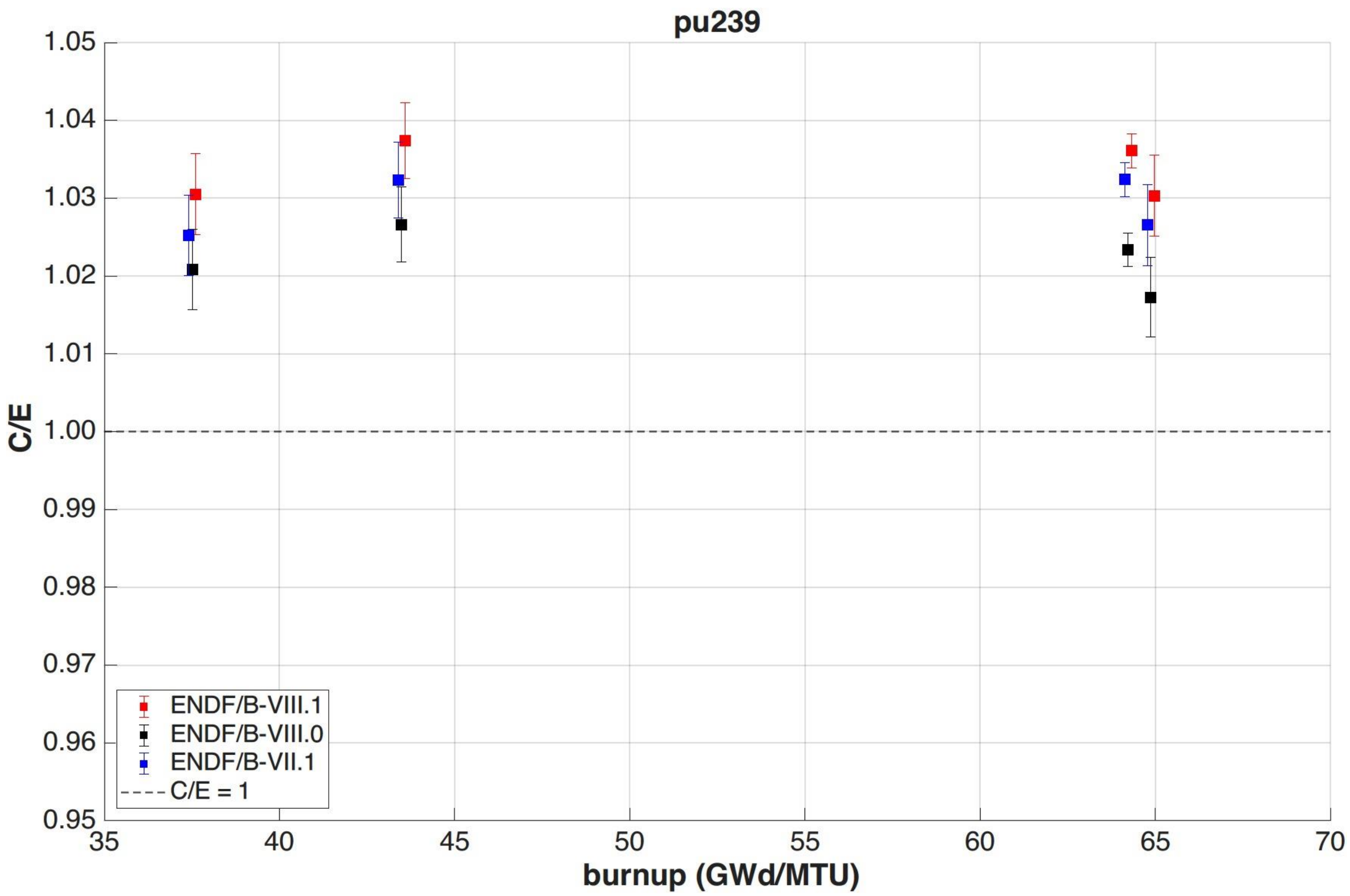
Comparison of calculated and experimental nuclide inventories

C/E vs burnup for ^{235}U: Significant underestimation relative to measurement is observed for ENDF/B-VIII.0 (6% at high burnup)



