

Fission Product Yields: SCALE/ORNL Perspective

Jesse Brown, Will Wieselquist, Steve Skutnik, Rike Bostelmann, Germina Ilas, Jordan McDonnell

Oak Ridge National Laboratory

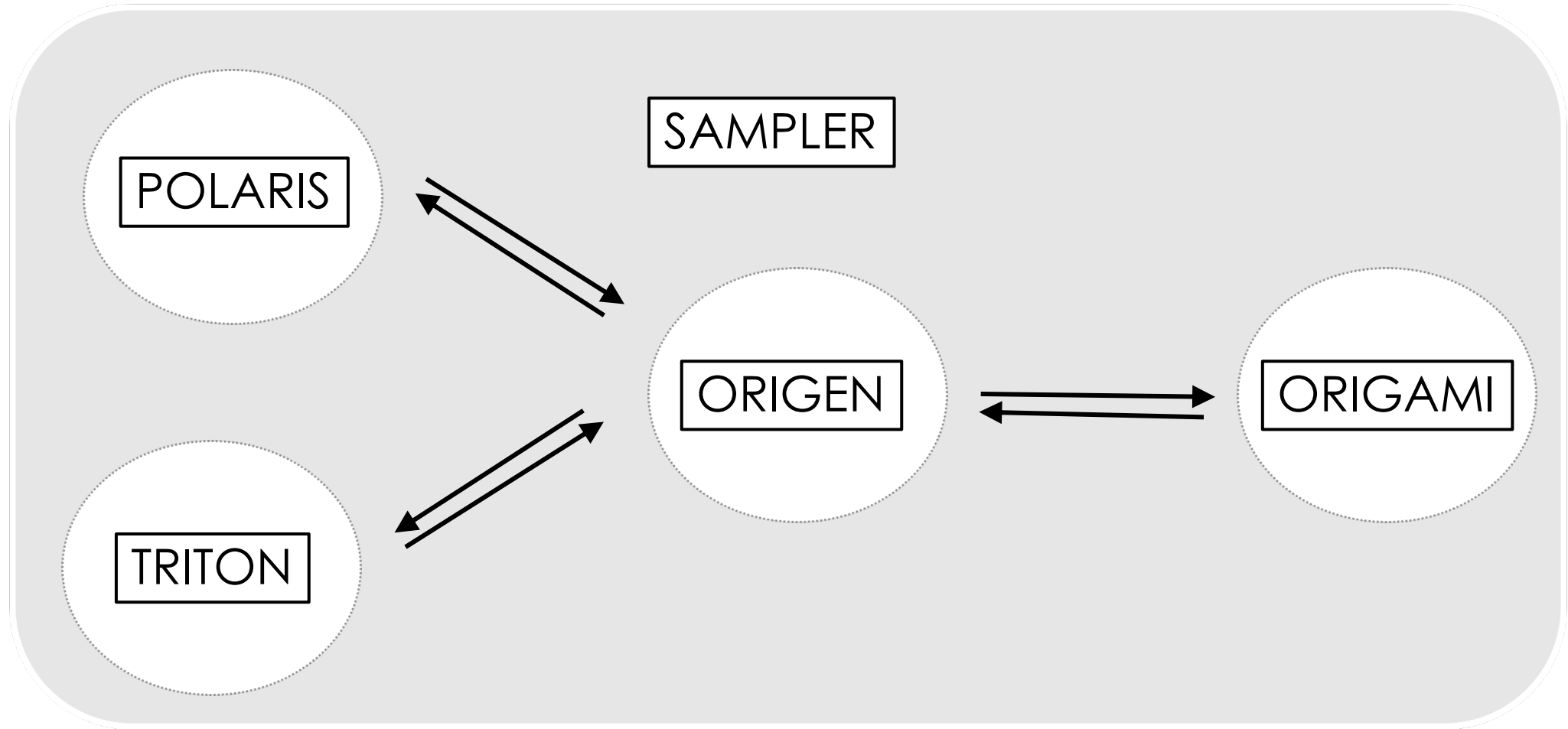
WANDA: Feb. 27- Mar 2, 2023

ORNL is managed by UT-Battelle, LLC for the US Department of Energy



U.S. DEPARTMENT OF
ENERGY

SCALE products using FPY



Critical Asset for Validation

ORIGEN

- Oak Ridge Isotope Generation code in SCALE
- Irradiation and decay simulation code for general purpose isotopic inventory tracking, **not** tracking an application-specific subset of isotopes
 - 2,237 isotopes
 - 176 actinides
 - 1151 fission products
 - 910 structural activation nuclides
 - 54,000 transitions between isotopes
 - All pathways in modern nuclear data for neutron transmutation, fission, & decay
 - All nuclides with half-lives > 1 ms

