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Verification of MCNP Critical Benchmark Model of U233-COMP-THERM-004

Riley Bulso, Jennifer L Alwin, Robbie MacQuigg, Ray Sartor, Jennifer Arthur, and Wim Haeck
Los Alamos National Laboratory
, P.O. Box 1663, E585, Los Alamos, NM 85745
rbulso@lanl.gov, jalwin@lanl.gov, robbie.macquigg@lanl.gov, sartor@lanl.gov, jennifera@lanl.gov , wim@lanl.gov

Kristina Y. Spencer
Idaho National Laboratory
1955 Freemont Ave, Idaho Falls, ID 83415
kristina.spencer@inl.gov

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ABSTRACT

Los Alamos National Laboratory (LANL) has been working on creating a new centralized repository for MCNP models of critical benchmark experiments. The initial model of U233-COMP-THERM-004 was derived from the Whisper Suite provided with MCNP6.2, and was compared against the ICSBEP handbook chapter for the benchmark. Many notable errors were found in the initial model and were revised accordingly. Comparing the computational model of the old and new models confirmed that any Whisper results that relied upon the old model are still valid.

Key Words: *Whisper, verification, validation, benchmark*

1 INTRODUCTION

A new centralized repository of high-quality Monte Carlo n-Particle (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 [1], and the initial set of benchmark models are derived from the Whisper Suite provided with MCNP6.2 [2]. This effort is a collaboration among Nuclear Criticality Safety, Nuclear Data, and Monte Carlo code development/application organizations at LANL. The goal is to build a single LANL benchmark collection that is up-to-date with the latest ICSBEP revision, 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 verification of the model U233-COMP-THERM-004, "D_2O Moderated Lattice of $^{233}UO_2$-$^{232}ThO_2$" [3]. The MCNP model was compared to the initial revision of U233-COMP-THERM-004, which consists of one unique case. This experiment considers a critical configuration of two different fuel types within a single reactor, moderated with either light or heavy water depending upon the region of the reactor. The benchmark experiment contains one case, which was modeled using MCNP [4]. The inner reactor vessel (also called the "test region") of the reactor contains D_2O-moderated of $^{233}UO_2$-$^{232}ThO_2$ fuel, surrounded by the outer secondary region (also called the "driver region") of H_2O-moderated TRX (^{235}U) fuel.

2 REVIEW OF U233-COMP-THERM-004 MODEL

The initial MCNP input file of U233-COMP-THERM-004 was taken from the Whisper Suite included in the MCNP 6.2 release package [3]. The benchmark review of the model identified differences in element placement and dimensions, and in material definitions when compared to the ICSBEP Handbook [1]. This also includes typographical errors in input comments and an inadequate source definition:

- The source was distributed in a cylindrical definition that covers the fissile material radially; the vertical distribution started far below the fuel and ended somewhere in the middle of the fuel pin. This source definition was corrected to cover all fissile material.
- Input file geometry did not follow best practices, having nested universes with edges overlapping exactly. This caused multiple geometry errors shown in red in the plotter and could result in lost particles. The universe structure of the model was redefined to avoid these errors.
- The surface cards defining the test region fuel rods were generally incorrect, and were recreated to match the ICSBEP Handbook specifications [1].
- The bottom of the driver region fuel rods were also generally incorrect, and were recreated to match the ICSBEP Handbook specifications [1].
- The spacer rods in the driver region were placed at incorrect positions, and their surface cards were updated accordingly.
- The support rods in the test region were placed at incorrect positions to avoiding overlapping the lattice structure. These positions were corrected without overlap by redefining the universe structure.
- Nuclide densities for Ti-46 and Ti-47 in the aluminum 6061 material card were slightly incorrect and updated accordingly.
- Nuclide densities for iron isotope in the SS 304 material card did not match the expected isotopic distribution and did not add to the ICSBEP-specified atom density of iron for the material. These densities and the total atom density were updated accordingly.
- Many comments were unclear and were reworded as deemed necessary for clarity
- Given the size of the problem/reactor, the previous number of neutrons per kcode cycle (10,000) was increased by an order of magnitude.