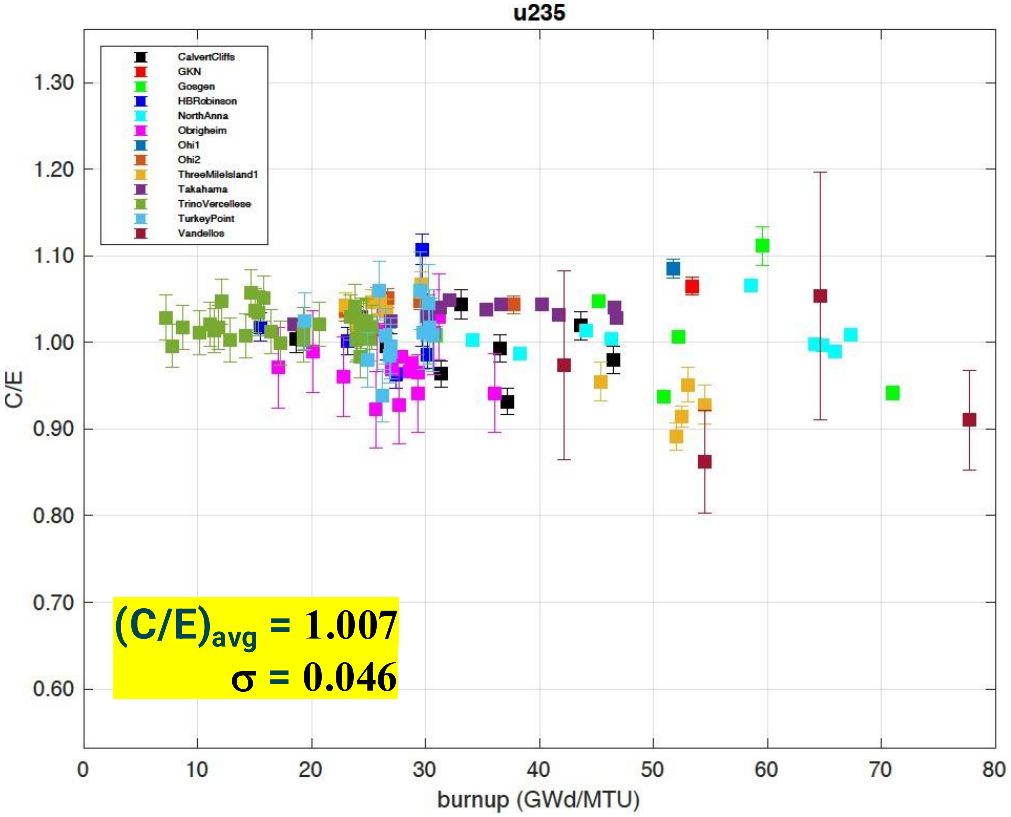
Error bars reflect only the reported measurement uncertainties (2σ).

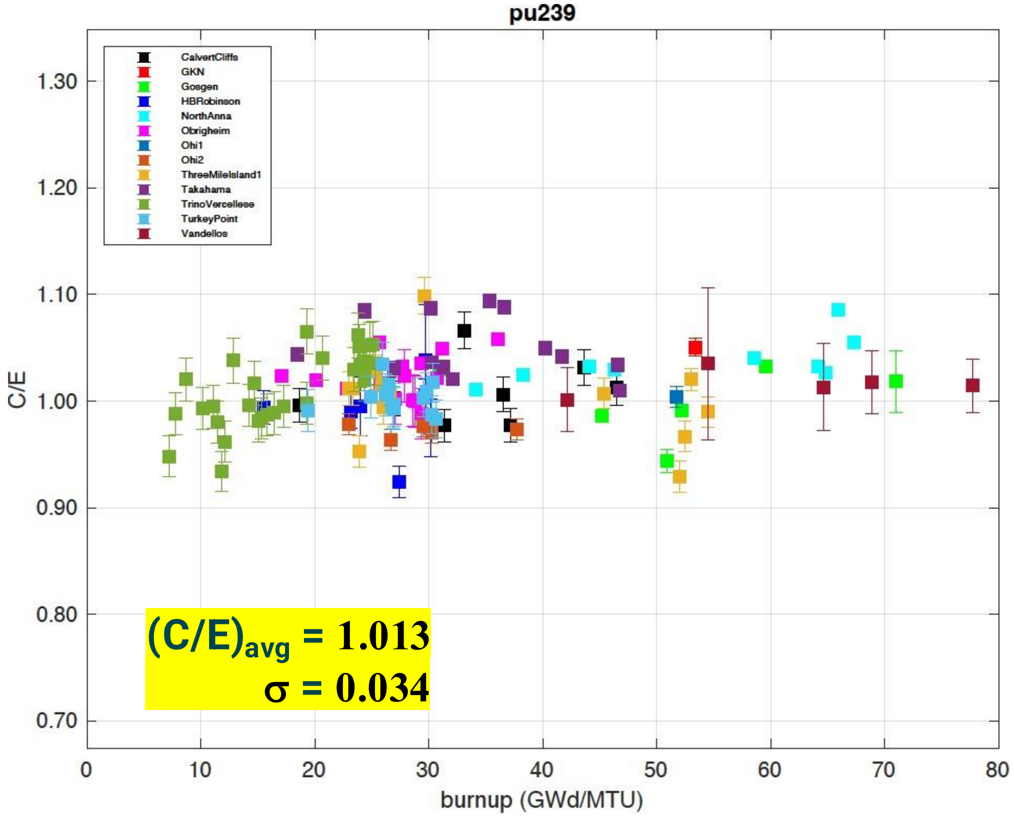
C/E vs burnup for ^{239}Pu: General agreement is observed among results obtained with different libraries



Error bars reflect only the reported measurement uncertainties (2σ).

