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Summary of LANL Critical Benchmark Comparison Study and Revisions for Cases Involving HEU, LEU, MIX, and Pu

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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:

"CEA and IRSN published a summary of the results of an extensive benchmark Intercomparison study of French analytic methods using JEFF-3.1.1 nuclear data in the proceedings of the International Conference on Nuclear Criticality Safety (ICNC 2015). While JEFF data is available in many NCSP codes (e.g., COG, MCNP), due to resource limitations it has not been tested as rigorously as the US national database ENDF/B. The proposal is for IRSN to lead a new Intercomparison based on the MORET code with the latest JEFF-3.2 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 Highly Enriched Uranium (HEU), Intermediate Enriched Uranium (IEU), a mixture of Pu and Uranium (MIX), as well as Pu cases. A previous summary of revisions for HEU an Pu cases was reported [2] and additional investigations into four cases originally presented therein uncovered further revisions which led to better agreement with other transport codes, those cases are updated in this report. The summary of all cases reported in Reference 2 is updated in this report. In addition, a previous summary of revisions for LEU and MIX was reported [3], a summary of those revisions in reproduced in this report for a comprehensive summary of changes to benchmarks beginning in fiscal year 2020 to current date.

The report focuses 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 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 [4] 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 [5-7]. 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 [8-9].

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 benchmarks which 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, LEU, MIX, 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 because of the comparison were documented [2-3]. This report updates and summarizes all results thus far for benchmark review and revision.

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 [8-9]. 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 [8-9]. 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. Another group of input files were reviewed and did not result in revisions, which is also indicated in Table 1. Finally, there was a benchmark experiment that was removed from the library entirely. HEU-MET-FAST-077 cases 1 through 8 were added at a time in which it was expected they would also be added to the Handbook. Although the authors could find little documentation for the experiments, they were deemed unacceptable to be added to the Handbook (see further information in Appendix) and therefore have been removed from the library. Appendix A contains a summary of review/revision; complete formal documentation is retained in accordance with [8].

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
HEU-COMP-INTER-003-006	1. Changed the material in the iron sleeve to Fe, previously it was steel. 2. The radius of case 6 changed to 10.0609 cm. Previous was radius for case 5. 3. Nitrogen revised to N-14 and N-15, previous was 100% N-14. 4. Material 1 – incorrect total atom density, revised to 0.101763 (sum of the reported values in Table 9 of handbook). 5. Material 3 – incorrect value for Carbon, revised to 1.9893E-04, and incorrect value for the total atom density revised to 0.101844. 6. Material 6 – Fe nuclides was a factor of 10 off from Table 9, revised to match handbook. The	1.00000	0.00470	0.99642 ~~0.99558~~	0.00011	Not yet known

Benchmark	Revisions	k_{bmk}	σ_{bmk}	k_{MCNP6}	σ_{MCNP6}	Revision Impact
	total atom density is also off, revised to 0.096476. 7. Material 10 – incorrect total atom density, revised to 0.098727. Note: Did not change to only O-16 and Fe abundances overall, although did change Fe abundances for material 6 using MCNP6 mattool.					
HEU-MET-FAST-005-001	Atom densities revised: M1 4.85498810e-02, M2 5.82275520e-02, M3 6.12760150e-02, M4 1.17349015e-01, M5 4.68055200e-03	1.00000	0.00360	0.99509 ~~0.99510~~	0.00009	Results closer to MORET after revision
HEU-MET-FAST-005-002	Atom densities revised: M1 4.85498810e-02, M2 5.82275520e-02, M3 6.12760150e-02, M4 1.17349015e-01, M5 4.68055200e-03	1.00070	0.00360	0.99796 ~~0.99795~~	0.00010	Results closer to MORET after revision
HEU-MET-FAST-007-035	Changed material densities to match handbook values for HEU. Changed surfaces 1 and 7 to match handbook.	1.00030	0.00180	1.00226 ~~0.99489~~	0.00011	Result is strongly improved: discrepancies between codes now < 60 pcm, pre-revision > 750 pcm. Also closer to k_{exp}.
HEU-MET-FAST-018-002	Simple Model benchmark uncertainty changed to 0.0016. Prior to revision, it was 0.0014.	1.00000	0.00160 ~~0.00140~~	0.99971	0.00008	Pre-revision failed to specify simple model. Now within 10 pcm of KENO.
HEU-MET-FAST-020-002	Simple model benchmark uncertainty changed to 0.0030. Prior to revision, it was 0.0028. Material 1 revised to include W-180. Material 2 revised to exclude H-2.	1.00000	0.00300 ~~0.00280~~	1.00071 ~~1.00063~~	0.00010	
HEU-MET-FAST-021-002	Simple model benchmark uncertainty changed to 0.0026. Prior to revision, it was 0.0024.	1.00000	0.00260 ~~0.00240~~	0.99760	0.00009	

