#### Summary Report

# IAEA Contract TAL-NAPC20200423-003 1 June 202 to 15 September 2020

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The work performed under this contract is in support of the IAEA Nuclear Data Section's Compilation of Nuclear Data Experiments for Radiation Characterization (CoNDERC) Activity.

Four Appendices are attached to this report, each describing a different aspect of the work performed during the current contract period.

Appendix A relates to the International Criticality Safety Benchmark Evaluation Project's Handbook. This Handbook provides benchmark descriptions for thousands of critical assembly configurations. However, as a Crit Safety document it is primarily focused on integral criticality, i.e., the ability of accurately calculate k<sub>eff</sub>. While a crucial quantity, for those involved in nuclear data testing it is important to assess not only criticality but other assembly parameters such as individual reaction rates, power distributions, reactivity coefficients, etc. Such information is rarely presented in an ICSBEP evaluation, but its existence is often acknowledged in a "Supplemental Information" section. Hence, in Appendix A we have searched many of the ICSBEP evaluations and summarize those for which additional data may be available. However, we emphasize "may", as these fleeting mentions of additional data may or may not include the appropriate citation, and even when references are given, they are often for decades old Progress Reports which may no longer exist. Nevertheless this summary provides a starting point to expand upon the basic criticality data for these evaluations.

Nuclear data testing by the major regional cross section library organizations (CSEWG/ENDF in the USA, the JEFF community in Europe, JAEA/JENDL in Japan, and more) are focused mostly on the evaluations available from the ICSBEP Handbook noted above. Other well-known but lessor used compilations include the Cross Section Evaluation Working Group's (CSEWG) Benchmark Book, the Reactor Physics Handbook from the International Reactor Physics Evaluation Project (IRPhEP) and the Shielding community's SINBAD Database.

A lesser known document is the IAEA's "Technical Research Series No. 480 - Research Reactor Database: Facility Specification and Experimental Data". Appendix B performs a similar function as Appendix A, but does so for the 15 reactors is noted therein. The TRS-480 document was first published in 2015 with an expanded second edition in 2020. This report represents the work of IAEA sponsored Coordinated Research Projects 1496 on Innovative Methods in Research Reactor Analysis: Benchmark Against Experimental Data on Neutronics and Thermalhydraulic Computational Methods and Tools for Operation and Safety Analysis of Research Reactors and T12029 on Benchmarks of Computational Tools Against Experimental Data on Fuel Burnup and Material Activation for Utilization, Operation and Safety Analysis of Research Reactors.

Appendices A and B summarize literature research into the availability of data not generally known to the nuclear data testing community. In Appendices C and D we summarize the results of MCNP6<sup>©</sup> criticality and reaction rate calculations for a select few of these benchmarks under varying conditions.

Appendix C provides the results of kcode calculations for the IRPhEP's KRITZ evaluation (4 cases; 2 at room temperature and two at ~245 °C as well as calculations for benchmarks described in the ICSBEP LEU-COMP-THERM-005 (LCT5), -007 (LCT7) and -008 (LCT8) evaluations. These are room temperature, light-water moderated and reflected, low-enriched <sup>235</sup>U-UO<sub>2</sub> fueled rod lattice assemblies. The calculations were performed using a light-water (h-h<sub>2</sub>o) thermal scattering kernel and with both the light-water kernel and fuel system (u-uo<sub>2</sub> and o-uo<sub>2</sub>) scattering kernels. As explained in the Appendix, the resulting k<sub>calc</sub> values suggest that the presence of the generally omitted fuel system scattering kernels increases k<sub>calc</sub> by several tens of pcm, with slight evidence that the k<sub>calc</sub> bias is 50 pcm or larger for systems with very low EALFs (Energy of Average Lethargy causing Fission).

Appendix D expands upon a previous study that examined the accuracy of MCNP's k<sub>calc</sub> uncertainty estimate to review the uncertainty estimate for reaction rates, spectral indices and pin power predictions. As discussed in this Appendix, the uncertainties for single quantities such as reaction rates or pin powers are calculated accuracy, but the when calculating the uncertainty of a spectral index, which is the ratio of two individual reaction rates, the legacy assumption of independent uncertainties for the individual rates may be inadequate. Rather correlation in these rates will lead to an overestimate of the spectral index uncertainty. The degree of correlation can vary greatly, depending upon details of the cross sections involved and assembly flux spectrum.