Key Capabilities

- Calculation of isotopic inventories and source terms
 - Nuclide concentrations (atoms and mass)
 - Activities
 - Decay heat
 - Radiation emission rates and spectra (neutron and gamma)
 - Radiotoxicity
- Application environments
 - operating reactors
 - spent fuel storage/handling
 - Structural material activation (in-core, ex-core)
 - Fuel cycle analysis (Material feed and removal processing)
- Methods and data enable comprehensive isotopic characterization of fuel **over a large time scale (milliseconds to billions of years)**

Note that FPY is very important immediately after shutdown!



Accuracy of **ORIGEN** is determined by the accuracy of the **nuclear data**

– **Decay data**

- Half lives
- Branching fractions,
- Decay energy release (reaction Q-value)

– Cross sections (Multigroup)

- ENDF/B-VII.0, -VII.1
- JEFF-3.1/A special purpose activation file

– Gamma ray production data

- X-ray and gamma ray emissions per decay

– **Fission product yields**

- Energy-dependent data

– Neutron production data

- Alpha decay energies
- Stopping powers
- (a,n) yield cross sections
- Spontaneous fission spectral parameters
- Delayed neutron spectra

Fission product yield data used by SCALE

- Energy dependent FPY from ENDF/B-VII.0
 - 30 actinides: $^{227,228,232}\text{Th}$, ^{231}Pa , $^{232-238}\text{U}$, $^{238-242}\text{Pu}$, $^{241,242\text{m},243}\text{Am}$, $^{237,238}\text{Np}$, $^{242-246,248}\text{Cm}$, $^{249,252}\text{Cf}$, and ^{254}Es
 - Data are from England and Rider compilations
 - Energy-dependent yields tabulated at
 - **Thermal fission:** 0.0253 eV
 - **Fast fission:** 500 keV
 - **High energy fission:** 14 MeV
 - Actual yields are interpolated using the mean energy of neutrons causing fission (EALF)
- As of *SCALE-7.0-beta* we have incorporated spontaneous FPY from ENDF/B-VIII.0