How well are major actinides generally predicted with ENDF/B-VII.1? C/E results obtained for 129 PWR spent fuel samples

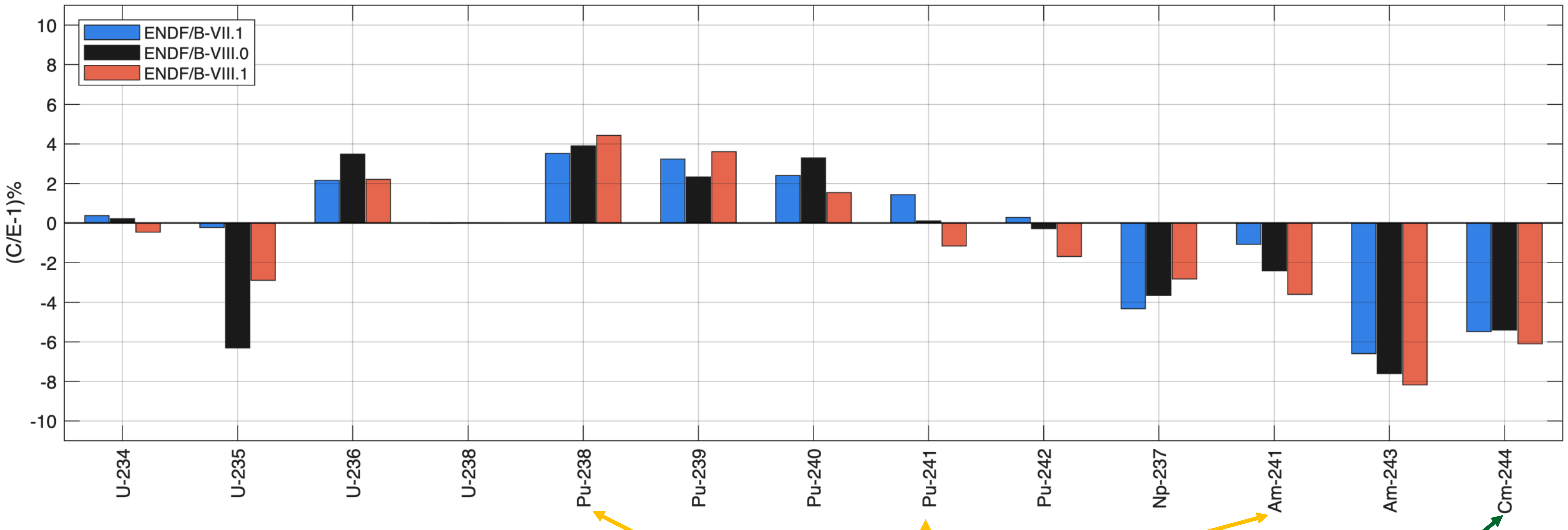




The 4 samples used as basis here are part of the North Anna 9 samples data set (cyan color).

Ref: G. Procop, R. Elzohery, B. Hiscox, U. Mertyurek, "SCALE 6.3 Validation: Spent Nuclear Fuel", ORNL/TM-2023/2884/v3, Oak Ridge National Laboratory (2025). https://doi.org/10.2172/2587031

Actinides: comparison calculation-experiment for sample #3 (64 GWd/MTU)

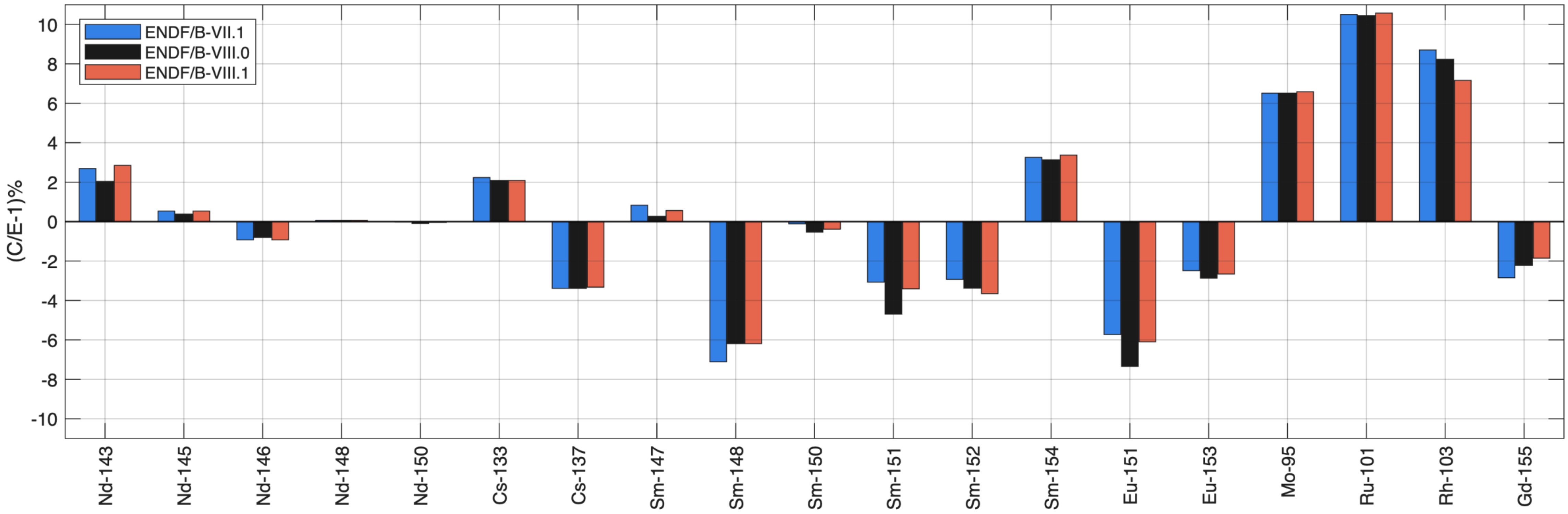


Most of these actinides are important for reactivity (crit safety with burnup-credit)