#### Appendix A

#### ICSBEP Handbook Supplemental Information (Section 1.4 or 1.5) Summary

## IAEA Contract TAL-NAPC20200423-003 September 2020

Evaluated experiments in the Handbook published by the International Criticality Safety Benchmark Evaluation Project (ICSBEP) are categorized by a series attributes, including fuel type (HEU, IEU and LEU for highly-enriched, intermediate-enriched and low-enriched uranium, PU for <sup>239</sup>Pu, U233 for <sup>233</sup>U and MIX for uranium-plutonium mixtures and SPEC for other fissile materials), fuel form (MET for metal, SOL for solution, COMP for molecular compounds) and spectrum (FAST, INTER and THERMAL). Identifiers such as "MIX" or "MISC" are also used if there is no single dominant characteristic.

These evaluations are focused on defining the necessary information to create a computer model to support critical eigenvalue calculations. Of lessor interest to the criticality safety community are those supplemental measurements that provide data that might be used for nuclear data qualification, or in many cases there simply are no supplemental information.

The following summarizes whether additional supplemental information might be available for many of the evaluations in the ICSBEP Handbook. We say "... might be ..." because these data were not the focus of the current evaluation effort and the presence of such data is often only mentioned in passing with limited or no accompanying citation. Hence it is not obvious whether these data can be recovered and used in a nuclear data qualification effort. Nevertheless it does provide a starting point to search for information beyond a global  $k_{eff}$  value.

The evaluation categories that were reviewed include (i) HEU-MET-FAST, (ii) IEU-MET-FAST, (iii) PU-MET-FAST, (iv) MIX-MET-FAST, (v) HEU-MET-INTER, (vi) LEU-COMP-THERM, (vii) HEU-SOL-THERM, and (viii) PU-SOL-THERM.

The 2019 edition of the ICSBEP Handbook, the latest available at this time, was used for this review.

#### (i) HEU-MET-FAST:

HEU-MET-FAST-001: Yes. Numerous references plus Appendix E (which is taken from the CSEWG Benchmark Book (CSEWG Fast Benchmark #5)).

HEU-MET-FAST-002: Yes. See reference 4 ... L. B. Engle, G. E. Hansen, and H. C. Paxton, "Reactivity Contributions of Various Materials in Topsy, Godiva, and Jezebel," Nucl. Sci. Eng., **8**, No. 6, p. 543, December 1960.

HEU-MET-FAST-003: Yes. See references 2 and 3 ... (2) J. D. Orndorff, H. C. Paxton, and G. E. Hansen, "Critical Masses of Oralloy at Reduced Concentrations and Densities," LA-1251, May 1951; (3) L. B. Engle, G. E. Hansen, and H. C. Paxton, "Reactivity Contributions of Various Materials in Topsy, Godiva, and Jezebel," Nucl. Sci. Eng., **8**, No. 6, p. 543, December 1960.

HEU-MET-FAST-004, -005: None

HEU-MET-FAST-006: Re-assigned to HEU-MET-THERM-003.

HEU-MET-FAST-007: None

HEU-MET-FAST-008: None. This and many other evaluations of experiments performed at VNIITF mention reactivity worth measurements that are documented in various log-books. It is not clear that these are publicly available.

HEU-MET-FAST-009 through -012: None, but see HMF8 comment.

HEU-MET-FAST-013 through -023: None

HEU-MET-FAST-024: None, but see HMF8 comment.

HEU-MET-FAST-025 through -027: None

HEU-MET-FAST-028: Yes. Data tabulated in the CSEWG Handbook are reproduced in this evaluation's Appendix C.

HEU-MET-FAST-029 through -034: None

HEU-MET-FAST-035: Yes. Re-assigned to HEU-MET-INTER-001 (ZPR-9/34).

HEU-MET-FAST-036 through -044: None

HEU-MET-FAST-045: Unassigned identifier.

HEU-MET-FAST-046: Unassigned identifier.

