LANL Critical Benchmark Comparison Study and Subsequent Revision for Cases Involving LEU and MIX

Jennifer Alwin[1], Nicolas Leclaire[2], Robbie MacQuigg[1]

1: Los Alamos National Laboratory, Radiation Transport Applications XCP-7
2: Institut De Radioprotection et De Sûreté Nucléaire (IRSN)

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Introduction

As part of an international collaboration within the DOE Nuclear Criticality Safety Program (NCSP), LANL is involved in a comparison study to quantify differences in k-effective results from neutron transport simulations of critical benchmark experiments. The DOE NCSP Mission and Vision details the activity in which the French Institut de Radioprotection et de Sûreté Nucléaire (IRSN) leads the study with LANL, ORNL, and LLNL to compare results of various neutron transport codes and nuclear data libraries for ICSBEP benchmarks held in common by the entities. The task statement from the DOE NCSP Five-Year Execution Plan [1] is given below:

The proposal is for IRSN to lead a new intercomparison based on the MORET code with the latest JEFF-3.3 data and ENDF/B-VIII.0 data, when available, using their existing comprehensive selection of 2,714 benchmarks and collate their results together with those from LLNL (COG), LANL (MCNP) and ORNL (SCALE). Due to the large number of benchmarks involved, this effort is envisioned to take three years with an additional year for IRSN to complete a summary report. The benchmark development will be performed independently to minimize modeling errors through discovery and resolution of discrepant results. A summary report will be generated (led by IRSN) to document the results of this study.

This report documents results obtained for revisions made to cases involving Intermediate Enriched Uranium (IEU) and a mixture of Pu and Uranium (MIX), with a focus on the changes made to LANL benchmarks modeled with MCNP6 using ENDF/B-VII.1 nuclear data that appeared to have discrepant results when compared with results of other codes. Feedback was used to pinpoint review of particular benchmark input files and to revise them when necessary. This report documents the results of review and revision of specific benchmarks highlighted as possibly discrepant in the comparison study. In addition, there is an effort tied to this work involving collaboration between LANL XCP and NCS Divisions in the development of a shared review/revision procedure and use of a new benchmark repository.

LANL has a benchmark library of critical experiments from the International Criticality Safety Benchmark Evaluation Project (ICSBEP) Handbook [2] modeled for use with MCNP. This collection is now over 1100 benchmarks, referred to as the Whisper-1.1 library because it is used with the sensitivity/uncertainty package, Whisper, which supports nuclear criticality safety validation and is released with MCNP6.2 [3-5]. The collection, originally created several decades ago, is a combination of smaller collections, which has been revised and expanded, by various groups at LANL over the years. The original authors are no longer at the laboratory and little formal documentation of review and revision of these benchmarks exists today. A branch of the benchmark collection was already the subject of a formal review undertaken by the LANL NCS Division and expanded to include XCP Division.

Benchmark Review and Revision

It takes a significant amount of work to generate and maintain a benchmark collection. There are now at least three organizations at LANL, which utilize criticality benchmark collections with MCNP6. It is believed each collection within those organizations originated from the same input files that have been revised and expanded to meet specific needs. One such effort uses criticality benchmarks (~1100 total benchmarks) and associated nuclear data sensitivity/uncertainty information with the recently released tool, Whisper-1.1, to support nuclear criticality safety validation. Another effort uses a benchmark collection (~800 total benchmarks) for traditional nuclear criticality safety validation in the NCS Division. A third effort uses a benchmark collection (~1400 total benchmarks) for nuclear data testing and evaluation. It is widely believed these collections have the same origin, however over several decades they have been revised and expanded individually without integration or formal documentation of review and revision.

Feedback on particular benchmarks that exhibit discrepant k-effective results when compared with those from IRSN, LLNL, and ORNL is very valuable as a starting place for a modern, formal benchmark review process. In a previous study HEU and Pu benchmarks found to be in common between LANL, IRSN, LLNL, and ORNL. Results in common between all four benchmark collections were compared as well as benchmarks in common between two or three collections. Discrepant results were investigated further, sometimes differing only by about a hundred percent millirho (pcm) and subsequent changes to LANL benchmarks as a result of the comparison were documented [6].

The investigation into results for MCNP6.2 with ENDF/B-VII.1 nuclear data sometimes led to revisions in the benchmark input files and subsequent calculation of k-effective. This report presents those results pre- and post-revision. This work is the beginning of a larger effort to centralize a single LANL collection that is up-to-date with the latest ICSBEP Handbook revision, that documents the type of benchmark model (simplified/detailed), 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. Future efforts are contingent upon funding.