Key long-term contributors to decay heat

Largest contributor to neutron source for LWR spent fuel

Fission products: comparison calculation-experiment for sample #3 (64 GWd/t)



Most of these are key absorbers relevant to for reactivity (crit safety with burnup-credit)

^{137}Cs is key nuclide for decay heat and shielding applications, burnup monitor

Important for reactor operation: strong neutron absorbers such as ^{155}Gd and Sm isotopes

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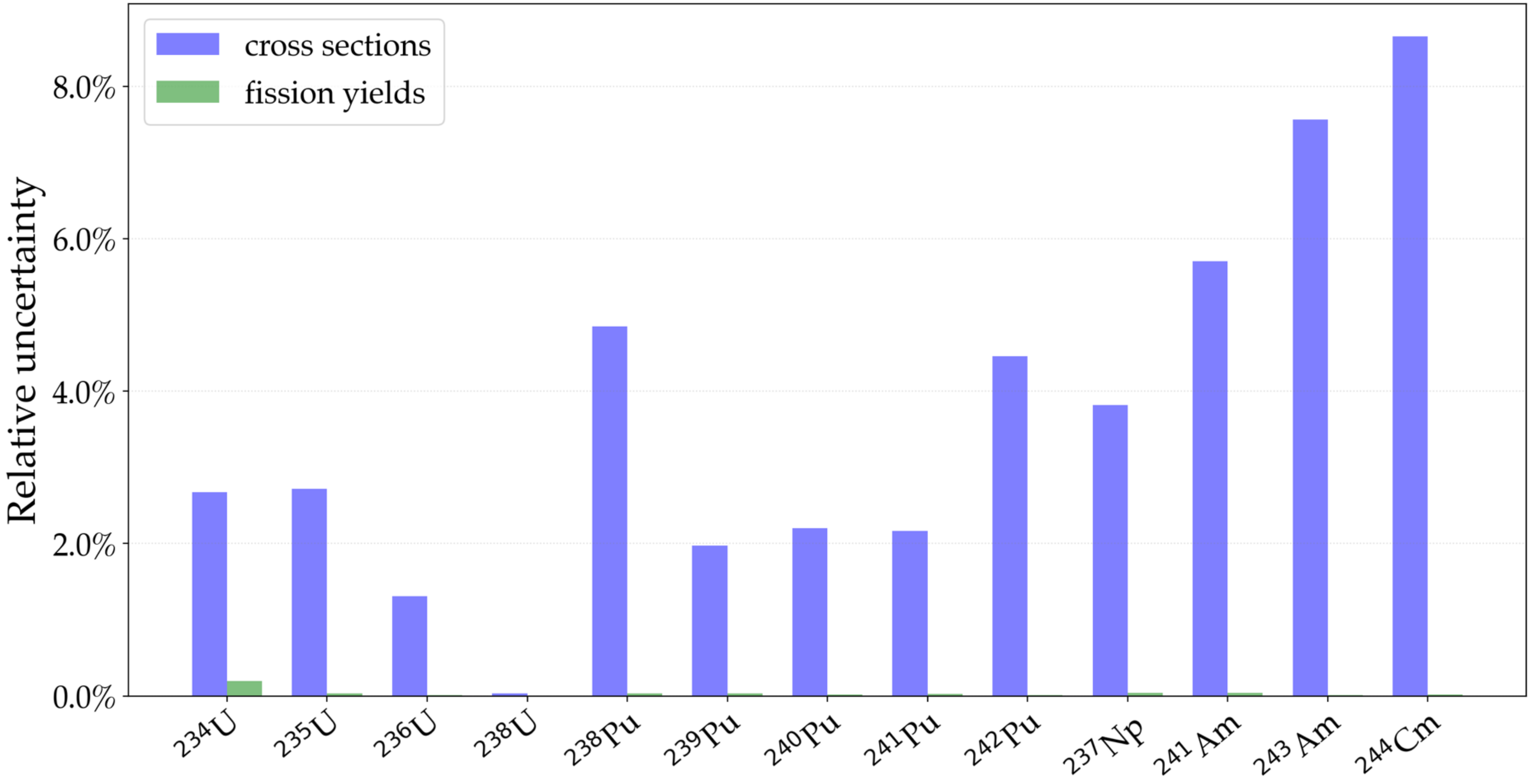
Uncertainties in calculated nuclide inventories that result from uncertainties in cross section (XS) and fission product yield (FPY) data