Benchmark	Revisions	k_{bmk}	σ_{bmk}	k_{MCNP6}	σ_{MCNP6}	Revision Impact
HEU-MET-FAST-022-002	Simple model benchmark uncertainty changed to 0.0021. Prior to revision, it was 0.0019. The atom densities of tungsten, including W-180, and iron in material m1 corrected. The atom densities of iron in material 2 corrected.	1.00000	0.00210 ~~0.00190~~	0.99734 ~~0.99763~~	0.00009	
HEU-MET-FAST-026-011	Simple model benchmark keff changed to 0.9982 and uncertainty changed to 0.0042. Prior to revision, it was 1.000 and 0.0038, respectively. The atom densities of Si, Cr, Fe, and Ni in material 2 corrected. Revisions to model.	0.99820 ~~1.00000~~	0.00420 ~~0.00380~~	0.99867 ~~1.00330~~	0.00009	Previous discrepancy with MORET and COG now corrected with revision.
HEU-MET-FAST-051-001	Updated to match revision 3. Updated Ag nuclides to natural abundance values.	0.99690 ~~0.99900~~	0.00050 ~~0.00120~~	0.99522 ~~0.99803~~	0.00009	Post-revision within 50 pcm of other codes.
HEU-MET-FAST-051-002	Updated to match revision 3. Updated Ag nuclides to natural abundance values.	0.99660 ~~0.99710~~	0.00050	0.99547 ~~0.99505~~	0.00009	Pre-revision failed to specify results are for detailed model.
HEU-MET-FAST-051-003	Updated to match revision 3 detailed model. Updated Ag nuclides to natural abundance values. Removed extra Sb. Updated N values to match natural abundances.	0.99710 ~~0.99680~~	0.00050	0.99498 ~~0.99546~~	0.00009	Pre-revision failed to specify results are for detailed model.
HEU-MET-FAST-051-004	Updated to match revision 3 detailed model. Updated Ag nuclides to natural abundance values and from .66c to .80c, changed elemental Sb to isotopic Sb.	0.99660 ~~0.99740~~	0.00050	0.99509 ~~0.99497~~	0.00008 ~~0.00009~~	Pre-revision failed to specify results are for detailed model.
HEU-MET-FAST-051-009	Updated to match revision 3 detailed model. Updated Ag nuclides to natural abundance values.	0.99780 ~~0.99690~~	0.00020 ~~0.00050~~	0.99494 ~~0.99517~~	0.00009	Pre-revision failed to specify results are for detailed model.
HEU-MET-FAST-051-014	Updated to match revision 3 detailed model. Updated Ag nuclides to natural abundance values. Removed extra Sb. Reordered materials to be sequential for reviewing.	0.99960 ~~0.99820~~	0.00020	0.99858 ~~0.99489~~	0.00008 ~~0.00009~~	Pre-revision failed to specify results are for detailed model.

Benchmark	Revisions	k_{bmk}	σ_{bmk}	k_{MCNP6}	σ_{MCNP6}	Revision Impact
HEU-MET-FAST-051-015	Updated to match revision 3 detailed model. Updated Ag nuclides to natural abundance values.	0.99970 ~~0.99960~~	0.00010 ~~0.00020~~	0.99810 ~~0.99861~~	0.00009 ~~0.00008~~	Pre-revision failed to specify results are for detailed model.
HEU-MET-FAST-051-016	Updated to match revision 3 detailed model. Updated Ag nuclides to natural abundance values. Updated Ag and Sb from .66c to .80c. Updated Ni values to match natural abundances. Changed elemental Sb to isotopic Sb. Changed N-14 from 2.4039e-5 to 2.4093e-5.	0.99790 ~~0.99980~~	0.00010	0.99640 ~~0.99805~~	0.00009 ~~0.00008~~	Pre-revision failed to specify results are for detailed model.
HEU-MET-FAST-051-017	Updated to match revision 3 detailed model. Updated Ag and N nuclides to natural abundance values. Updated Ag and Bi from .66c to .80c. Updated Sb values from elemental to isotopic to match natural abundances. Changed elemental Sb to isotopic Sb. Changed N-14 from 2.4039e-5 to 2.4093e-5.	0.99650 ~~0.99810~~	0.00010	0.99526 ~~0.99636~~	0.00009	Pre-revision failed to specify results are for detailed model.
HEU-MET-FAST-051-018	Updated to match revision 3 simple model. Updated Ni and N nuclides to natural abundance values. Updated Ag and Bi from .66c to .80c. Changed geometry to match revised simplified model.	0.99790 ~~0.99690~~	0.00020 ~~0.00010~~	0.99392 ~~0.99546~~	0.00008	Pre-revision failed to specify results are for simplified model.
HEU-MET-FAST-063-001	Benchmark uncertainty changed to 0.0040. Prior to revision, it was 0.0049. The LiD material revised to exclude lwtr.20t or hwtr.20t (fast system).	0.99930	0.00400 ~~0.00490~~	1.00064	0.00009	
HEU-MET-FAST-065-001 ~~HEU-MET-FAST-065-002~~	This should be HEU-MET-FAST-065-001 instead of HMF-065-002.	0.99950	0.00130	0.99812	0.00009	
HEU-MET-FAST-067-001	Benchmark keff changed to 0.9959 and uncertainty changed to 0.0024. Prior to revision, it was 1.0086 and 0.0004, respectively. The number density of W-180 separated from	0.99590 ~~1.00860~~	0.00240 ~~0.00040~~	1.00099 ~~1.00112~~	0.00008	Discrepancies with MORET improved with ENDF/B-VIII.0 data. (kcalc =