Table 1 lists the benchmarks that were reviewed and provides brief remarks of revisions. In addition, the benchmark k-effective and experimental uncertainty as well as the MCNP6.2 using ENDF/B-VII.1 calculated k-effective and uncertainty are displayed.

The reviews were conducted by comparing the most recent revision in the ICSBEP Handbook with the input files. XCP began reviewing the particular cases pointed out by the DOE NCSP intercomparison collaboration with IRSN, LLNL, and ORNL. In parallel, LANL NCS Division had begun a formal review of all benchmarks, in accordance with recent procedures and documentation requirements [7, 8]. This report includes the results of both of those efforts.

Table 1 contains a brief description of the changes to the input files and contains a comparison of calculational k-effective results. The pre-revision result is indicated with a strikethrough if the post-revision calculated k-effective or uncertainty resulted in a change.

Table 1. Benchmark experiments reviewed and summary of revisions, along with experiment k-effective and uncertainty and MNCP6 k-effective and uncertainty.

Benchmark	Revisions	k_{bmk}	σ_{bmk}	k_{MCNP6}	σ_{MCNP6}	Revision Impact
LCT-011 Case 15	1. Corrected atom fraction for Cu in cladding material from 5.1174E-04 to 5.1174E-05 to match Table 35 of Handbook. 2. Removed plugs (end caps) from bottom of rods. 3. Corrected 0.3-cm layer of water at bottom of rods.	1.0010	0.0018	0.99781 ~~0.99619~~	0.00011	Small improvement in bias
LCT-027 Case 1	Model updated from Revision 1 (September 30, 2000) to Revision 2. 1. Material compositions revised to match Table 14 and 15 of the Handbook. 2. Model revised to use air instead of void in cells that contain air. 3. Surfaces revised slightly to match current revision in Handbook.	1.0014 ~~1.0000~~	0.0015 ~~0.0011~~	1.00068 ~~1.00425~~	0.00011	Results closer to MORET, correcting ~300 pcm discrepancy
LCT-027 Case 2	Model updated from Revision 1 (September 30, 2000) to Revision 2. 1. Material compositions revised to match Table 14 and 15 of the Handbook. 2. Model revised to use air instead of void in cells that contain air. Surfaces revised slightly to match current revision in Handbook.	1.0014 ~~1.0000~~	0.0012 ~~0.0011~~	1.00326 ~~1.00664~~	0.00011	Results closer to MORET, correcting ~300 pcm discrepancy
LCT-027 Case 3	Model updated from Revision 1 (September 30, 2000) to Revision 2. 1. Material compositions revised to match Table 14 and 15 of the Handbook. 2. Model revised to use air instead of void in cells that contain air.	1.0014 ~~1.0000~~	0.0015 ~~0.0011~~	1.00382 ~~1.00699~~	0.00010	Results closer to MORET, correcting ~300 pcm discrepancy

Benchmark	Revisions	k_{bmk}	σ_{bmk}	k_{MCNP6}	σ_{MCNP6}	Revision Impact
	Surfaces revised slightly to match current revision in Handbook.					
LCT-027 Case 4	Model updated from Revision 1 (September 30, 2000) to Revision 2. 1. Material compositions revised to match Table 14 and 15 of the Handbook. 2. Model revised to use air instead of void in cells that contain air. Surfaces revised slightly to match current revision in Handbook.	1.0014 ~~1.0000~~	0.0015 ~~0.0011~~	1.00604 ~~1.00921~~	0.00011	Results closer to MORET, correcting ~300 pcm discrepancy
MST-001 Case 6	1. Multiple material compositions corrected. 2. Solution height corrected.	1.0000	0.0016	0.99867 ~~0.99557~~	0.00012	Improvement in bias
MST-001 Case 11	1. Multiple material compositions corrected. 2. Cd inner layer corrected.	1.0000	0.0052	1.00580 ~~1.03581~~	0.00012	Substantial improvement in bias

The k-effective results presented in Table 1 are for MCNP6.2 calculations using ENDF-B/VII.1 nuclear data. A comparison of these results with MCNP6.2 results using ENDF-B/VIII.0 nuclear data is shown in Table 2.