Combining ORIGIN with Transport Applications

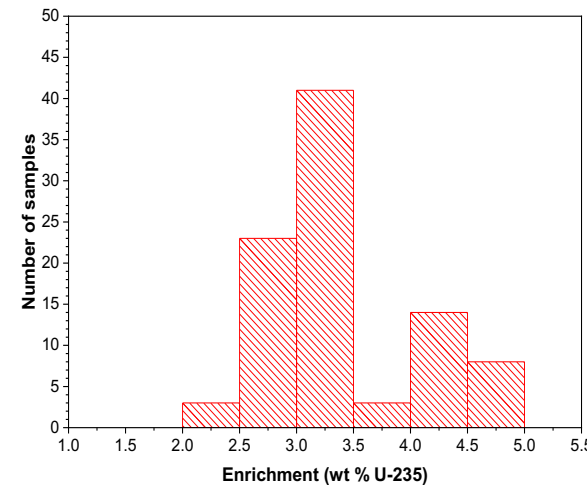
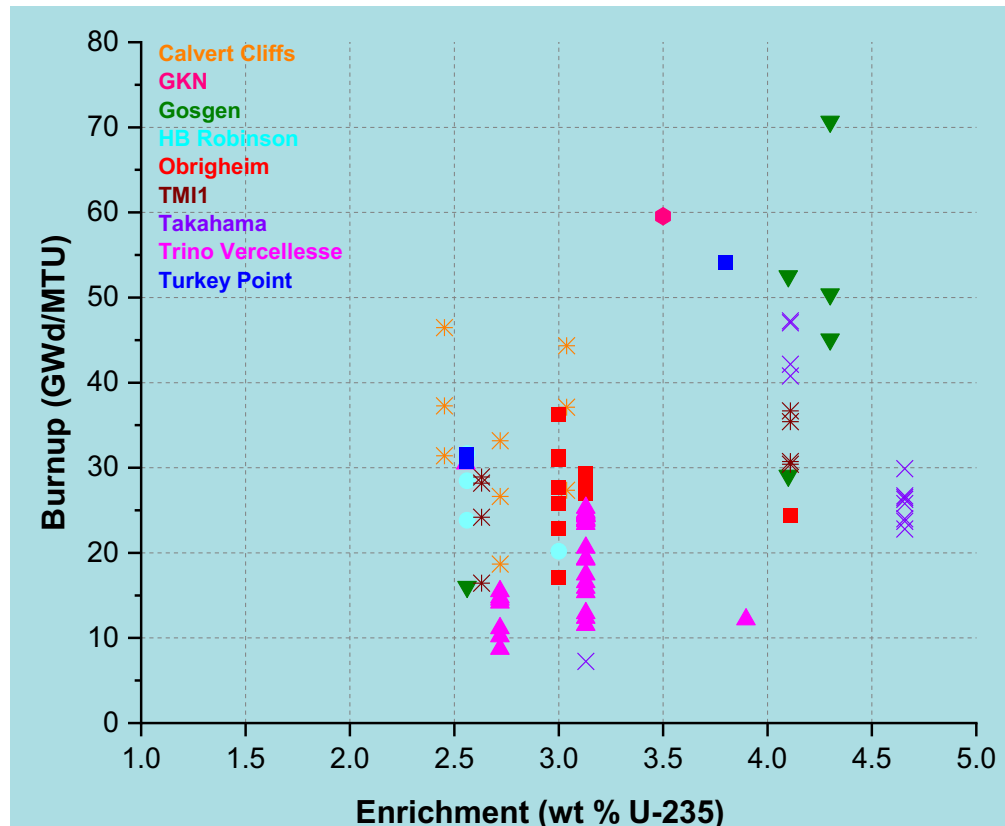
POLARIS

TRITON

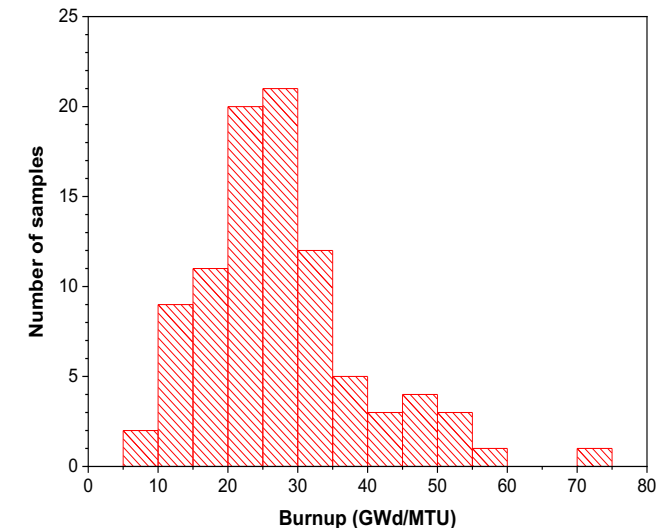
- Employ ORIGIN as a depletion solver in their coupled transport-depletion sequences
- Use detailed models (assemblies, reactors, etc.) to predict inventory of those models over time

Validation: Comparisons to radiochemical assay experiments

Nuclide inventory from experimental data for PWR fuel (92 samples)