Benchmark	Revisions	k_{bmk}	σ_{bmk}	k_{MCNP6}	σ_{MCNP6}	Revision Impact
	W-182 in material 1 and W values revised to match Handbook values in Section 3.3 and updated abundances. Thermal scattering treatment for graphite added.					1.00124 0.00008
~~HEU-MET-FAST-077-001~~	Removed from library.	~~1.00010~~	~~0.00310~~	~~1.00068~~	~~0.00010~~	
~~HEU-MET-FAST-077-002~~	Removed from library.	~~0.99950~~	~~0.00270~~	~~1.00068~~	~~0.00010~~	
~~HEU-MET-FAST-077-003~~	Removed from library.	~~0.99950~~	~~0.00400~~	~~0.99787~~	~~0.00011~~	
~~HEU-MET-FAST-077-004~~	Removed from library.	~~0.99980~~	~~0.00320~~	~~0.99836~~	~~0.00010~~	
~~HEU-MET-FAST-077-005~~	Removed from library.	~~0.99940~~	~~0.00270~~	~~1.00012~~	~~0.00009~~	
~~HEU-MET-FAST-077-006~~	Removed from library.	~~0.99960~~	~~0.00330~~	~~0.99969~~	~~0.00010~~	
~~HEU-MET-FAST-077-007~~	Removed from library.	~~0.99940~~	~~0.00560~~	~~1.00057~~	~~0.00010~~	
~~HEU-MET-FAST-077-008~~	Removed from library.	~~0.99940~~	~~0.00350~~	~~0.99833~~	~~0.00010~~	
HEU-MET-MIXED-017-001	Benchmark keff changed to 1.0000. Prior to revision, it was 0.9995.	1.00000 ~~0.99950~~	0.00080	0.99547	0.00011	
HEU-MET-THERM-010-002 ~~HEU-MET-THERM-010-001~~	Simple model for 15-mil thick Gd. Changed to HEU-MET-THERM-010-002 to correspond to DICE convention as there is no case name given in the handbook. Benchmark uncertainty changed to 0.0070. Prior to revision, it was 1.0065 and 0.0072, respectively.	1.00650	0.00700 ~~0.00720~~	1.00875	0.00012	Pre-revision failed to specify 15-mil thick case for simple model, now named HMT-010-002 for future comparison.
HEU-SOL-THERM-001-001	Benchmark keff and uncertainty revised to match handbook revision.	1.00040 ~~1.00000~~	0.00600 ~~0.00250~~	0.99828	0.00016	