HEU-MET-FAST-047: None

HEU-MET-FAST-048: Yes. See Appendix B for component reactivity worth data.

HEU-MET-FAST-049 through -054: None

HEU-MET-FAST-055: Yes. ZPR-3/23, but no published documentation, 😕.

HEU-MET-FAST-056 through -059: None

HEU-MET-FAST-060: Yes. ZPR-9/4. See references 1 through 6.

HEU-MET-FAST-061: Yes. ZPPR-21 Phase F. Undocumented sub-crits.

HEU-MET-FAST-062: Yes. "... many neutronic experiments ...". See references.

HEU-MET-FAST-063 through -066: None

HEU-MET-FAST-067: Yes. ZPR-9/5 & 9/6. See references 1 through 6.

HEU-MET-FAST-068: Yes. Many spectral index measurements are claimed, but no data nor any specific reference is cited. A number of references are given in Section 5 that could be reviewed.

HEU-MET-FAST-069: None

HEU-MET-FAST-070: Yes. ZPR-9/7, -9/8 & 9/9. See references 1 through 7.

HEU-MET-FAST-071 through 074: None

HEU-MET-FAST-075: Yes. ZPPR-20. A tabulation of integral measurements is provided, but no data nor specific references are cited. A technical conference reference is cited in Section 5.

HEU-MET-FAST-076 through -094: None

HEU-MET-FAST-095: Unassigned identifier.

HEU-MET-FAST-096: Yes. Reactivity worth of various rods.

HEU-MET-FAST-097: Unassigned identifier.

HEU-MET-FAST-098: Unassigned identifier.

HEU-MET-FAST-099: See ORCEF-SPACE-EXP-001 in the IRPhEP Handbook.

HEU-MET-FAST-100: Yes. See citations.

(ii) IEU-MET-FAST:

IEU-MET-FAST-001: None

IEU-MET-FAST-002: Yes. See reference 1 ... H. C. Paxton, "Bare Critical Assemblies of Oralloy at Intermediate Concentrations of U-235," Los Alamos Scientific Laboratory report LA-1671 (declassified), pp. 46, July 7, 1954.

IEU-MET-FAST-003 through -006: None

IEU-MET-FAST-007: Yes. Big-10. See Appendix C and other references.

IEU-MET-FAST-008, -009: None

IEU-MET-FAST-010: Yes. ZPR-9/36 & ZPR-6/9 (also known as "U9"). See references 1 through 3 ... (1) K. S. Smith and R. W. Schaefer, "Recent Developments in the Small-Sample Reactivity

Discrepancy," Nuclear Science and Engineering, **87**, 314-332 (1984); (2) E. F. Bennett, R. W. Schaefer, and G. J. Dilorio, "Spectrum and Kinetics Parameters from the U9 Critical Assemblies," *Trans. Am. Nucl. Soc.*, **43**, 719, Washington, DC (November, 1982); (3) R. W. Schaefer and R. G. Bucher, "Calculated and Measured Reactivities in the U9 Critical Assemblies," *Proceedings of the Topical Meeting on Advances in Reactor Physics and Core Thermal Hydraulics*, Kiamesha Lake, NY, Sept. 22-24, 1982 NUREG-CP-0034, Vol. I, 93-107 (1982)

IEU-MET-FAST-011: Yes. See ZEBRA-FUND-RESR-001 in the IRPhEP Handbook. But evaluation title says "K-Infinity" so not sure how useful this might be.

IEU-MET-FAST-012: Yes. ZPR-3/41. No specific citation, but general references in Section 5.

IEU-MET-FAST-013: Yes. ZPR-9/1. See Section 5, reference 1 through 6.

IEU-MET-FAST-014: Yes. ZPR-9/2 & -9/3. See Section 5, reference 1 through 6.

IEU-MET-FAST-015: Yes. ZPR-3/6F. No references cited here, but there is a footnote to see the CSEWG Benchmark Book (CSEWG Fast Benchmark #7).

IEU-MET-FAST-016: Yes. ZPR-3/11. No references cited here, but there is a footnote to see the CSEWG Benchmark Book (CSEWG Fast Benchmark #8).