Table 2. MCNP6.2 Results using ENDF-B/VII.1 and ENDF-B/VIII.0 Nuclear Data

Benchmark	$K_{MCNP6.2}$ +/- 1-sigma ENDF-B/VII.1	$k_{MCNP6.2}$ +/- 1-sigma ENDF-B/VIII.0
LCT-011 Case 15	0.99774 +/- 0.00009	0.99768 +/- 0.00009
LCT-027 Case 1	1.00068 +/- 0.00011	1.00082 +/- 0.00010
LCT-027 Case 2	1.00326 +/- 0.00011	1.00318 +/- 0.00011
LCT-027 Case 3	1.00382 +/- 0.00010	1.00377 +/- 0.00011
LCT-027 Case 4	1.00604 +/- 0.00011	1.00593 +/- 0.00011
MST-001 Case 6	0.99867 +/- 0.00012	0.99650 +/- 0.00013
MST-001 Case 11	1.00580 +/- 0.00012	1.00183 +/- 0.00012

Summary of Results

There exist 209 LEU benchmarks in the Whisper-1.1 library and 73 MIX benchmarks in the Whisper-1.1 library. The cases in common with other codes were examined during the intercomparison collaboration. There were 7 input files that were found to warrant further examination based upon discrepancies. All required revisions, in summary:

- 1 experiment, LEU-COMP-THERM-011, case 15, was found to have errors in geometry and required a slight correction to material, resulting in ~160 pcm improvement:
  - A correction was made to the atom fraction of copper in the cladding material to revise from 5.1174E-04 to 5.1174E-05.
  - The model was revised to remove end caps on fuel rods to be consistent with the Handbook.
  - A layer of water at the bottom of the rods was slightly modified to be 0.3-cm.
- 1 experiment, LEU-COMP-THERM-027, cases 1-4 were revised to update to the current revision in the Handbook, resulting in ~300 pcm improvement in all cases:
  - Material compositions were updated to current revision.
  - Instead of void the cells with air were modeled as air per the Handbook.
  - Several surfaces were revised slightly to match current revision in Handbook.
  - Experimental k-effective and uncertainty were revised to match revision in Handbook.
- 1 experiment, MIX-SOL-THERM-001, cases 6 and 11, was revised for material changes and geometry errors, resulting as much as 3000 pcm improvement:
  - Case 6 was revised to correct material compositions and solution height.
  - Case 11 was revised to correct material compositions and Cd layer.

As can be observed from the results, the largest differences in k-effective occur when geometry is revised.

Impact of Revisions

Benchmarks are ultimately used for nuclear criticality safety validation, to determine the appropriate bias and uncertainty in transport code simulations. Errors resulting in a significant bias in a long-standing benchmark collection have already been corrected because they are easier to identify. Eliminating smaller errors in the benchmark models is more difficult, may improve bias, and has the potential to influence validation. Comparison of upper subcritical limits (USLs) determined using the benchmark collection pre- and post-revision is a way to quantify the effect of correcting low-level errors on validation.

In a study conducted under a related NCSP task, LANL has participated in a comparison of USLs with IRSN and ORNL. LANL results using MCNP6.2 with nuclear data from ENDF/B-VII.1 evaluation to model the benchmarks, and Whisper-1.1 to compute USL, were compared with IRSN's MORET/MACSENS and ORNL's SCALE/TSURFER also using nuclear data from ENDF/B-VII.1 evaluation. In four total cases with HEU and Pu in thermal or fast energy applications, the changes to the benchmark collection did not result in overall significant change to the Upper Subcritical Limit (USL) for the cases studied [9].

Conclusions and Future Work

While participating in a study comparing k-effective results obtained with MCNP6 using nuclear data from ENDF/B-VII.1 evaluation with those obtained by IRSN using MORET, ORNL using SCALE, and LLNL using COG for ICSBEP benchmarks shared in common between laboratories, there were some LANL results identified as being discrepant. That information was used to examine particular benchmark models more closely, which resulted in revision to a total of 7 cases.

- All revisions in cases resulted in improvements in the bias, ranging from ~160 to 3000 pcm.
- All of the cases resulted in updates to material composition and isotopic abundances using data that are more recent.
- A few benchmarks had changes to geometry, one resulting in substantial improvement to the bias.

Benchmark collections are used for validation of transport codes. Ultimately, it is necessary to understand how revisions to the benchmark library affect validation. MCNP6.2 comes with a sensitivity/uncertainty tool, Whisper-1.1, used to support nuclear criticality safety validation. Using that tool, and the corresponding methodology, the benchmark revisions documented in the previous study [6] were shown not to affect validation significantly with respect to four well-characterized applications involving HEU and Pu in thermal and fast energy applications [9]. However, the revisions documented in this report for LEU and MIX cases should be used for future validation and to assess the impact on other methods or applications.

As discussed in the beginning of this report, the information and work done to review this subset of critical benchmarks has prompted a larger effort to combine efforts within XCP and NCS Divisions for review, revision, expansion, and maintenance of an open-source repository of LANL benchmarks.

Acknowledgments

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