Benchmark	Revisions	k_{bmk}	σ_{bmk}	k_{MCNP6}	σ_{MCNP6}	Revision Impact
HEU-SOL-THERM-001-002	Benchmark keff and uncertainty revised to match handbook revision. The stainless steel material in case 2 revised to include the natural abundance of Sulphur (previously only included S-32).	1.00210 ~~1.00000~~	0.00720 ~~0.00250~~	0.99604 ~~0.99603~~	0.00016 ~~0.00015~~	
HEU-SOL-THERM-001-003	Benchmark keff and uncertainty revised to match handbook revision.	1.00030 ~~1.00000~~	0.00350 ~~0.00250~~	1.00177	0.00016	
HEU-SOL-THERM-001-004	Benchmark keff and uncertainty revised to match handbook revision.	1.00080 ~~1.00000~~	0.00530 ~~0.00250~~	0.99852	0.00015	
HEU-SOL-THERM-001-005	Benchmark keff and uncertainty revised to match handbook revision.	1.00010 ~~1.00000~~	0.00490 ~~0.00250~~	0.99868	0.00014	
HEU-SOL-THERM-001-006	Benchmark keff and uncertainty revised to match handbook revision.	1.00020 ~~1.00000~~	0.00460 ~~0.00250~~	1.00196	0.00013	
HEU-SOL-THERM-001-007	Benchmark keff and uncertainty revised to match handbook revision.	1.00080 ~~1.00000~~	0.00400 ~~0.00250~~	0.99779	0.00014	
HEU-SOL-THERM-001-008	Benchmark keff and uncertainty revised to match handbook revision.	0.99980 ~~1.00000~~	0.00380 ~~0.00250~~	0.99823	0.00015	
HEU-SOL-THERM-001-009	Benchmark keff and uncertainty revised to match handbook revision.	1.00080 ~~1.00000~~	0.00540 ~~0.00250~~	0.99435	0.00015	
HEU-SOL-THERM-001-010	Benchmark keff and uncertainty revised to match handbook revision.	0.99930 ~~1.00000~~	0.00540 ~~0.00250~~	0.99257	0.00013	
HEU-SOL-THERM-010-001	Reviewed, didn't find any issues. Possibly due to O-17 in model or steel abundances needing update. Will update in next revision.	1.00000	0.00290	1.00115	0.00012	Results within 20 pcm of other codes. Typo in comparison corrected.
HEU-SOL-THERM-019-001	Benchmark keff changed to 1.0000. Prior to revision all cases were 0.9991	1.00000 ~~0.99910~~	0.00410	0.99737	0.00014	Input file states Rev. 2, still ~200 pcm discrepancies with other codes. Further investigation.

Benchmark	Revisions	k_{bmk}	σ_{bmk}	k_{MCNP6}	σ_{MCNP6}	Revision Impact
HEU-SOL-THERM-019-002	Benchmark keff changed to 1.0000. Prior to revision all cases were 0.9991	1.00000 ~~0.99910~~	0.00410	0.99895	0.00013	
HEU-SOL-THERM-019-003	Benchmark keff changed to 1.0000. Prior to revision all cases were 0.9991	1.00000 ~~0.99910~~	0.00670	0.99459	0.00013	
HEU-SOL-THERM-038-010	Support structure material is missing Mg, revised to add Mg to material definition and total atom density.	1.00000	0.00260	0.99726 ~~0.99742~~	0.00014	
LCT-011 Case 15	8. Corrected atom fraction for Cu in cladding material from 5.1174E-04 to 5.1174E-05 to match Table 35 of Handbook. 9. Removed plugs (end caps) from bottom of rods. 10. 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. 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.	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
	2. Model revised to use air instead of void in cells that contain air. 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
LCT-079 case 7	Hexagon dimension for grid plate corrected.	1.0003	0.0008	0.99937 ~~0.99778~~	0.00011	Results improved.
LCT-079 case 8	Model was missing driver element, which has been added. Hexagon dimension for grid plate corrected.	1.0008	0.0008	1.00053~~0~~ ~~.99904~~	0.00011	Results improved.
LCT-079 case 9	Model was missing driver element, which has been added. Hexagon dimension for grid plate corrected.	1.0003	0.0008	0.99984 ~~0.99858~~	0.00011	Results improved.
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
PU-COMP-MIXED-001-005	Reviewed, didn't find issues.	0.99890	0.00720	1.00865	0.00014	Only 2 codes results and as the C-E are not good for both, difficult to conclude. Further investigation.
PU-COMP-MIXED-002-001	Reviewed, didn't find issues. Density of Plexiglas different values in handbook could lead to difference.	0.99900	0.00460	1.03110	0.00012	PCM002 only 2 code results and as the C-E are not good for both, difficult to conclude which

Benchmark	Revisions	k_{bmk}	σ_{bmk}	k_{MCNP6}	σ_{MCNP6}	Revision Impact
						is wrong. Further investigation.
PU-COMP-MIXED-002-023	Reviewed, didn't find issues. Density of Plexiglas different values in handbook could lead to difference.	1.00000	0.00680	1.00690	0.00012	"
PU-COMP-MIXED-002-024	Reviewed, didn't find issues. Density of Plexiglas different values in handbook could lead to difference.	1.00000	0.00680	1.00761	0.00013	"
PU-COMP-MIXED-002-025	Reviewed, didn't find issues. Density of Plexiglas different values in handbook could lead to difference.	1.00000	0.00680	1.00764	0.00014	"
PU-COMP-MIXED-002-026	Reviewed, didn't find issues. Density of Plexiglas different values in handbook could lead to difference.	1.00000	0.00680	1.00871	0.00014	"
PU-COMP-MIXED-002-027	Reviewed, didn't find issues. Density of Plexiglas different values in handbook could lead to difference.	1.00000	0.00680	1.00917	0.00013	"
PU-COMP-MIXED-002-028	Reviewed, didn't find issues. Density of Plexiglas different values in handbook could lead to difference.	1.00000	0.00680	1.00916	0.00013	"
PU-COMP-MIXED-002-029	Reviewed, didn't find issues. Density of Plexiglas different values in handbook could lead to difference.	1.00000	0.00680	1.01014	0.00013	"
PU-MET-FAST-001	Added new model. Latest revision by J. Favorite.	0.99999 ~~1.00000~~	0.00110 ~~0.00200~~	1.00101 ~~1.00001~~	0.00008	
PU-MET-FAST-003-001	Revised, material density for Pu-240 was incorrect (2.2936E-03 changed to 2.9236e-03) Also, was labeled PMF003-103.	1.00000	0.00300	0.99606 ~~0.99873~~	0.00008 ~~0.00009~~	