IEU-MET-FAST-017: Yes. Re-assigned to MIX-MISC-MET-001. See BFS1-FUND-EXP-002 and -001 in the IRPhEP Handbook.

IEU-MET-FAST-018: None. Re-assigned to HEU-MET-FAST-036.

IEU-MET-FAST-019: None

IEU-MET-FAST-020: Yes. See Section 1.5. IEU-20, -21 & -22 are related.

IEU-MET-FAST-021: Yes. See Section 1.5. IEU-20, -21 & -22 are related.

IEU-MET-FAST-022: Yes. See Section 1.5. IEU-20, -21 & -22 are related.

IEU-MET-FAST-023: None. Re-assigned to HEU-MET-FAST-036.

IEU-MET-FAST-024: Yes. See FCA-LMFR-EXP-001 in the IRPhEP Handbook.

(iii) PU-MET-FAST:

PU-MET-FAST-001: Yes. Numerous references plus Appendix E (which is taken from the CSEWG Benchmark Book (CSEWG Fast Benchmark #1)).

PU-MET-FAST-002: Yes. Appendix D (which is taken from the CSEWG Benchmark Book (CSEWG Fast Benchmark #21).

PU-MET-FAST-003: Yes. See reference 2 ... "J. R. Morton, G. A. Pierce, L. L. Gardner, and C. J. Ball, "Summary Report of Critical Experiments, Plutonium Array Studies, Phase 1," UCRL-50175, 1966".

PU-MET-FAST-004, -005: None

PU-MET-FAST-006: Yes. Numerous references plus Appendix C (which is taken from the CSEWG Benchmark Book (CSEWG Fast Benchmark #23)).

PU-MET-FAST-007: None

PU-MET-FAST-008: Yes. Numerous references plus Appendix C (which is taken from the CSEWG Benchmark Book (CSEWG Fast Benchmark #25)).

PU-MET-FAST-009 through -011: None

PU-MET-FAST-012: Yes. Internal IPPE reports and reference 4 ... "Experimental and Calculational Investigations of Cross Section Ratios for Many Nuclides in the BR-1 Reactor (in Russian)". Also see FUND-IPPE-FR-MULT-RRR-001.

PU-MET-FAST-013: Yes. Internal IPPE reports and reference 4 ... "Experimental and Calculational Investigations of Cross Section Ratios for Many Nuclides in the BR-1 Reactor (in Russian)". Also see FUND-IPPE-FR-MULT-RRR-001.

PU-MET-FAST-014: Yes. Internal IPPE reports and reference 4 ... "Experimental and Calculational Investigations of Cross Section Ratios for Many Nuclides in the BR-1 Reactor (in Russian)". Also see FUND-IPPE-FR-MULT-RRR-001.

PU-MET-FAST-015: Yes. Internal IPPE reports and reference 4 ... "Experimental and Calculational Investigations of Cross Section Ratios for Many Nuclides in the BR-1 Reactor (in Russian)". Also see FUND-IPPE-FR-MULT-RRR-001.

PU-MET-FAST-016 through -042: None

PU-MET-FAST-043: Unassigned identifier.

PU-MET-FAST-044: None

PU-MET-FAST-045: Yes. See reference 2 ... H. G. Barkman, D. M. Holm, R. M. Kiehn, and R. E. Peterson, "Preliminary Critical Experiments on a Mock-Up of the Los Alamos Molten Plutonium Reactor Experiment," LA-2142, June 1957.

PU-MET-FAST-046: None

#### (iv) MIX-MET-FAST:

MIX-MET-FAST-001 through -005: None

MIX-MET-FAST-006: Yes. See BFS1-LMFR-EXP-002 in the IRPhEP Handbook.

MIX-MET-FAST-007: None

MIX-MET-FAST-008: Yes. See IEU-MET-FAST011 and ZEBRA-FUND-RESR-001 in the IRPhEP Handbook.

MIX-MET-FAST-009 through -011: None

MIX-MET-FAST-012: None. ZPPR-21A. Re-assigned to PU-MET-FAST-033.

MIX-MET-FAST-013: None

MIX-MET-FAST-014: Unassigned identifier.

