

Comparison of Revision Two and Three for the Flattop HEU Benchmark (HEU-MET-FAST-028)

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INTRODUCTION

The International Criticality Safety Benchmark Evaluation Project (ICSBEP) is a collection of evaluated nuclear criticality experiments [1] that provides safety basis for criticality safety evaluations as well as a validation suite for neutron transport codes. The 2024 version contains 598 benchmarks with 5,168 total configurations. Some of the experiments are historic benchmarks dating from the dawn of the nuclear industry in the 1940s and 50s. The first time many of these configurations were evaluated as benchmarks was in the mid-to late- 1990s. Benchmarks are designed to have simple materials and geometry so they can readily validate fundamental transport physics making them paramount to criticality safety evaluations and stockpile stewardship priorities. Expectations for benchmark evaluations have changed dramatically since the early days of the ICSBEP, as experimental measurements are taken at ever higher fidelities and modern computational power along with code features allow for more complete uncertainty quantification.

The Flattop high enriched uranium (HEU) experiment validates metallic HEU systems in the fast neutron spectrum [2]. It was originally built at Los Alamos National Lab in the 1950s. An idealized configuration was evaluated as a critical ICSBEP benchmark in 1999 under the designation HEU-MET-FAST-028.¹ A second revision to the Flattop experiment was written in 2016 based off the historical experimental results. The evaluators reported that, "uncertainty in k_{eff} was based upon engineering judgment...considering unknown factors in the final configuration and in correction methods"[3]. Besides a passing mention of analysis with the ONEDANT code comparing mass uncertainty, the benchmark did not include any additional efforts to quantify the experimental or model uncertainty. The revision two benchmark stands at 23 pages of analysis including appendices.

The Flattop benchmark is a fundamental validation experiment for HEU in the fast energy spectrum. A more thorough analysis was warranted for a benchmark which validates such an important component in many criticality safety evaluations. So, a complete re-evaluation of Flattop HEU was commissioned, including new high fidelity measurements of the critical configuration at National Criticality Experiments Research Center [4, 5, 6] culminating in a third revision to the Flattop HEU experiment in the ICSBEP [7]. HEU-MET-FAST-028 revision three is considerably more detailed standing at over 226 pages of experimental data (including dimensional measurements using a coordinate measuring machine), model descriptions, and uncertainty analysis. The detail in it is an exemplar modern benchmarks where uncertainty is rigorously

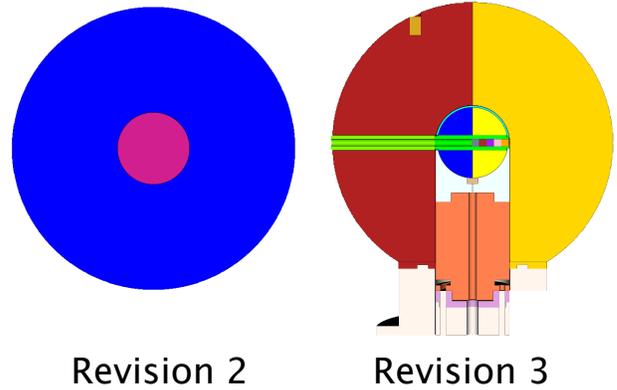


Fig. 1. Rendered models of Flattop HEU benchmark revisions at a y-plane slice at $x = z = 0$. Colors are non-transferable between renderings.

quantified and itemized with every model simplification from the physical experiment.

This re-evaluation gives us an opportunity to compare a traditional benchmark evaluation with a modern one and make comparisons to scalar flux, sensitivities for various reactions to k_{eff} , and emissions spectra produced from each model. In this work we compare the HEU-MET-FAST-028 revision two model to full-detailed HEU-MET-FAST-028 revision three model which we will call revision two and three for the remainder of this work. We examine the scalar flux, fission emission spectra, and sensitivities to k_{eff} for various reactions in the HEU core of each revision's model.

MODELS

Flattop HEU experiment consists of a highly enriched uranium core surrounded by a natural uranium reflector. The reflector has a stationery hemispherical portion and two quarter-sphere portions on rails aligned at 45° from the axis. When conducting the experiment the quarter-sphere reflectors are fully closed on the core. At this point the system is still subcritical and an approach to critical is done by moving control rods within the assembly. Further description, schematics, and images of the model can be found in revision three of the benchmark [7] as well as in the published literature [6, 2].

