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Validation of MCNP Critical Benchmark Models of Highly Enriched Uranium Cylinders

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INTRODUCTION

A new centralized repository of high-quality MCNP models of critical benchmark experiments is currently under development at Los Alamos National Laboratory (LANL). The benchmark experiments are described in the International Criticality Safety Benchmark Evaluation Project (ICSBEP) Handbook, and the initial set of benchmark models are derived from the Whisper Suite provided with MCNP6.2 [1]. This effort is a collaboration among the Nuclear Criticality Safety, Nuclear Data, and Monte Carlo code development/application organization at LANL. The objective is to create a current single LANL benchmark collection that includes the latest ICSBEP revision that has a formal review and revision process, is contained in an open-source repository, and utilizes new Python tools for improved input and output file review.

This paper describes the validation of the models associated with HEU-MET-FAST-051, "Uranium Metal Cylinders (7-inch, 9-inch, 11-inch, 13-inch, and 15-inch diameter) and two 11-inch-diameter Interacting Uranium Metal Cylinders" [2]. The Monte Carlo n-Particle (MCNP) models were compared to the third revision of HEU-MET-FAST-051. The experiment considered critical configurations of unreflected and unmoderated highly enriched uranium (HEU) metal cylinders in various geometric configurations in 10 unique cases. [2]

The uranium cylinder assemblies were separated into two units with a mobile unit built onto a hydraulic lift that was lowered down adjacent to a stationary unit. All uranium cylinder assemblies were constructed by layering many central disks as shown in Figure 1.

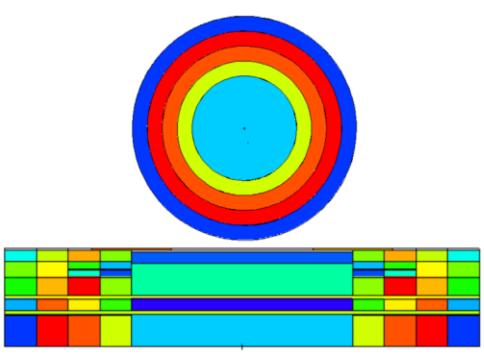

Fig. 1. MCNP graphic plot of HEU-MET-FAST-051, case 18.

The various colors in the figure represent different unique disks of highly enriched uranium that were machined to high precision.

REVIEW OF HEU-MET-FAST-051 MCNP MODELS

The initial MCNP input files of HEU-MET-FAST-051 were taken from the Whisper Suite included in the MCNP 6.2 package [1]. The benchmark review of the models identified differences in the geometry and material specifications compared to the experiment model described in the ICSBEP Handbook [2]. This includes rounding errors, typos, and incorrect material and geometry definitions shown below:

- Total number densities are not written out to full precision in some cases.
- Material definitions were not given at natural abundance values in all cases.
- Surface definition values were miscalculated in multiple cases.
- Material data files were updated to .80c in some cases.

It is important to note that only cases 2, 9, 16, and 18 had any updates to the geometry, but all cases had changes to the material properties. Other changes were made to the input files such as reordering material cards or removing unnecessary comments. However, these are judged to not have any effect on the results of the models.

Any assumptions given in the ICSBEP handbook for these models were reflected in the input decks. This includes neglecting supporting structures, room floor and walls, and evenly distributing small interstitial gaps that may exist between the uranium disks.

METHODOLOGY

Computational models of critical benchmarks are used to quantify the bias of calculation techniques and to establish margins of subcriticality for operations with fissionable materials. Therefore, the impact of the model revisions can be quantified by the change in the calculated bias.

The bias in the benchmark case is defined as the difference between the calculated model k_{eff} and the experimentally derived k_{eff}. This is shown in Eq. 1.

$$\text{Bias} = k_{Calc} - k_{Bmk} \quad (1)$$

The bias uncertainty must also be considered as various uncertainties arise from the calculation method, calculational model, and uncertainties in the benchmark [3]. Equation 2 shows the formula for bias uncertainty, which is the linear propagation of the standard deviations in the calculated k_{eff} and the benchmark k_{eff}.

$$\sigma_{Bias} = \sqrt{(\sigma_{keff,Calc})^2 + (\sigma_{keff,Bmk})^2} \tag{2}$$

The changes in bias between the two versions of the models show if the model has improved. If the magnitude of the new bias is smaller than that of the previous bias, then the model is closer to the experimental value. Some of these changes could be negligibly small, which was determined statistically using a z-test. Equation 3 shows the formula for a z-test with two uncertain numbers.

$$z = \frac{|Y_2 - Y_1|}{\sqrt{\sigma_2^2 + \sigma_1^2}} \tag{3}$$

Here, Y represents the nominal value for two sets of data, and σ represents their standard deviation. In this paper, Y may be either k_{eff} or Bias. This formulation assumes that the null hypothesis proves the two uncertain values are equal to each other. Any z-value greater than 1.96 proves that the two values are not equal (95% confidence, two-sided test).

Computations were performed using MCNP6 Version 1.0 with ENDF/B-VII.1 cross sections on the Blowfish High Performance Computing cluster at LANL. This computational technique has been validated within the LANL Nuclear Criticality Safety Division in accordance with ANSI/ANS-8.24 [4].