MIX-MET-FAST-015: Yes. Re-assigned to MIX-MISC-FAST-001, but see BFS1-FUND-EXP-002 and -001 in the IRPhEP Handbook.

#### (v) HEU-MET-INTER:

HEU-MET-INTER-001: Yes. ZPR-9/34. Many measurements, some described in Section 5 references 1, 2 and 3. Others in Argonne National Laboratory internal memoranda.

HEU-MET-INTER-002: None. Re-assigned to HEU-MET-FAST-034.

HEU-MET-INTER-003: None. Re-assigned to HEU-MET-FAST-030.

HEU-MET-INTER-004: None. Re-assigned to HEU-MET-MIXED-004.

HEU-MET-INTER-005: Yes. Re-assigned to HEU-MET-MIXED-005.

HEU-MET-INTER-006: Yes. Rossi- $\alpha$  is tabulated. Also sample activation whose "... results should appear in a future LANL report".

HEU-MET-INTER-007: None. Re-assigned to HEU-MET-FAST-007.

HEU-MET-INTER-008: Yes. Re-assigned to HEU-MET-FAST-068.

HEU-MET-INTER-009: Yes. Decay constants & Rossi-α.

HEU-MET-INTER-010: None. Re-assigned to HEU-MET-THERM-027.

#### (vi) LEU-COMP-THERM:

LEU-COMP-THERM-001 through -004: None

LEU-COMP-THERM-005: Yes. Maybe in PNL-4976 ... S. R. Bierman, E. S. Murphy, E. D. Clayton, and R. T. Clayton "Criticality Experiments with Low Enriched UO2 Fuel Rods in Water Containing Dissolved Gadolinium," (PNL-4976) - February 1984.

LEU-COMP-THERM-006, -007: None

LEU-COMP-THERM-008: Yes. Appendix B and more ... 1. M. N. Baldwin and M. E. Stern, "Physics Verification Program, Part III, Task 4, Summary Report," Babcock & Wilcox report BAW-3647-20, March 1971.

LEU-COMP-THERM-009 through -014: None

LEU-COMP-THERM-015: Yes, see ZR6-VVER-EXP-001 in the IRPhEP Handbook.

LEU-COMP-THERM-016 through -018: None

LEU-COMP-THERM-019: Yes, flux & energy distribution data (figures only). No specific reference is cited but three are tabulated in Section 5.

LEU-COMP-THERM-020: Yes, flux & energy distribution data (figures only). No specific reference is cited but three are tabulated in Section 5.

LEU-COMP-THERM-021: Yes, flux & energy distribution data (figures only). No specific reference is cited but three are tabulated in Section 5.

LEU-COMP-THERM-022 through -025: None

LEU-COMP-THERM-026: Yes, 200+ °C but not recommended as criticality safety benchmarks.

LEU-COMP-THERM-027 through -029: None

LEU-COMP-THERM-030: Yes. Reactivity coefficients, but unpublished, 😕.

LEU-COMP-THERM-031: Yes, flux & energy distribution data (figures only). No specific reference is cited but three are tabulated in Section 5.

LEU-COMP-THERM-032: Yes, flux & energy distribution data (figures only). No specific reference is cited but two are tabulated in Section 5.

LEU-COMP-THERM-033: Yes. No specific references are cited but six are tabulated in Section 5.

LEU-COMP-THERM-034: None

LEU-COMP-THERM-035: Yes. Temperature coefficients are mentioned but no citation given. Two are tabulated in Section 5.

LEU-COMP-THERM-036: Yes. Fission rate distributions and spectral indices are given in the references.

LEU-COMP-THERM-037 through -040: None

LEU-COMP-THERM-041: Yes. See text and references.

LEU-COMP-THERM-042 through -046: None

LEU-COMP-THERM-047: Yes. Brief description but no specific reference citation. See reference 1 and citations therein.

LEU-COMP-THERM-048: Yes. See DIMPLE-LWR-EXP-001 in the IRPhEP Handbook.

LEU-COMP-THERM-049 through -052: None

LEU-COMP-THERM-053: Yes. Reactivity coefficients, but unpublished, 😕.

LEU-COMP-THERM-054: None

LEU-COMP-THERM-055: Yes. See DIMPLE-LWR-EXP-002 in the IRPhEP Handbook.