For sample #3, burnup 64 GWd/MTU

Covariance data **ENDF/B + BLO**

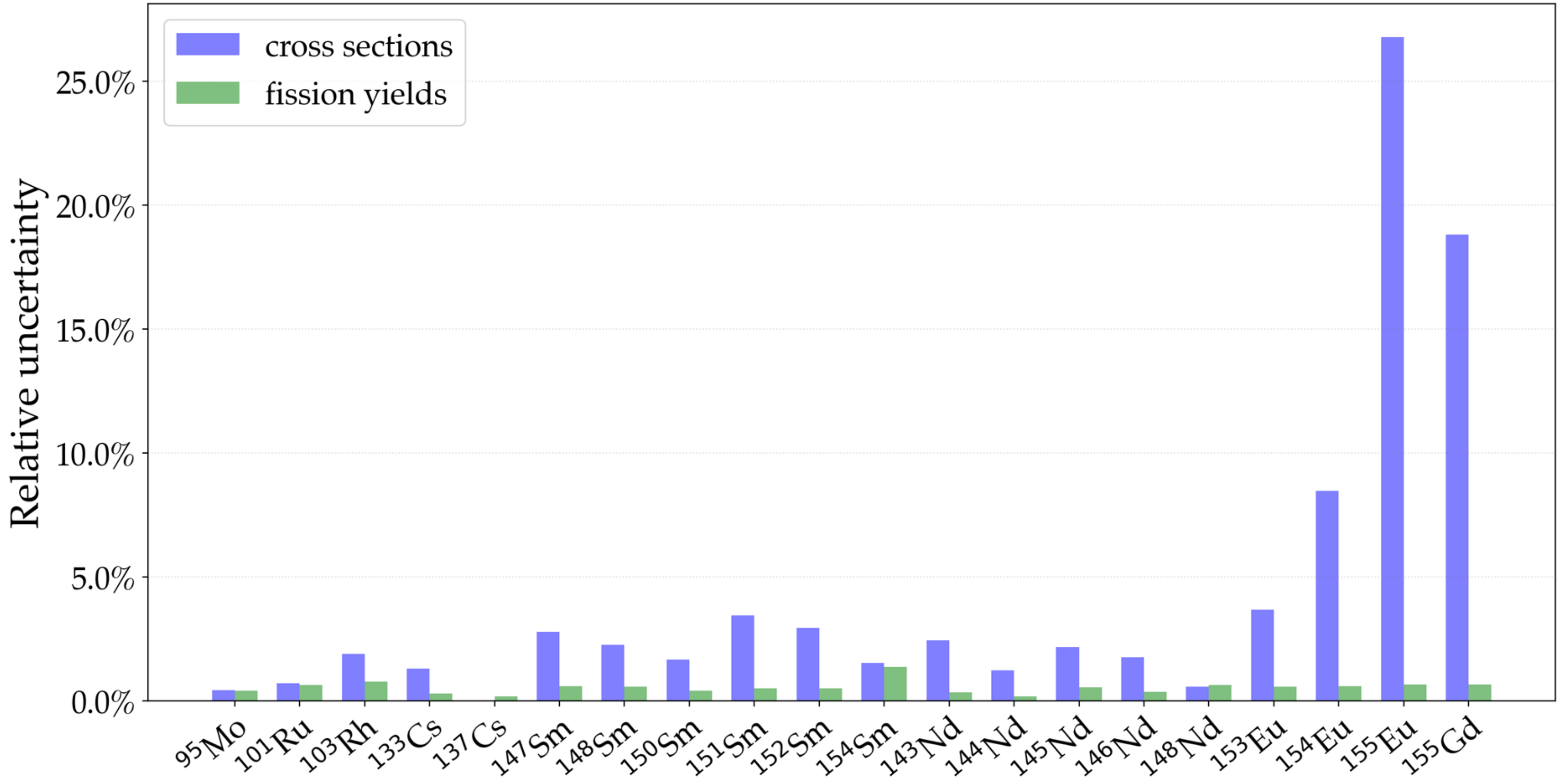
ENDF/B-VII.1 : Effect of uncertainty in XS and FPY data on calculated actinides inventories



Relative uncertainty > 5%
^{238}Pu, ^{241}Am, ^{243}Am, ^{244}Cm

Cross section uncertainties are major drivers for uncertainties of calculated actinide concentrations, no significant impact of fission yield uncertainties.

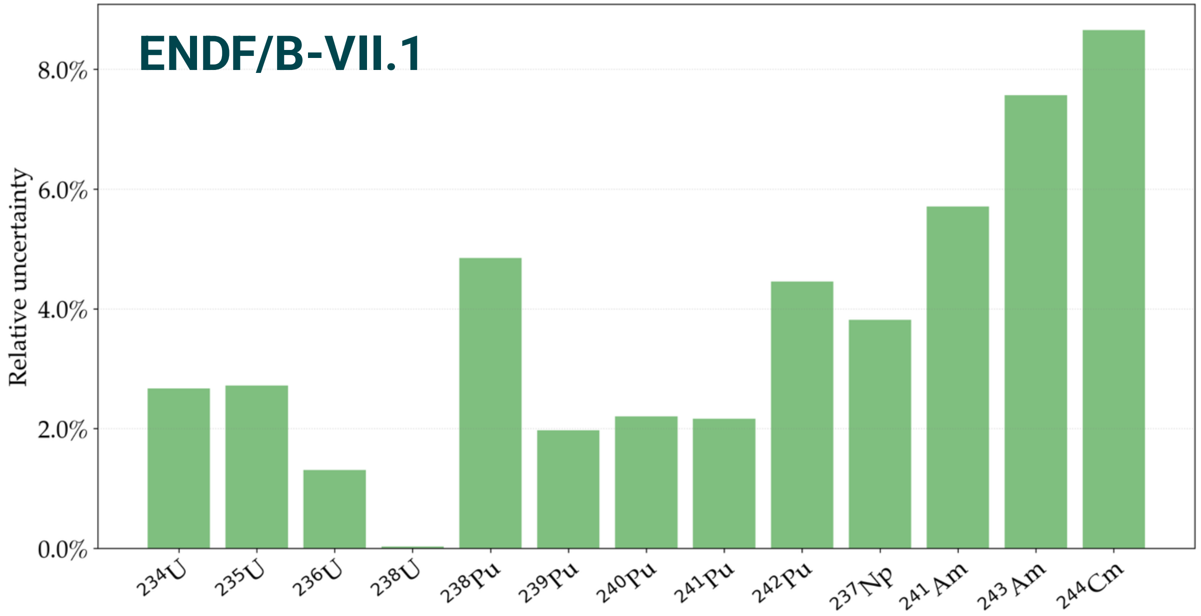
ENDF/B-VII.1 : Effect of uncertainty in XS and FPY nuclear data on calculated FP inventories