During the review, a couple issues were found in the Handbook chapter that were clarified with the original independent reviewer (Michael L. Zerkle). He referred the authors to engineered drawings within technical report B-TM-1640 [5]. Zerkle and John Bess initiated a revision of the chapter, which has been approved by the ICSBEP and is to be includedin the new edition of the ICSBEP handbook, to address the following issues:

- The dimensions of the indent in the fuel pin bottom end were not described in Figure 24 or Table 20, but the indent is displayed in the figure as being part of the experimental model. Zerkle recommended using the dimensions from Fig. A-38 in Reference R2: “So the lengths of the bottom end plug sections from Figure A-38 (in inches) should be 0.375" (0.9525 cm) conical section modeled as rcc, the indent for the locking nut should be 0.158" (0.40132) long, the upper section of the bottom end plug below the clad should be 0.279" (0.70866 cm) long, for a total bottom end plug length below the clad of 0.812" (2.06248 cm).”
- The active fuel length in Table 20 does not correspond to the active fuel length in Figure 24. Drawing B-TM-1640 agrees with the length in Figure 24.

In the process of this revision, some assumptions and “local (LANL NCS) practices/policies” were applied as follows: Hydrogen was modeled as 100% ^{1}H; Carbon was modeled on an elemental basis using the 6000.80c cross section table; Oxygen was modeled as 100% ^{16}O; and an unused material was removed from the input file. All iterations of this model were run at room temperature, with $S(\alpha, \beta)$ cross sections utilized where applicable.

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

$$Bias = k_{calc} - k_{bmk} \tag{1}$$

The bias uncertainty must also be considered as various uncertainties arise from the calculation method, calculational model, and uncertainties in the benchmark. Equation 2 shows the formula for bias uncertainty, which is a linear propagation of the standard deviations in the calculated k_{eff} and the benchmark k_{eff}. 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 95% confidence, two-sided z-test. Equation 3 shows how the z-value was determined for two uncertain numbers.

$$\sigma_{bias} = \sqrt{(\sigma_{keff,calc})^2 + (\sigma_{keff,bmk})^2} \tag{2}$$

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

Here, Y represents the nominal value for two data sets and σ represents their standard deviation; in this paper, Y is either k_{eff} or bias. This methodology 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 values are statistically not equal.

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 [6].

4 RESULTS

Models were run with various levels of revision: no revisions (i.e., the original MCNP model), revisions only to material cards, revisions only to geometry, and complete revision. The results of these models were compared to the benchmark k_{eff} values and between each other to understand the impact of the revisions. Table I depicts the k_{eff} values of the experimental benchmark cases, original models, partially and completely revised models. Note that geometry had the greatest effect on the revised model, and moved k_{eff} farther away from the k_{bmk}. Upon further investigation, it was noted that the output file states "warning: 864 fission cell elements had no neutron tracks entering; warning: 864 fission cell elements had no neutron collisions; warning: 864 fission cell elements had no fission source points. The k_{eff} results could be too small because cells with fissionable material were not sampled." Since 864 corresponds to the number of fuel rods in the test region, it was determined that this warning was referring to the test region not being properly sampled by the volumetric source definition. In an effort to mitigate this, an explicit source calling out fuel rods was added to the input, as seen in row 5 of Table I. However, this edit did not correct this warning or significantly change the resulting k_{eff}. Given that this source definition specified all fuel rods as an individual repeated-structure/lattice source, the review team suspects that this may a false warning to be further investigated.

TABLE I. Reactivity Results and Comparison

Case:	k_{eff}	σ	z-value from k_{bmk}
Original Model	0.99811	8E-5	1.79
Geometry Change	0.99541	3E-5	3.14
Material Change	0.99772	8E-5	1.99
Final Model	0.99496	3E-5	3.37
Final with explicit source definition	0.99497	3E-5	3.36
Benchmark value	1.0017	2E-3	N/A

As seen above, the changes resulted in a significant change from the benchmark value of reactivity. Additionally, as seen below in Table II, there was also significant change in the revised biases from the original model bias.

TABLE II. Bias Results and Comparisons

Case:	Bias	σ_{bias}	z-value from original bias
Original Model	0.00359	0.00200	N/A
Geometry Change	0.00629	0.00200	31.6
Material Change	0.00398	0.00200	3.45
Final Model	0.00674	0.00200	36.9
Final with explicit source definition	0.00673	0.00200	36.8

5 CONCLUSIONS

The verification of U233-COMP-THERM-004 contributed to the centralized LANL benchmark repository currently under development. These revisions lead to significant results in both the calculated multiplication factor and in the calculated bias. While z-test results indicate that the bias was substantially changed, the magnitude of the bias is for this model is relatively small in comparison to other uranium benchmark biases, and thus it is not expected that these updates will have a significant impact on the USL. However, due to the false warning regarding neutron sampling, further investigation into the cause of this error may be required before final incorporation of the model into the new Los Alamos Benchmark Suite.

6 REFERENCES

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