Benchmark	Revisions	k_{bmk}	σ_{bmk}	k_{MCNP6}	σ_{MCNP6}	Revision Impact
PU-MET-FAST-016-001	Benchmark keff changed to 0.9974 to match handbook. Prior to revision was 0.9976. Homogenized Al sleeve submerged in water did not have water, revised to include water in material and overall density. Dimensions of cylinders revised to be consistent with ICSBEP Handbook.	0.99740 ~~0.99760~~	0.00420	1.01551 ~~1.01764~~	0.00011	MCNP6 results consistent with MORET.
PU-MET-FAST-026-001	Simplified model. Benchmark uncertainty changed to 0.0026 to match handbook. Prior to revision was 0.0022. Reflector material Mn atom density revised to match handbook Table 7, from 3.2805e-04 to 3.2850e-4.	1.00000	0.00260 ~~0.00220~~	0.99866 ~~0.99867~~	0.00009	Pre-revision failed to specify simple model. Now more consistent with other codes.
PU-MET-FAST-029-001	Simplified model. Benchmark uncertainty changed to 0.0022 to match handbook. Prior to revision was 0.0024.	1.00000	0.00220 ~~0.00240~~	0.99580	0.00008	Pre-revision failed to specify simple model. Now more consistent with other codes.
PU-MET-FAST-045-001	Detailed model. Revised, number density for Pu was incorrect. Should be 0.03996 instead of 0.03966. Top height of reactor was incorrect, revised.	1.00000	0.00470	1.00711 ~~1.00164~~	0.00010 ~~0.00009~~	Worse results when looking at c-E and bigger discrepancies than previously with other codes. Pre-revision failed to specify detailed model. Further investigation.
PU-MET-FAST-045-002	Revised, number density for Pu was incorrect. Should be 0.03996 instead of 0.03966. Top height of reactor was incorrect, revised.	1.00000	0.00460	1.01356 ~~1.00785~~	0.00010	“
PU-MET-FAST-045-003	Revised, number density for Pu was incorrect. Should be 0.03996 instead of 0.03966. Top height of reactor was incorrect, revised.	1.00000	0.00440	1.01100 ~~1.00536~~	0.00009	“

Benchmark	Revisions	k_{bmk}	σ_{bmk}	k_{MCNP6}	σ_{MCNP6}	Revision Impact
PU-MET-FAST-045-004	Revised, number density for Pu was incorrect. Should be 0.03996 instead of 0.03966. Top height of reactor was incorrect, revised.	1.00000	0.00460	1.01025 ~~1.00462~~	0.00009	"
PU-MET-FAST-045-005	Revised, number density for Pu was incorrect. Should be 0.03996 instead of 0.03966. Top height of reactor was incorrect, revised. Surface 16 was 7.5663 revised to 7.56663.	1.00000	0.00450	1.01447 ~~1.00858~~	0.00009	"
PU-MET-FAST-045-006	Revised, number density for Pu was incorrect. Should be 0.03996 instead of 0.03966. Top height of reactor was incorrect, revised.	1.00000	0.00490	1.01055 ~~1.00483~~	0.00009	"
PU-MET-FAST-045-007	Revised, number density for Pu was incorrect. Should be 0.03996 instead of 0.03966. Top height of reactor was incorrect, revised.	1.00000	0.00500	1.01108 ~~1.00541~~	0.00010 ~~0.00009~~	"
PU-SOL-THERM-001-003	Revised, number densities for N were incorrected. Updated isotopic abundances for Fe, Cr, Ni.	1.00000	0.00500	1.01050 ~~1.01135~~	0.00013	Reduced discrepancies with other codes (< 150 pcm)
PU-SOL-THERM-002-006	Updated isotopic abundances for Fe, Cr, Ni.	1.00000	0.00470	1.00518	0.00012	< 50 pcm discrepancies with other codes