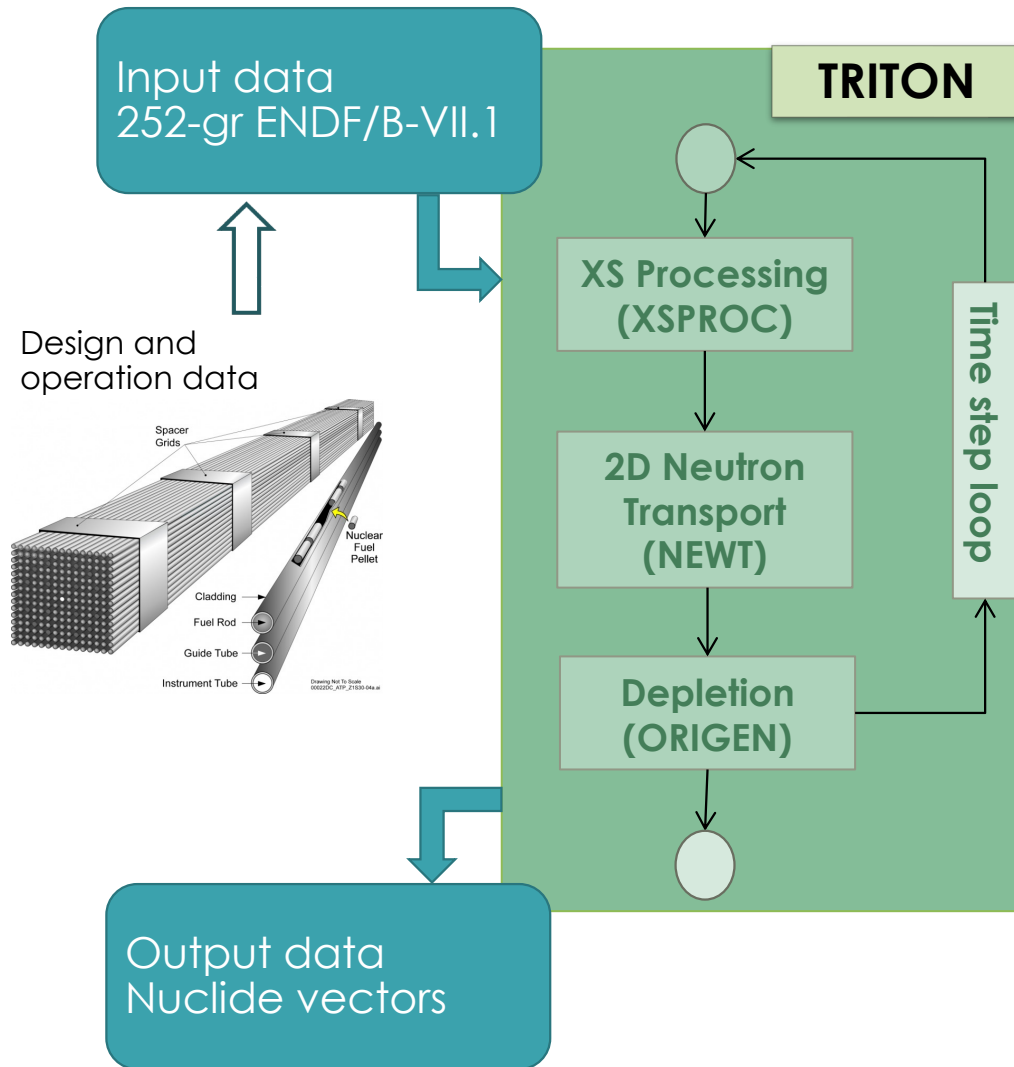


Burnup & enrichment space covered

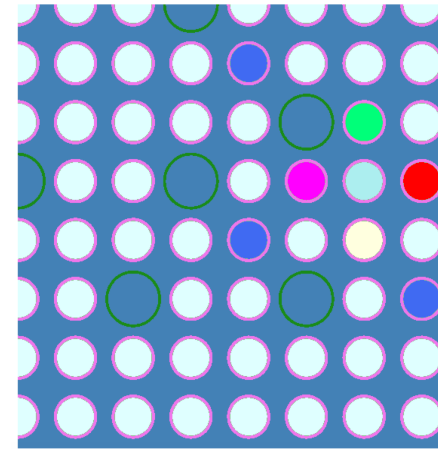


G. Ilas, J. Burns, B. Hiscox, U. Mertyurek, *SCALE 6.2.4 Validation: Reactor Physics*, ORNL/TM/2020-1500/V3 (2022) <https://www.osti.gov/biblio/1902818>