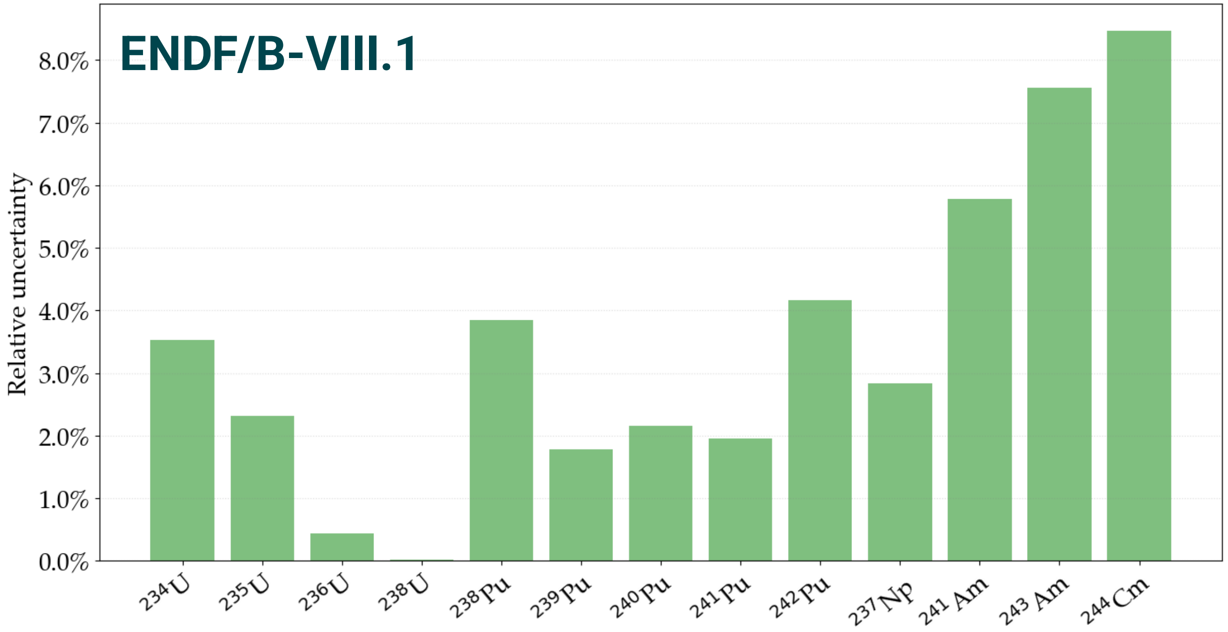


Relative uncertainty > 5%
^{154}Eu, ^{155}Eu, ^{155}Gd

Cross section uncertainties are major drivers for uncertainties of calculated fission products concentrations, generally no significant impact of fission yield uncertainties.

ENDF/B-VII.1 vs ENDF/B-VIII.1: Effect of XS data uncertainty on uncertainties in calculated actinides inventories