LEU-COMP-THERM-056: Yes. See reference 1 ... BORAX-V Project Staff, "Design and Hazards Summary Report Boiling Reactor Experiment (BORAX-V)," ANL-6302, Argonne National Laboratory, May 1961.

LEU-COMP-THERM-057: None

LEU-COMP-THERM-058: Yes. Water worth.

LEU-COMP-THERM-059: Unassigned identifier.

LEU-COMP-THERM-060: Yes. See references.

LEU-COMP-THERM-061: Yes. See PFacility-VVER-EXP-001 in the IRPhEP Handbook.

LEU-COMP-THERM-062: Yes. No specific references are cited but two are tabulated in Section 5.

LEU-COMP-THERM-063: Yes. See reference 1.

LEU-COMP-THERM-064: Yes. Reactivity coefficients, but unpublished, 😕.

LEU-COMP-THERM-065: Yes. Unpublished internal report only, 😕.

LEU-COMP-THERM-066 through -069: None

LEU-COMP-THERM-070: Unassigned identifier.

LEU-COMP-THERM-071 through -074: None

LEU-COMP-THERM-075: Yes. Reactivity coefficients, but unpublished, 😕.

LEU-COMP-THERM-076: Yes. See reference 1.

LEU-COMP-THERM-077: Yes. See IPEN(MB01)-LWR-RESR-001 in the IRPhEP Handbook.

LEU-COMP-THERM-078 through -080: None

LEU-COMP-THERM-081: Yes. But incomplete description so not benchmark quality.

LEU-COMP-THERM-082 through -084: None

LEU-COMP-THERM-085: Yes. Reactivity coefficients, but unpublished, 😕.

LEU-COMP-THERM-086: Yes.

LEU-COMP-THERM-087: Yes.

LEU-COMP-THERM-088 through -092: None

LEU-COMP-THERM-093: Re-assigned to DCA-HWR-EXP-001 in the IRPhEP Handbook.

LEU-COMP-THERM-094: Yes. Reactivity coefficients and fission rate distributions, but unpublished, 🙁.

LEU-COMP-THERM-095: Unassigned identifier.

LEU-COMP-THERM-096, -097: None

LEU-COMP-THERM-098: Yes. See reference 1 ... Taylor, E. G. Saxton Plutonium Program. Critical Experiments for the Saxton Partial Plutonium Core. WCAP-3385-54. Dec. 1965.

LEU-COMP-THERM-099, -100: None

LEU-COMP-THERM-101: Unassigned identifier.

LEU-COMP-THERM-102: Unassigned identifier.

LEU-COMP-THERM-103: None

LEU-COMP-THERM-104 (Kritz): Scheduled for review and publication in 2020, but see Kritz evaluations in the IRPhEP handbook.

(vii) HEU-SOL-THERM:

HEU-SOL-THERM-001 through -003: None

HEU-SOL-THERM-004: Yes. See reference 1 ... Olcott, R. N. "Homogeneous Heavy Water Moderated Critical Assemblies. Part 1. Experimental," Nucl. Sci. Eng., **1**, 327-341, 1956.

HEU-SOL-THERM-005 through -010: None

HEU-SOL-THERM-011: Yes. Radial flux traverse, but no data nor reference cited, 😕.

HEU-SOL-THERM-012: None

HEU-SOL-THERM-013: Yes. Maybe something in reference 2 ... R. Gwin and D. W. Magnuson, "Critical Experiments for Reactor Physics Studies," ORNL-CF-60-4-12, Oak Ridge National Laboratory, 1960.

HEU-SOL-THERM-014 through -019: None

HEU-SOL-THERM-020: Yes. See reference 1 ... Olcott, R. N. "Homogeneous Heavy Water Moderated Critical Assemblies. Part 1. Experimental," Nucl. Sci. Eng., **1**, 327-341, 1956.

HEU-SOL-THERM-021: Nothing to support nuclear data testing.