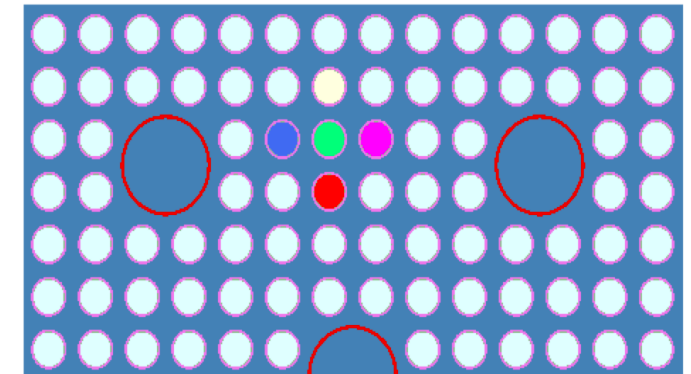
Validation: SCALE simulations for nuclide inventory



Sample irradiation and decay history modeling

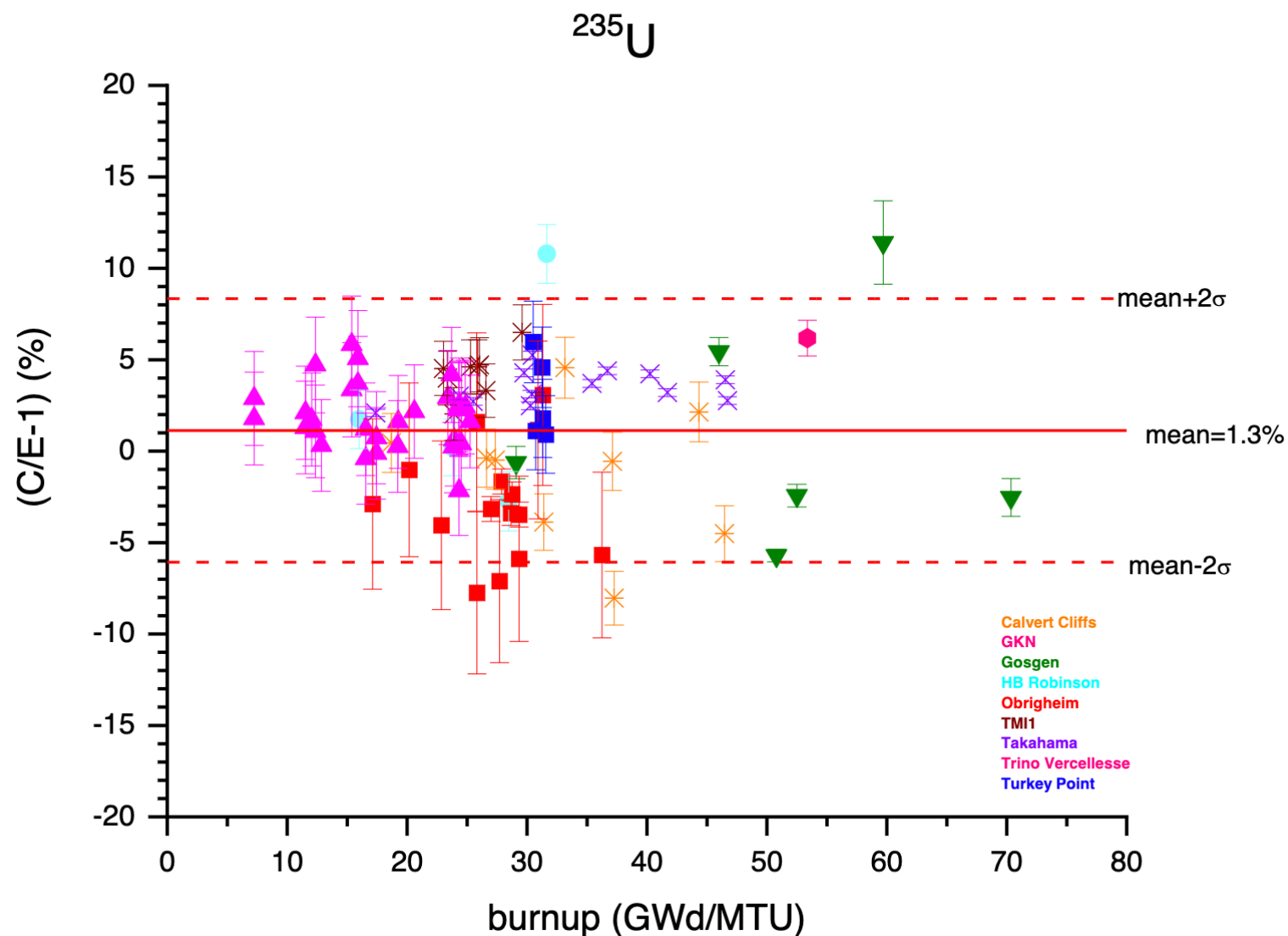


1/4 assembly model for Gosgen GU3 sample