HEU-MET-FAST-028 revision two benchmark is a simple spherical core of highly enriched uranium inside a thick spherical shell reflector made of the natural uranium. Figure 1 at left shows the simple model used in revision two. No additional elements from the physical Flattop HEU experiment are modeled such as the glory hole, mass adjustment buttons, control rods, structural mechanisms or other physically present

¹HEU: highly enriched uranium, MET: metallic configuration, FAST: fast neutron spectra, 028: the 28th benchmark accepted in that category.

masses. For this reason the revision two model is colloquially called the "ball-in-ball" model. Revision two experimental k_{eff} was reported as exactly $1.0000 \pm 300\text{pcm}^2$ [3].

HEU-MET-FAST-028 revision three is considerably more complex including details as small as the HEU core cap, control rods, and mass adjustment buttons. Figure 1 at right shows the dramatically increased model fidelity as compared to revision two at left. In this benchmark every physically present feature of the Flattop HEU experiment is either modeled or simplified with a reported uncertainty incurred. The reevaluation experimentally measured k_{eff} as $1.00151 + 0.00129 / -0.00130$. We use the "detailed" benchmark model for these comparisons though revision three also includes a "simplified" model with slightly larger justified uncertainties [6].

RESULTS

To compare the models to one another we look at total scalar flux as a function of energy, total fission emission spectra, both for the HEU core and sensitivity to k_{eff} for U235 and U238 for various reaction types in fissile regions. We ran both models using MCNP6.3, ENDF/B-VIII.1, and use the SCALE-238 energy group structure as our bin structure. We ran MCNP's kcode subroutine with 100 inactive and 600 active cycles and 2×10^6 particles per cycle. When ran with these settings the revision two model calculates $k_{\text{eff}} = 1.000702(62)$ and revision three detailed model $k_{\text{eff}} = 0.998413(58)$. The statistical error from the Monte Carlo process associated k_{eff} was ± 6 pcm. We conducted a convergence study (increasing particle and cycle counts) to ensure that the stochastic error was sufficiently small to observe difference in the quantities of interest.

We make examinations between models by defining the U238 dominant reflector region and the U235 dominant HEU core region. In revision two this is simply the outer natural uranium spherical shell and the inner HEU sphere respectively. However as revision three is considerably more complex we have to define the HEU core region as: male and female HEU hemispheres, full core cap, the glory hole fillers, glory hole reducer, mass adjustment buttons. Similarly for the U238 dominant reflector we define as the: hemisphere and quarter-sphere shell components, reflector sleeve, lifting fixtures, control rods, pedestal base, and reflector adapter ring.

Flux

We first compare revisions by computing the scalar flux (ϕ) in the HEU core. We used MCNP's f4:n tally, a volumetric track length estimator for neutrons. To select the core a single cell is specific for revision two. For revision three both the male and female hemispheres of the HEU core are selected as a single region. This is consistent in subsequent presented calculations.

Figure 2 on top shows the scalar flux for the HEU core as a function of energy. The peak neutron flux is, as expected, around 1 MeV which is within the fast region, where the assembly is supposed to have most reactions. Figure 2 on bottom shows the percent difference between the flux produced from

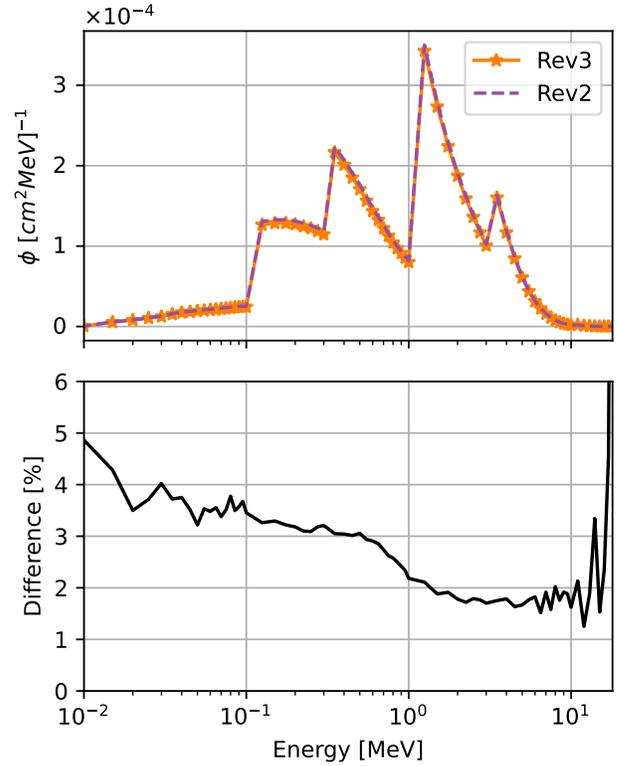


Fig. 2. Top: Scalar flux (ϕ) produced in the HEU core of Flattop comparing revision 2 and 3. Bottom: percent difference between ϕ from revision 2 and 3.

revision two and three in the energy region of interest. In the region of highest flux (far from zero) the deviation ranges from 5% to 1%.