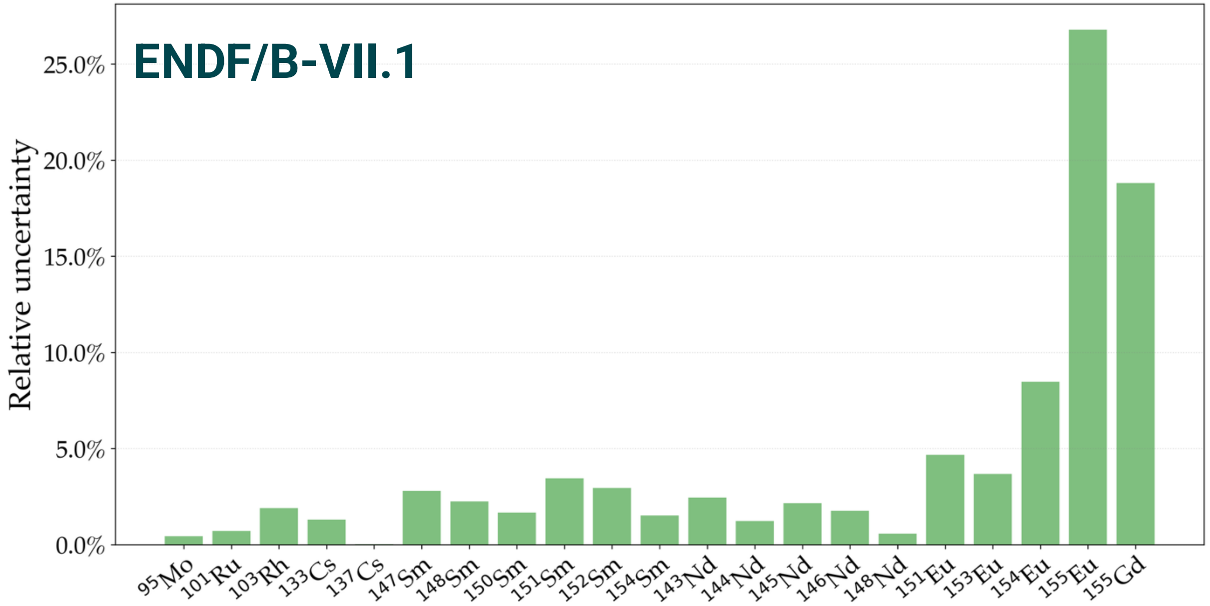


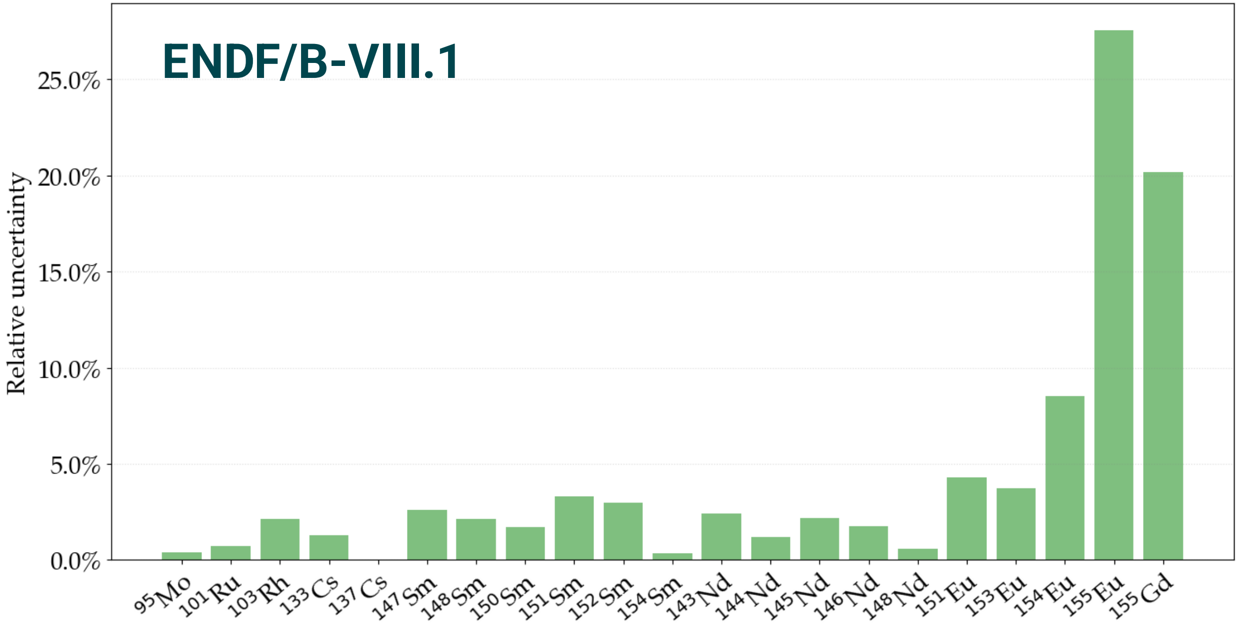


Differences in uncertainty estimates between ENDF/B-VIII.1 and ENDF/B-VII.1 are:

- **> 1%** for ^{238}**Pu** (-1.01%)
- **0.5% - 1%** for ^{234}**U**, ^{236}**U**, ^{237}**Np**
- **< 0.4%** for the other nuclides shown

ENDF/B-VII.1 vs ENDF/B-VIII.1: Effect of XS data uncertainty on uncertainties in calculated fission products inventories