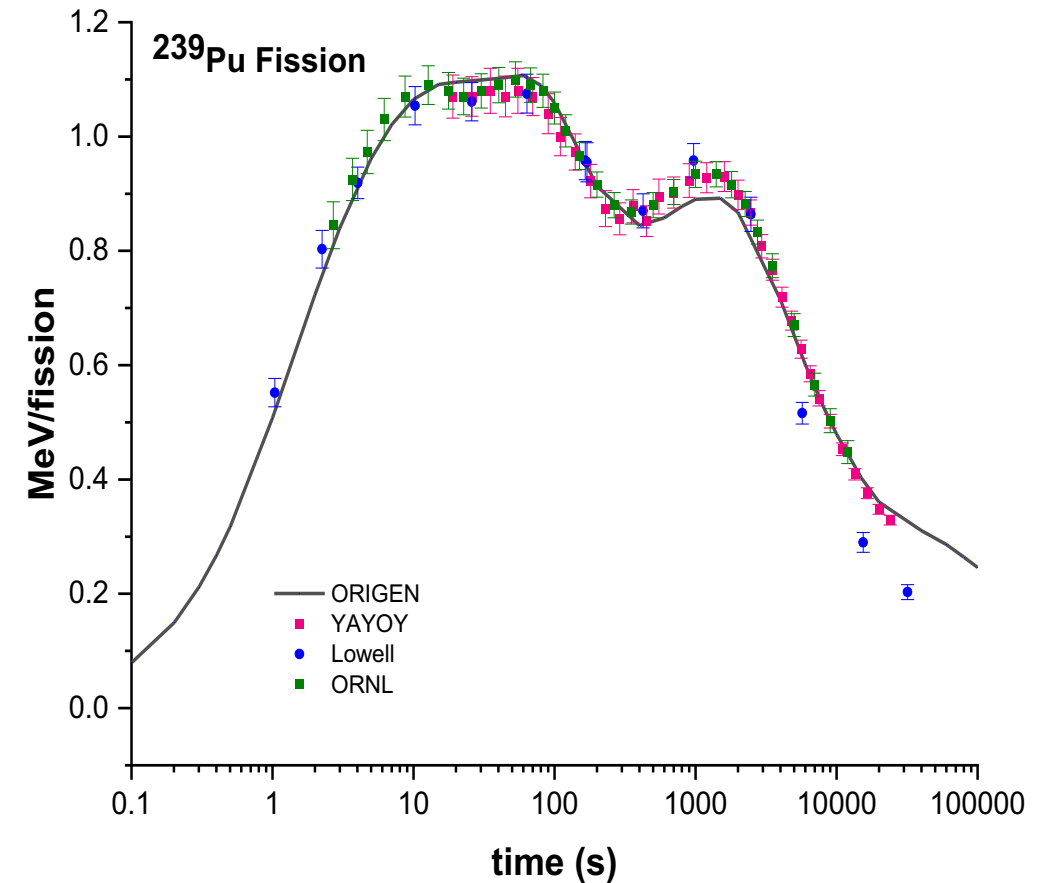
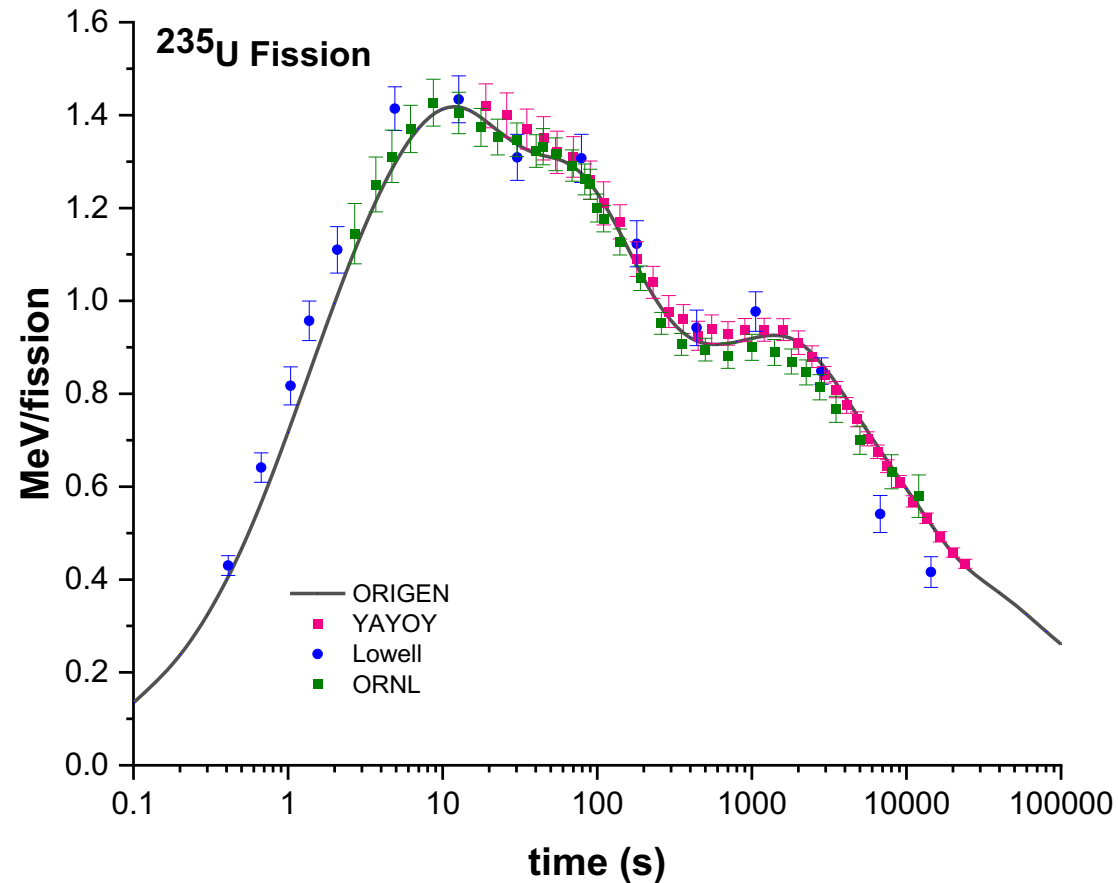
1/2 assembly model for Calvert Cliffs MKP109-CC sample