HEU-SOL-THERM-022 through -031: None

HEU-SOL-THERM-032: Yes. See references 1 and 2 ... (1) R. Gwin, and D. W. Magnuson, "Critical Experiments for Reactor Physics Studies," ORNL-60-4-12, Oak Ridge National Laboratory, September, 1960; (2) R. Gwin, and D. W. Magnuson, "The Measurement of Eta and Other Nuclear Properties of U233 and U235 in Critical Aqueous Solutions," Nuclear Science and Engineering, **12**,364-

380 (1962).

HEU-SOL-THERM-033 through -037: None

HEU-SOL-THERM-038: Yes, sub-critical, Rossi- $\alpha$ , <sup>252</sup>Cf source driven noise

HEU-SOL-THERM-039, -040: None

HEU-SOL-THERM-041: Unassigned identifier.

HEU-SOL-THERM-042: Yes. See references 1 and 2 ... (1) R. Gwin, and D. W. Magnuson, "Critical Experiments for Reactor Physics Studies," ORNL-60-4-12, Oak Ridge National Laboratory, September, 1960; (2) R. Gwin, and D. W. Magnuson, "The Measurement of Eta and Other Nuclear Properties of U233 and U235 in Critical Aqueous Solutions," Nuclear Science and Engineering, **12**,364380 (1962).

HEU-SOL-THERM-043 through -045: None

HEU-SOL-THERM-046: Yes. See references 1 and 2 ... (2) J. Bertrand, P. Bonnaure, C. Clouet d'Orval, J. Corpel, J de Lamare, P. Lecoustey, I. Prevot, R. Roche, M. Sauve, J. Tachon, and G. Vendryes - Proceedings of the second United Nations International Conference on the Peaceful Uses of Atomic Energy – Geneva -1 September – 13 September 1958 – Volume 12 Reactor Physics "Proserpine," A Homogeneous Critical Experiment with Plutonium; (3) Jean Tachon - Rapport CEA n° 1547 - année 1960, Etude Neutronique d'une Pile a NeutronsThermiques au Plutonium: "Proserpine" Corrélations Entre Neutrons dans une Réaction en Chaîne.

HEU-SOL-THERM-047 through -051: None

#### (viii) PU-SOL-THERM:

PU-SOL-THERM-001: Yes. See references 1 & 7 ... (1) R. C. Lloyd, C. R. Richey, E. D. Clayton, D. R. Skeen, "Criticality Studies with Plutonium Solutions," Nucl. Sci. Eng., **25**, 165-173, 1966; (7) R. C. Lloyd, D. R. Skeen, E. D. Clayton, "Criticality of Plutonium Nitrate Solutions in Spherical Geometry," Physics Research Quarterly Report, April, May, June, 1964, HW-83187, General Electric Company Hanford Atomic Products Operation, July 1964.

PU-SOL-THERM-002 through -006: None

PU-SOL-THERM-007: Yes. See reference 1 ... (1) R. C. Lloyd, C. R. Richey, E. D. Clayton, D. R. Skeen, "Criticality Studies with Plutonium Solutions," Nucl. Sci. Eng., **25**, 165-173, 1966.

PU-SOL-THERM-008: Yes. See references 1 & 8 ... (1) R. C. Lloyd, C. R. Richey, E. D. Clayton, D. R. Skeen, "Criticality Studies with Plutonium Solutions," Nucl. Sci. Eng., **25**, 165-173, 1966; (8) R. C. Lloyd, D. R. Skeen, E. D. Clayton, "Criticality of Plutonium Nitrate Solutions in Spherical Geometry," Physics Research Quarterly Report, April, May, June, 1964, HW-83187, General Electric Company Hanford Atomic Products Operation, July 1964.

PU-SOL-THERM-009 through -018: None

PU-SOL-THERM-019: Yes. See references 2 & 3 ... (2) J. Bertrand, P. Bonnaure, C. Clouet d'Orval, J. Corpel, J de Lamare, P. Lecoustey, I. Prevot, R.Roche, M. Sauve, J. Tachon, and G. Vendryes - Proceedings of the second United Nations International Conference on the Peaceful Uses of Atomic Energy – Geneva -1 September – 13 September 1958 – Volume 12 Reactor Physics. "Proserpine", a Homogeneous Critical Experiment with Plutonium; (3) Jean Tachon -Rapport CEA n° 1547 - année 1960

