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LANL Critical Benchmark Comparison Study and Subsequent Revision

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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 and in conjunction with ORNL and LLNL to compare results of various neutron transport codes and nuclear data libraries to compute k-effective for ICSBEP benchmarks held in common by the entities. The task statement from the DOE NCSP Five-Year Execution Plan [1]:

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 through partial completion of the overall effort 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. The feedback received through participation in the comparison collaboration has prompted an effort to review particular input files for benchmarks and revise when necessary. This report documents the results of review and revision of specific benchmarks highlighted as possibly discrepant in the comparison study. In addition, this effort prompted a new 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, is referred to as the Whisper-1.1 library because it is used with a sensitivity/uncertainty package, Whisper, which helps support 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), 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 (~1100 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 atypical 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. The work documented in this report is the start of a larger effort to centralize a single LANL collection that is up-to-date with the latest ICSBEP Handbook 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. Future efforts are contingent upon funding. Forty-seven HEU benchmarks and twenty-three Pu benchmarks have been reviewed in this particular study based upon feedback collected as a part of the LANL collaboration with IRSN, LLNL, and ORNL. MCNP6.2 using ENDF/B-VII.1 nuclear data results for k-effective are presented pre- and post-revision.

The particular benchmarks, which have been reviewed and brief remarks of revisions are given in Table 1. 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 [5]. 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. Some of the benchmarks did not have any changes to the input file itself, though there was a change to the experimental k-effective and/or uncertainty as reported in the ICSBEP Handbook and those differences indicated with a strikethrough. Another group of input files were reviewed and did not result in revisions, this 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 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 [6].

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

Benchmark	Revisions	Benchmark k-effective	Benchmark uncertainty	MCNP6 k-effective	MCNP6 uncertainty
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 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.	1.00000	0.00470	0.99642 ~~0.99558~~	0.00011
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
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
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
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

Benchmark	Revisions	Benchmark k-effective	Benchmark uncertainty	MCNP6 k-effective	MCNP6 uncertainty
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
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.	0.99820 ~~1.00000~~	0.00420 ~~0.00380~~	1.00306 ~~1.00330~~	0.00011
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
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
HEU-MET-FAST-051-003	Updated to match revision 3. 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
HEU-MET-FAST-051-004	Updated to match revision 3. 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~~
HEU-MET-FAST-051-009	Updated to match revision 3. Updated Ag nuclides to natural abundance values.	0.99780 ~~0.99690~~	0.00020 ~~0.00050~~	0.99494 ~~0.99517~~	0.00009
HEU-MET-FAST-051-014	Updated to match revision 3. 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~~
HEU-MET-FAST-051-015	Updated to match revision 3. Updated Ag nuclides to natural abundance values.	0.99970 ~~0.99960~~	0.00010 ~~0.00020~~	0.99810 ~~0.99861~~	0.00009 ~~0.00008~~

Benchmark	Revisions	Benchmark k-effective	Benchmark uncertainty	MCNP6 k-effective	MCNP6 uncertainty
HEU-MET-FAST-051-016	Updated to match revision 3. 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~~
HEU-MET-FAST-051-017	Updated to match revision 3. 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
HEU-MET-FAST-051-018	Updated to match revision 3. Updated Ni and N nuclides to natural abundance values. Updated Ag and Bi from .66c to .80c. Changed elemental Sb to isotopic Sb. Changed N-14 from 2.4039e-5 to 2.4093e-5. Changed Na-23 from 1.3238e-5 to 1.3262e-5, Changed surfaces 4 – 12, 22 – 31, 42 – 51, 62 – 68 to match revised model.	0.99790 ~~0.99690~~	0.00020 ~~0.00010~~	0.99546	0.00008
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 W-182 in material 1 and W values revised to match Handbook values in Section 3.3 and updated adundances.	0.99590 ~~1.00860~~	0.00240 ~~0.00040~~	1.00085 ~~1.00112~~	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~~

Benchmark	Revisions	Benchmark k-effective	Benchmark uncertainty	MCNP6 k-effective	MCNP6 uncertainty
~~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-010-001	Benchmark keff changed to 1.0065 and 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
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
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

Benchmark	Revisions	Benchmark k-effective	Benchmark uncertainty	MCNP6 k-effective	MCNP6 uncertainty
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
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
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
PU-COMP-MIXED-001-005	Reviewed, didn't find issues.	0.99890	0.00720	1.00865	0.00014
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
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

Benchmark	Revisions	Benchmark k-effective	Benchmark uncertainty	MCNP6 k-effective	MCNP6 uncertainty
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~~
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.	0.99740 ~~0.99760~~	0.00420	1.01710 ~~1.01764~~	0.00012
PU-MET-FAST-026-001	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
PU-MET-FAST-029-001	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
PU-MET-FAST-045-001	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~~
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
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

Benchmark	Revisions	Benchmark k-effective	Benchmark uncertainty	MCNP6 k-effective	MCNP6 uncertainty
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
PU-SOL-THERM-002-006	Updated isotopic abundances for Fe, Cr, Ni.	1.00000	0.00470	1.00518	0.00012

Summary of Results

Overall, 70 benchmarks were reviewed based upon information received during the intercomparison collaboration. There were 32 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
- 12 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

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 ENDF/B-VII.1 to model the benchmarks and Whipser-1.1 to compute USL were compared with IRSN's MORET/MACSENS and ORNL's SCALE/TSURFER also using ENDF/B-VII.1 nuclear data. In four different cases, for HEU and PU, and thermal or fast energy applications, the changes to the benchmark collection documented in this report did not result in overall significant change to the Upper Subcritical Limit (USL) for the cases studied [7].

Conclusions and Future Work

While participating in a study comparing k-effective results obtained with MCNP6 using ENDF/B-VII.1 nuclear data 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 atypical. That information was used to examine those particular benchmark models more closely, which resulted in revision to some of the benchmarks.

- Many of the cases resulted in updates to isotopic abundances using data that are more recent.
- In several benchmarks, W-180 nuclear data was not available at the time of the experiment including into the Handbook. Some of those benchmarks have been updated to include the proper amount of W-180 in the material. Exceptions remain for consistency with the Handbook, when experiment k-effective was stated without modeling W-180.
- A few benchmarks had changes to geometry, although improvement in bias is minor.
- HEU-MET-FAST-077 is removed from the library; this series was never accepted into the Handbook although were added to the library at the time they were proposed for inclusion in the Handbook.
- Finally, there were cases in which no error could be identified and they are kept in the library as is.

Benchmark collections are used for validation of transport codes. MCNP6.2 comes with a sensitivity/uncertainty tool used to support nuclear criticality safety validation. Ultimately, it is necessary to understand how revisions to the benchmark library affects validation. The revisions documented in this report, for HEU and Pu, have little effect on the USL for HEU and Pu applications studied.

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.

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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 22 – changed N-14 from 2.4039e-5 to 2.4093e-5.
    - Material 29 – updated N nuclides to natural abundance values.
    - Material 50 – change Na-23 from 1.3238e-5 to 1.3262e-5.
    - All materials – Updated Ag and Bi nuclides from 66c to 80c, changed natSb to isoSb.
    - changed surfaces 4 – 12, 22 – 31, 42 – 51, 62 – 68

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.

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.

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.