Validation: SCALE simulations for nuclide inventory



Validation: Fissile material irradiation

experiment-to-calculation comparisons



G. Ilas, J. Burns, B. Hiscox, U. Mertzyurek, *SCALE 6.2.4 Validation: Reactor Physics*,
ORNL/TM/2020-1500/V3 (2022) <https://www.osti.gov/biblio/1902818>

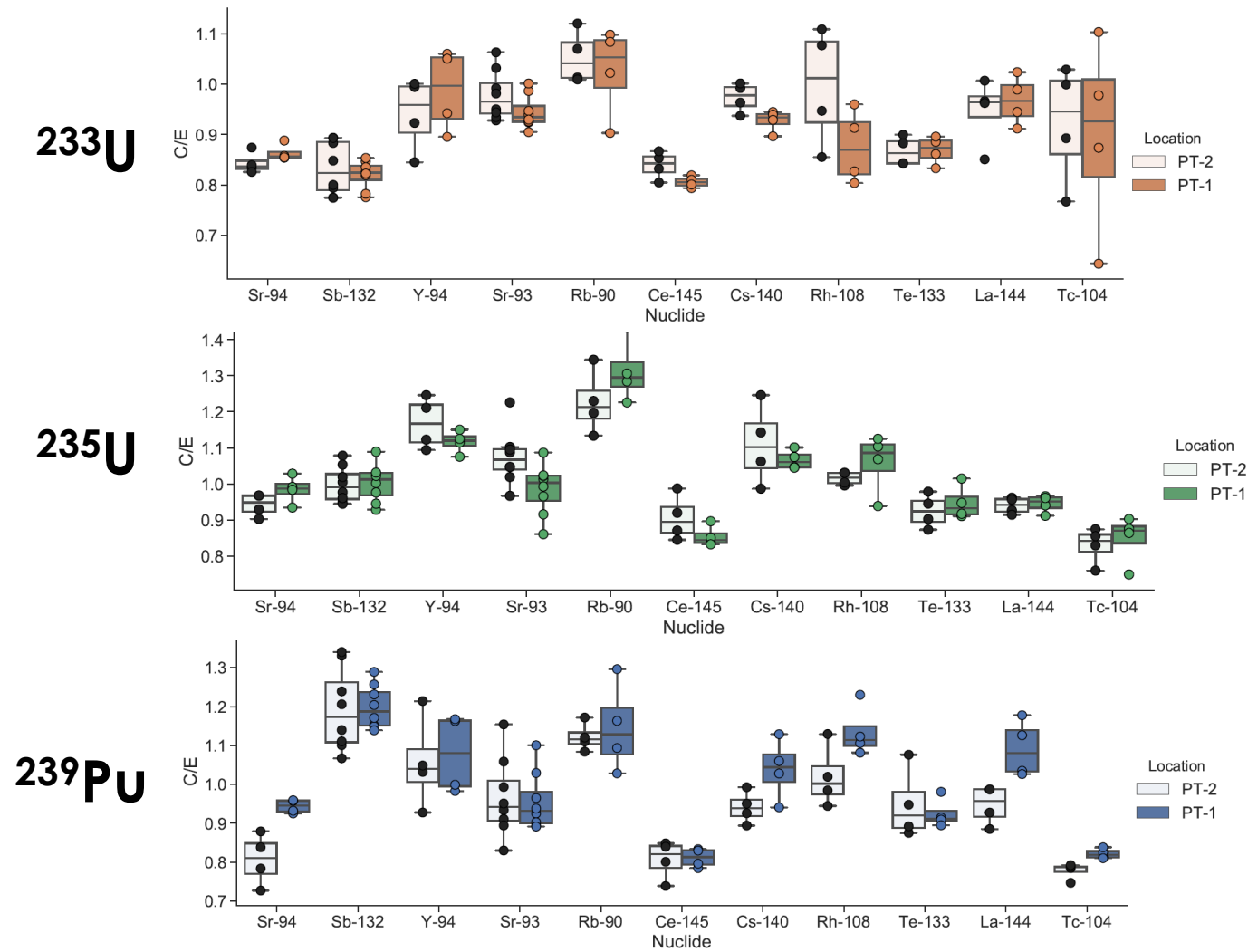
Proposal for New Validation Efforts

- Overall decay heat from burst fission
- Fission product measurements

Notes on comparison:

- New measurements for Tc-104 beta feeding / gamma emissions
- Rb-90 branching fractions issue identified

ORIGEN vs. HFIR meas. via HPGe



S. Skutnik, J. Knowles, and D. Glasgow, "Quantification of Trace-Level Fissile Samples via Short-Lived Delayed Gamma Spectroscopy," *IEEE Transactions on Nuclear Science*, 66(9), September 2019. DOI: [10.1109/TNS.2019.2934677](https://doi.org/10.1109/TNS.2019.2934677)

Key takeaways

- ORIGIN is a **consumer** of FPY data
- TRITON & POLARIS are assets which can be used to **validate** new FPY data
 - e.g., from **existing** radiochemical benchmarks and **new** irradiation experiments
- New capabilities with covariance data should be developed
- V&V methods and analysis also needed for the covariance data

Acknowledgements

This work was supported by the Nuclear Criticality Safety Program, funded and managed by the National Nuclear Security Administration for the Department of Energy

The entire Nuclear Energy and Fuel Cycle Division at ORNL