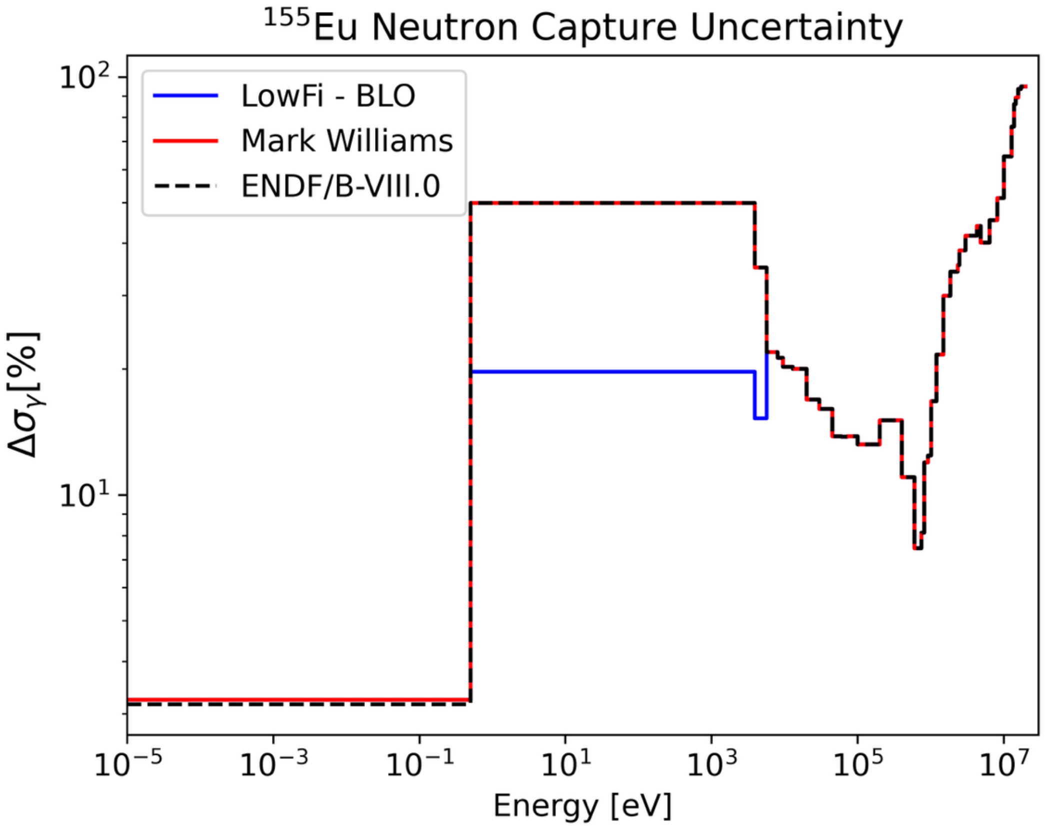




Differences in uncertainty estimates between ENDF/B-VIII.1 and ENDF/B-VII.1 are:

- **> 1%** for **^{155}Gd** (+1.4%) and **^{154}Sm** (-1.2%)
- **0.5% - 1%** for **^{155}Eu** (+0.8%)
- **< 0.4%** for the other nuclides shown

Large differences among ENDF/B libraries for Eu-155(n,g) uncertainty may be confusing to and are impactful for the end users of the data



- ENDF/B-VII.1 library had covariance data from the LowFi project; *SCALE used Mark Williams's "special" E7.1 file instead*
- ENDF/B-VIII.0 data looks similar, though is not the same, with Mark Williams's evaluation
- ENDF/B-VIII.1 ***provides zero covariance***

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^{155}Gd is only one example emphasizing the importance of reliable uncertainty data for thermal reactor safety and back-end of fuel cycle

Gd is a cornerstone of advanced fuel design and operation

^{155}Gd is one of the most effective neutron absorbers used to control reactivity during operation

Gd consideration goes well beyond LWR/UO_2 fuel

Accident tolerant fuel, (ATF), improved TRISO-based fuel, high-density fuel

Gd use can be critical to LWRs and advanced reactors operation

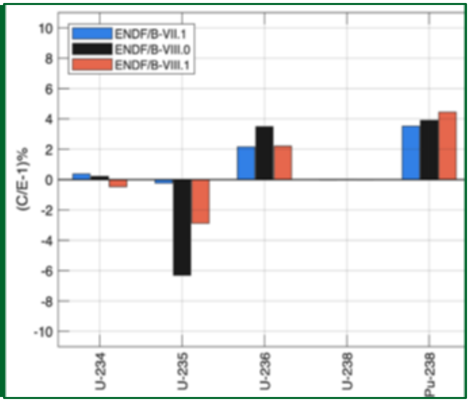
Enables passive and self-regulating reactivity control, longer fuel cycles, simplified operational strategies

Effective use of Gd requires effective computational tools and associated nuclear data

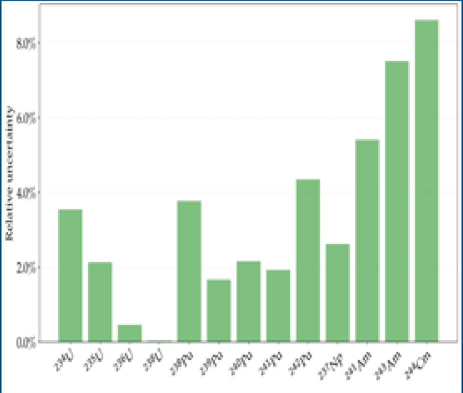
Well-validated depletion tools for accurate tracking of ^{155}Gd and ^{157}Gd, validated cross section data with well-understood uncertainty

Significance/impact of findings from an end-user perspective

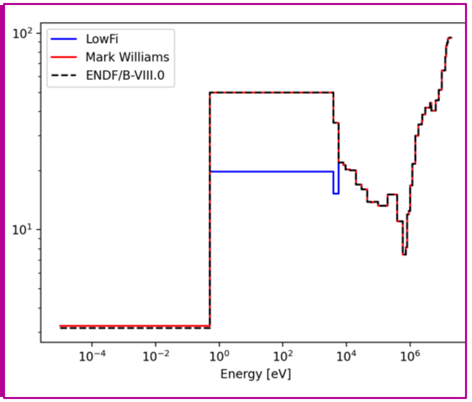
Change in the cross-section library has an important effect on calculated nuclide inventory. Which library should I use?



XS-induced uncertainty in calculated nuclides contents can be greater than that resulting from modeling data. How could I reduce it?



XS uncertainty data can vary significantly from library to library. Which one should I trust?



Small differences in ND and uncertainties might seem non-impactful. For user applications and regulatory purposes, the ultimate effect may be consequential.

How could we better embed the user experience in ND generation, evaluation, and validation?

Acknowledgments

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Questions ?

Indian Summer in Smoky Mtns, Dec 2025, Mount LeConte