RESULTS

Models were run at varying levels of revision to study the effects of the specific modifications including:

- Original MCNP models
- Changes only to the model geometry
- Changes only to the model material properties
- Revisions to both the model geometry and material properties.

This was done to determine which changes to the original model would most greatly affect the system multiplication factor.

A z-test was performed for all cases to determine the number of cases with significant changes in bias (95% confidence). Any changes to the geometry of the models did not result in significant change in bias. The only revisions that had a significant effect on the bias were from changes in material properties and that was only significant in case 3. The overall results from the revisions are given in Table 1. Revisions in case 3 included updating Ag and N nuclides to natural abundance values for two materials and this case did not have any changes to the geometry. Overall, the revisions had a mostly insignificant effect on the bias.

TABLE 1. Number of significant changes in bias based on type of revision.

Revision Type	Significant Changes	Insignificant Changes
Geometry	0	4
Material	1	9
Complete	1	9

The change in bias from completely revising the model is shown in Fig. 2. The data points are shown with 2σ error bars. Case 3 has the largest change in bias, around 0.00012 more than the next highest case. Cases with mostly geometry changes showed little increase or decrease in bias while those with mostly material changes showed much higher changes in bias.

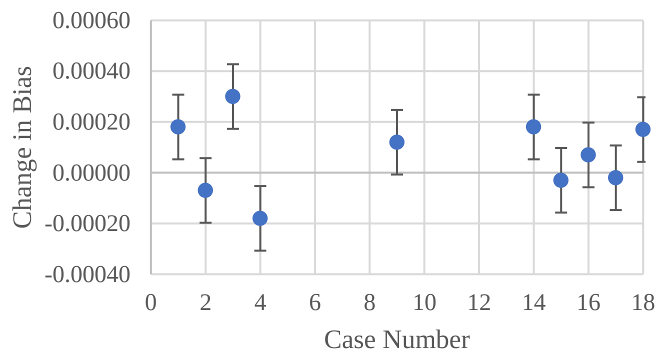

Fig. 2. Change in bias comparing original to completely revised models.

Fig. 3 shows the bias of the original and completely revised models for each case. Vertical error bars are shown to one standard deviation. This figure demonstrates that the revisions to the models resulted in relatively negligible changes to the bias. The difference in bias is largest in case 3, hence it being the only case with a statistically significant change.

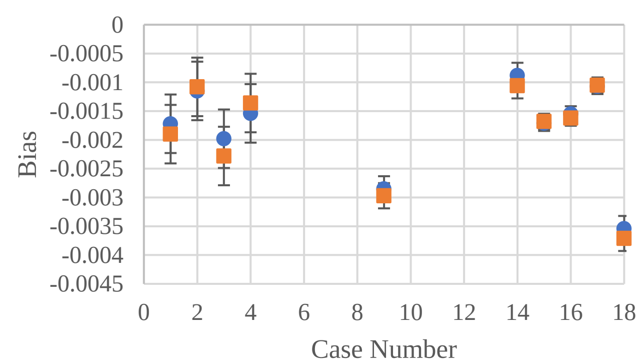

Fig. 3. Bias from the original model and the completely revised model.

Table II shows the bias and change in bias for the top three cases with the largest changes in bias from revisions of material properties. Table III shows the bias and change in bias for the top three cases with the largest changes in bias from revision of geometry properties. These data show that the material revisions have a strong effect on the multiplication factor of the models. The largest change in bias for material revisions was in case 3 at 0.00030 and the largest change in bias for geometry revision was in case 018 at 0.00023. The largest change in bias due to the geometry is more than double the next highest case.

TABLE II. Bias and change in bias for the three most significant cases with material revisions.

Case #	Bias	Bias σ	Change in Bias	Change in Bias σ
003	-0.00198	0.000508	0.00030	0.000127
016	-0.00142	0.000135	0.00020	0.000127
014	-0.00088	0.000219	0.00018	0.000127

TABLE III. Bias and change in bias for the three most significant cases with geometry revisions.

Case #	Bias	Bias σ	Change in Bias	Change in Bias σ
018	-0.00348	0.0002	0.00023	0.000127
009	-0.00308	0.0002	-0.00011	0.000127
002	-0.00117	0.0005	-0.00009	0.000127

Each of the cases in HEU-MET-FAST-051 was revised with between 3 and 11 multiplication factor altering changes. Many of the changes were relatively small for correcting geometry and correcting atom densities. Case 3 had many small changes to the atom densities and one isotope in the material definition resulting in the larger change in bias.

CONCLUSIONS

The validation of the models described here contributed to the centralized LANL benchmark repository currently under development [5]. While the revisions to the HEU-MET-FAST-051 model made statistically significant changes to the bias in one case, the changes were mostly negligible. Given the number of revisions made, the lack of substantial changes in multiplication factor and bias provide additional confidence in the Whisper collection.

NOMENCLATURE

k_{eff} = neutron multiplication factor
σ_{Bias} = bias uncertainty
$\sigma_{keff,Calc}$ = uncertainty in k_{eff} from the model
$\sigma_{keff,Bmk}$ = uncertainty in k_{eff} from the benchmark
Y_1, Y_2 = nominal value for data used in z test
σ_1, σ_2 = uncertainty in the nominal values of Y_1 and Y_2 respectively
z = value used to determine significance in z-test

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