Summary of Results

Overall, 70 HEU and Pu benchmarks were reviewed based upon information received during the intercomparison collaboration. There were 33 input files that were revised:

- 2 experiments were not known to have errors, rather they were updated to match the current handbook version:
  - pmf001, resulting in 100 pcm difference, and
  - hmf051 (10 cases) resulting in differences of 12 - 369 pcm
- 13 cases were revised for material changes, resulting in differences of less than ~50 pcm except for:
  - pmf003: 267 pcm difference due to typo in the number density for Pu-240, and
  - pst001: 85 pcm difference due to change in N abundances of plutonium nitrate solution
- 3 experiments (9 cases) were revised for material changes and geometry errors:
  - hci-003-006, 84 pcm difference
  - hmf-007-035, 737 pcm difference
  - pmf045, 7 cases all resulting in > 500 pcm difference

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 10 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, LEU-COMP-THERM-079, cases 7-9 were revised to correct modeling errors:
  - Model was missing driver element in cases 8 and 9, which has been added.

    - Hexagon dimension for grid plate corrected.
- 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 [10].

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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Appendix A: Benchmark Revision Remarks

HEU-COMP-INT-003-006: There are a number of changes made to the file:

1. The Handbook describes an iron sleeve, originally modeled as steel in the input file now revised to be 100% iron. The handbook can be somewhat confusing because it states, *“The steel sleeve extends the full length of the reflector. Its inner radius is 7.5489 cm, and its outer radius is 7.6759 cm. It is full-density iron with a thickness of 0.1270 cm.”*
2. The overall radius for case 6 was incorrect and has been revised to 10.0609 cm. The input file previously used the radius for case 5, this is also an error in the example input file for case 6 in the handbook; it is a repeat of the input file for case 5.
3. Nitrogen was changed from 100% N-14 to 99.636 at% N-14 and 0.364 at% N-15.
4. Material 1 atom density was changed to 0.10176 to match the handbook value. The previous value of is incorrect.
5. Material 3 carbon density 1.9893e-4 and overall material density was changed to 0.101844 to match handbook values.
6. Material 6 the atom densities were an order of magnitude low and were revised, the total atom density was revised to 0.096476.
7. Material 10 atom density was revised to 0.098727.

HEU-MET-FAST-005-001: Atom densities for material 1 revised to 4.85498810e-02, material 2 is 5.82275520e-02, material 3 is 6.12760150e-02, material 4 is 1.17349015e-01, material 5 is 4.68055200e-03

HEU-MET-FAST-005-002: Atom densities for material 1 revised to 4.85498810e-02, for material 2 to 5.82275520e-02, material 3 to 6.12760150e-02, material 4 to 1.17349015e-01, material 5 to 4.68055200e-03

HEU-MET-FAST-007-035: Material densities were revised to match Handbook and the precision of surface 1 revised to 5.36162 to match Handbook value.

HEU-MET-FAST-018, -020, -021 and -022: there is only one experiment with a detailed and a simplified model. They were named -002 (HMF-018-002) to indicate the simplified model. Thus, the benchmark uncertainty should be increase by 0.0002 as indicated in the Handbook:

"Because of the simplification procedure (See Section 3.1.3), a small additional uncertainty is associated with the simplified model. This uncertainty is not folded into the uncertainty presented with the benchmark keff. However, it is expected that the additional uncertainty associated with the simplified benchmark model keff is not greater than 0.0002. »

020: - Material 1 revised to include W-180, material 2 revised to exclude H-2

022: - The atom densities of tungsten, including W-180, and iron in material m1 corrected. The atom densities of iron in material 2 corrected.

HEU-MET-FAST-026-011: benchmark keff value should be 0.99820 +/- 0.0042 (and not 1 +/- 0.0038) as case 11 corresponds to experiment c-1 (see table below)

HEU-MET-FAST-026

Table 11. Benchmark k_{eff} Values.

Exp. I.D.	Benchmark k_{eff}	Uncertainty, Δk_{eff}
b-1, b-2, b-6, b-7, c-1, c-2, c-3, c-8, c-9, d-1, d-2, d-6, d-7	0.9982	0.0042
All the rest	1.0000	0.0038

The atom densities of Si, Cr, Fe, and Ni in material 2 corrected.

HEU-MET-FAST-051: All cases were updated benchmark revision 3, 2014. Updated benchmark model keff values to agree with Table 20 of the Handbook.