Sensitivity

Next we compare sensitivities to k_{eff} of elastic, inelastic and fission reactions for U235 and U238. When considering sensitivity to U235 in revision two we specify only the HEU core where U235 is the dominant isotope in the metallic Uranium. Revision three is more complex and we define the core as all HEU components the male and female HEU hemispheres, mass adjustment buttons, glory hole with its fillers, and the fuel cap. For U238 sensitivities we compute with respect to the outer reflector where U238 is dominant. We use MCNP6's ksen card which uses the CLUTCH method to compute how sensitive 1% deviation in the cross-section of interest.

Figure 3 on top shows the sensitivity profile (S) of the U235 fission cross-section per unit lethargy. This is the dominant sensitivity and is an order of magnitude larger than other considered parameters. The revision two and three lines lie on top of each other with no significant deviations one from the another. Details around the peak (≈ 1 MeV) are captured by both models. Figure 3 on bottom shows the percent difference between revision two and three. In the range considered no delta is greater than 1%.

²Per cent mille; 1 pcm is equivariant to $\pm 1 \times 10^{-5}$

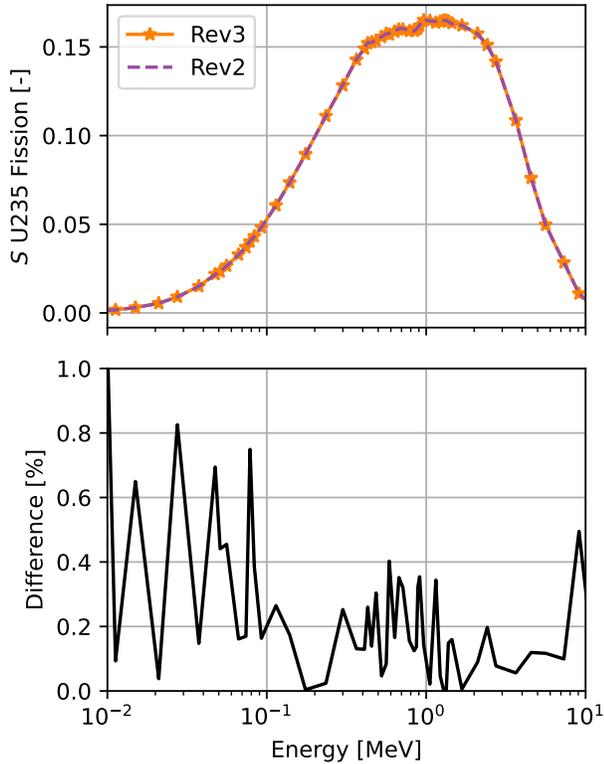


Fig. 3. Top: Sensitivity per unit lethargy (S) for fission reactions in the U235 core of Flattop, Bottom: % difference between sensitivities from versions

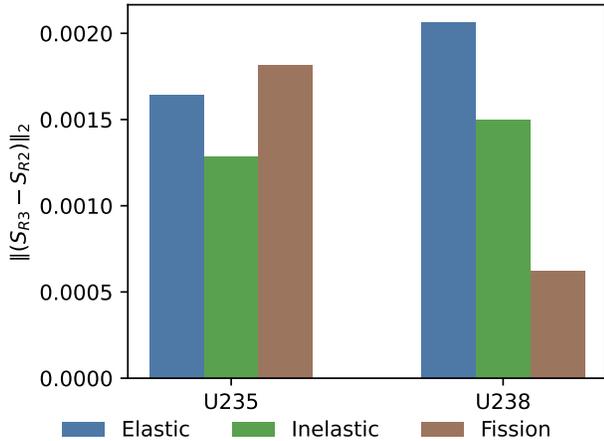


Fig. 4. The L_2 -norm between revision 2 and 3 various sensitivities

Figure 4 shows L_2 norms between revision 2 (S_{R2}) and 3 (S_{R3}) for elastic, inelastic, and fission reactions in the HEU core for uranium 235 and 238. A smaller norm means the sensitivities between the revisions are closer to one another. The greatest deviation between the two models is for the U238 elastic reaction which comes to about 0.0020. Deviations range down to 0.0005 with most centered around 0.0015.