- Case 1: Material 5 – updated Ag nuclides to natural abundance values.
- Case 2: Material 5 – updated Ag nuclides to natural abundance values.
- Case 3: Material 5 – updated Ag nuclides to natural abundance values.
    - Material 18 - removed extra uncommented line with old natural Sb.
    - Material 29 – updated N nuclides to natural abundance values.
- Case 4: All materials – Updated Ag and Bi nuclides from 66c to 80c, changed natSb to isoSb.
- Case 9: Material 5 – updated Ag nuclides to natural abundance values.
    - All materials – Updated Ag and Bi nuclides from 66c to 80c, changed natSb to isoSb.
- Case 14: Reordered materials to be sequential (easier editing).
    - Material 5 – updated Ag nuclides to natural abundance values.
    - All materials – Updated Ag and Bi nuclides from 66c to 80c, changed natSb to isoSb.
- Case 15: Material 8 – updated Ni nuclides to natural abundance values.
    - All materials – Updated Ag and Bi nuclides from 66c to 80c, changed natSb to isoSb.
- Case 16: surface 69 changed to 8.8940005 cm (Ref. 34 from Table 14).

    - Material 5 – updated Ag nuclides to natural abundance values.
    - Material 8 – updated Ni nuclides to natural abundance values.
    - Material 22 – changed N-14 from 2.4039e-5 to 2.4093e-5.
    - All materials – Updated Ag and Bi nuclides from 66c to 80c, changed natSb to isoSb.
- Case 17: Material 5 – updated Ag nuclides to natural abundance values.
    - Material 29 – updated N nuclides to natural abundance values.
    - All materials – Updated Ag and Bi nuclides from 66c to 80c, changed natSb to isoSb.
- Case 18: Material 8 – updated Ni nuclides to natural abundance values.
    - Material 29 – updated N nuclides to natural abundance values.
    - All materials – Updated Ag and Bi nuclides from 66c to 80c, changed natSb to isoSb.
    - changed geometry to match revised simplified version in Handbook

HEU-MET-FAST-063-001: Benchmark uncertainty changed to 0.0040. Prior to revision, it was 0.0049. The LiD material revised to not include lwtr.20t or hwtr.20t (fast system).

HEU-MET-FAST-065-001: This should be HEU-MET-FAST-065-001 instead of HMF-065-002.

HEU-MET-FAST-067-001: Benchmark keff changed to 0.9959 and uncertainty changed to 0.0024. Prior to revision, it was 1.0086 and 0.0004, respectively. The number density of W-180 separated from W-182 in material 1 and W values revised to match Handbook values in Section 3.3 with updated abundances. Thermal scattering treatment for graphite added. Agreement with MORET results for ENDF/B-VIII.0 data.

HEU-MET-FAST-077: These cases have been removed from the library. They were added at a time in which it was expected they would also be added to the Handbook. Although the authors could find little documentation for the experiments, they were deemed unacceptable to be added to the Handbook, excerpt of email (David P. Heinrichs, personal communication, March 7, 2019):

"I think your decks are from a preliminary evaluation of part of the NIMBUS program (e.g., HMF066). If my recollection is correct, the expectations for evaluations were increasing and when these were evaluated, reviewers were asking lots of questions about the machine and fixturing at which point the cost of doing this became prohibitive and the evaluation was effectively abandoned, and the evaluation number recycled …. I think. In any case, it's definitely not HMF077."

HEU-MET-MIXED-017-001: Benchmark keff changed to 1.0000. Prior to revision, it was 0.9995.

"Including the uncertainties described in Section 2, the benchmark-model k_{eff} value is 1.0000 ± 0.0008. The benchmark idealizations combined, give a total bias of -0.0005±0.0005. Because the uncertainty of the idealizations is equivalent to the calculated idealization, it is not statistically significant and ***no correction is required to the benchmark k_{eff}.***"

HEU-MET-THERM-010-001: Benchmark keff changed to 1.0065 and uncertainty changed to 0.0070. Prior to revision, it was 1.0065 and 0.0072, respectively.

HEU-SOL-THERM-001-001: Benchmark keff and uncertainty revised to match handbook revision.

HEU-SOL-THERM-001-002: Benchmark keff and uncertainty revised to match handbook revision. The stainless steel material in case 2 revised to include the natural abundance of Sulphur (previously only included S-32).

HEU-SOL-THERM-001-003: Benchmark keff and uncertainty revised to match handbook revision.

HEU-SOL-THERM-001-004: Benchmark keff and uncertainty revised to match handbook revision.

HEU-SOL-THERM-001-005: Benchmark keff and uncertainty revised to match handbook revision.

HEU-SOL-THERM-001-006: Benchmark keff and uncertainty revised to match handbook revision.

HEU-SOL-THERM-001-007: Benchmark keff and uncertainty revised to match handbook revision.

HEU-SOL-THERM-001-008: Benchmark keff and uncertainty revised to match handbook revision.

HEU-SOL-THERM-001-009: Benchmark keff and uncertainty revised to match handbook revision.

HEU-SOL-THERM-001-010: Benchmark keff and uncertainty revised to match handbook revision.

HEU-SOL-THERM-010-001: Reviewed, didn't find any issues.

HEU-SOL-THERM-019-001: Benchmark keff changed to 1.0000. Prior to revision all cases were 0.9991

HEU-SOL-THERM-019-002: Benchmark keff changed to 1.0000. Prior to revision all cases were 0.9991

HEU-SOL-THERM-019-003: Benchmark keff changed to 1.0000. Prior to revision all cases were 0.9991

HEU-SOL-THERM-038-010: - Material 7 revised to include the contribution from magnesium.

PU-COMP-MIXED-001-005: Reviewed, didn't find issues.

PU-COMP-MIXED-002-001: Reviewed, didn't find issues.

PU-COMP-MIXED-002-023: Reviewed, didn't find issues.

PU-COMP-MIXED-002-024: Reviewed, didn't find issues.

PU-COMP-MIXED-002-025: Reviewed, didn't find issues.

PU-COMP-MIXED-002-026: Reviewed, didn't find issues.

PU-COMP-MIXED-002-027: Reviewed, didn't find issues.

PU-COMP-MIXED-002-028: Reviewed, didn't find issues.

PU-COMP-MIXED-002-029: Reviewed, didn't find issues.

PU-MET-FAST-001: Revised to new model by J. Favorite.

PU-MET-FAST-003-001: Revised, material density for Pu-240 was incorrect (2.2936E-03 changed to 2.9236e-03) Also, was labeled PMF003-103

PU-MET-FAST-016-001: Benchmark keff changed to 0.9974 to match handbook. Prior to revision was 0.9976. Input file missing material for homogenized Al and water for the length of sleeve that is submerged. Dimensions of cylinders revised to be consistent with ICSBEP Handbook.

PU-MET-FAST-026-001: Benchmark uncertainty changed to 0.0026 to match handbook. Prior to revision was 0.0022. In Material 2, 25055.80c should be 3.2850E-4 per Handbook Table 8.

PU-MET-FAST-029-001: Benchmark uncertainty changed to 0.0022 to match handbook. Prior to revision was 0.0024.

PU-MET-FAST-045-001: Revised, number density for Pu was incorrect. Should be 0.03996 instead of 0.03966

- Surface 27, the top height of the reactor, was taken directly from the handbook and did not take into account where z = 0 was set for the MCNP model for any case. It should be 43.7478.

PU-MET-FAST-045-002: Revised, number density for Pu was incorrect. Should be 0.03996 instead of 0.03966

- Surface 27, the top height of the reactor, was taken directly from the handbook and did not take into account where z = 0 was set for the MCNP model for any case. It should be 43.7478.

PU-MET-FAST-045-003: Revised, number density for Pu was incorrect. Should be 0.03996 instead of 0.03966

- Surface 27, the top height of the reactor, was taken directly from the handbook and did not take into account where z = 0 was set for the MCNP model for any case. It should be 43.7478.

- Surfaces 16, 19, and 23 are all lower in the MCNP model than the values calculated using the handbook by 0.0036 cm.

PU-MET-FAST-045-004: Revised, number density for Pu was incorrect. Should be 0.03996 instead of 0.03966

- Surface 27, the top height of the reactor, was taken directly from the handbook and did not take into account where z = 0 was set for the MCNP model for any case. It should be 43.7478.

PU-MET-FAST-045-005: Revised, number density for Pu was incorrect. Should be 0.03996 instead of 0.03966

- Surface 27, the top height of the reactor, was taken directly from the handbook and did not take into account where z = 0 was set for the MCNP model for any case. It should be 43.7478.

- Surface 16 is given as 7.5663 but should be 7.56663.

PU-MET-FAST-045-006: Revised, number density for Pu was incorrect. Should be 0.03996 instead of 0.03966

- Surface 27, the top height of the reactor, was taken directly from the handbook and did not take into account where z = 0 was set for the MCNP model for any case. It should be 43.7478.

PU-MET-FAST-045-007: Revised, number density for Pu was incorrect. Should be 0.03996 instead of 0.03966

- Surface 27, the top height of the reactor, was taken directly from the handbook and did not take into account where z = 0 was set for the MCNP model for any case. It should be 43.7478.

PU-SOL-THERM-001-003: Revised number densities for N were incorrect. Updated isotopic abundances for Fe, Cr, Ni.

PU-SOL-THERM-002-006: Updated isotopic abundances for Fe, Cr, Ni.

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.

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.

LEU-COMP-THERM-079: cases 7-9 were revised to correct modeling errors: Model was missing driver element in cases 8 and 9, which has been added. Hexagon dimension for grid plate corrected.

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.