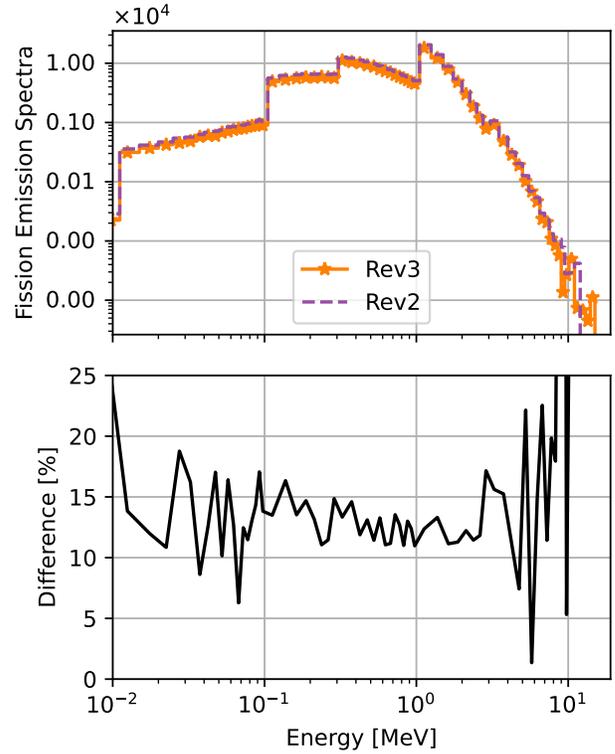


Fig. 5. Top: fission spectra for the HEU core as a function of energy, Bottom: percent difference between revision 2 and 3

Fission Spectra

Finally we compare the total emission spectra from all fission events in the HEU core of Flattop. We use MCNP's PTRAC card to generate a histogram of the total weight tallied when sourcing new particles from fission sites in the kcode subroutine. We normalize this weight as a post process.

Figure 5 on top shows the total weight tallied during simulation in the HEU core between revisions as a function of energy. As in previous figures only the fast portion of the neutron spectra is shown. Figure 5 on bottom shows percent error as a function of energy bin. Error ranges between 20% and 5%.

DISCUSSIONS AND CONCLUSIONS

ICSBEP benchmarks have many use cases, some are:

1. Providing safety basis for criticality safety evaluations;
2. Validating neutronics codes' criticality calculations;
3. Validating the nuclear data itself; and
4. Providing complex real-world tests for neutronics codes.

Adoption of the new revision may or may not be warranted under each use case. For example in criticality safety evaluations, sensitivities to k_{eff} are how evaluators provide experimental

safety basis as required by regulations. In that use-case, the maximum deviation to the k_{eff} is under a single percent which may be small enough. Crucially, this insensitivity between revisions was not known a priori the reevaluation. How revision one and two went from physical experiment to the simplified “ball-in-ball” model is unknown [3]. Revision three makes this benchmark—used very broadly in safety evaluations—*traceable* and *reproducible* down to the layout of the room where the experiment was conducted [7].

We show in this paper that more complex quantities of interest like scalar flux and the fission emission spectrum are sensitive between revisions. That means for applications like nuclear data validation revision three should be used.

While ICSBEP evaluations can only *validate* criticality results for given nuclear data and neutronics code, they also serve as real world integration³ and regression⁴ testing for quantities of interest and simulation parameters other than k_{eff} . When using HEU-MET-FAST-028 to test a neutronics code in this way we strongly recommend adoption of the much more complex revision three. Revision three more accurately reflects realistic needs of code users, including, complex geometries, repeated surfaces, and high fidelity isotopic configurations. The complexity of the revision three may elucidate inaccuracies in data processing, flaws in a given tracking method, or other code features that would otherwise go unnoticed in the much simpler revision two. For example, many modern Monte Carlo neutron transport applications are developing hybrid surface–delta tracking algorithms [8]. How events are sampled, crossings are evaluated, and quantities of interest tallied, vary on the simulation mode. For such a method revision three will stress calculations like the majorant-cross section evaluation⁵ (which can be compared for accuracy between codes and versions of the same code) while revision two will not.

HEU-MET-FAST-028 revision two to three is a natural progression of complexity from the halcyon days of the field through to the modern era. Revision three provides more sophisticated testing to match modern neutronics codes and further validates many criticality safety biases with a traceable and reproducible experiment.

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³If all components of a code work together to get a result

⁴Code-to-code comparison, comparison between versions of the same code

⁵The largest cross-section for all materials in a whole problem needed when delta tracking