# ETUDE NEUTRONIQUE D'UNE PILE A NEUTRONS THERMIQUES AU PLUTONIUM : "PROSERPINE" CORRELATIONS ENTRE NEUTRONS DANS UNE REACTION EN CHAINE

PU-SOL-THERM-020: Yes. See references 1 & 11 ... (1) R. C. Lloyd, C. R. Richey, E. D. Clayton, D. R. Skeen, "Criticality Studies with Plutonium Solutions," Nucl. Sci. Eng., **25**, 165-173, 1966; (11) R. C. Lloyd, D. R. Skeen, E. D. Clayton, "Criticality of Plutonium Nitrate Solutions in Spherical Geometry," Physics Research Quarterly Report, April, May, June, 1964, HW-83187, General Electric Company Hanford Atomic Products Operation, July 1964.

PU-SOL-THERM-021: Yes. See references 1 & 10 ... (1) R. C. Lloyd, C. R. Richey, E. D. Clayton, D. R. Skeen, "Criticality Studies with Plutonium Solutions," Nucl. Sci. Eng., **25**, 165-173, 1966; (10) R. C. Lloyd, D. R. Skeen, E. D. Clayton, "Criticality of Plutonium Nitrate Solutions in Spherical Geometry," Physics Research Quarterly Report, April, May, June, 1964, HW-83187, General Electric Company Hanford Atomic Products Operation, July 1964.

PU-SOL-THERM-022 through -026: None

PU-SOL-THERM-027: None. Re-assigned to MIX-MISC-THERM-003.

PU-SOL-THERM-028: Yes. See reference 1 ... CEA /D.U.S.I N° 13 Oct. 1963 & CEA/D.U.S.I 42 Dec. 1966.

PU-SOL-THERM-029 through -035: None

PU-SOL-THERM-036: Yes. See references 1 and 7b ... (1) Jean-Georges Bruna, Jean-Paul Brunet, Robert Caizergues, Christian Clouet d'Orval, Jacques Kremser, Henry Tellier, Philippe Verrière, Rapport CEA-R 2814, Alecto – Résultats des Expériences Critiques Homogènes Réalisées sur le 239Pu, 235U et 233U, Octobre 1965; (7b) J-G. Bruna, J-P. Brunet, R. Caizergues, C. Clouet d'Orval, J. Kremser, Rapport EC/S N° 126, 1963, Expérience de Criticalité sur une Solution de Plutonium - Résultats Expérimentaux et Calculs Concernant la Cuve N°2 (Φ=300).

PU-SOL-THERM-037 through -039: None

PU-SOL-THERM-040: None. Re-assigned to MIX-MISC-THERM-007.

#### Appendix B

# Summary Review of the IAEA's "Technical Report Series No. 480 – Research Reactor Database: Facility Specification and Experimental Data"

### IAEA Contract TAL-NAPC20200423-003 September 2020

In this Appendix we provide a <u>brief</u> summary of the research reactors and their associated experiments that are provided in the IAEA's Technical Report Series No. 480 - Research Reactor Database: Facility Specification and Experimental Data.

In this summary we do not fully explain the details of the many experiments that have been performed at these facilities over a period of years. Rather we simply seek to provide notice to the nuclear data benchmarking community of the availability of this information.

For many years the data testing of basic nuclear data files has relied upon a variety of benchmark compilations. One of the earliest was the CSEWG (Cross Section Evaluation Working Group) Benchmark Book (ENDF-202) which was initially published in 1974 with updates into the early 1990s. This compilation includes separate sections for unmoderated (Fast) and moderated (Thermal) critical systems, Shielding benchmarks and a Dosimetry benchmark.

More recently, starting in the mid-1990s and continuing today, the International Criticality Safety Benchmark Evaluation Project (ICSBEP) has published a Handbook of evaluated criticality safety benchmarks. In recent years the work to maintain and expand this Handbook has been coordinated by the US Department of Energy (USDOE) and the OECD's Nuclear Energy Agency (NEA). The focus of these evaluations has been to allow accurate modelling of the defined configurations with an emphasis on the calculation of criticality. On occasion there is a passing reference to other measured data. This compilation has been used extensively by the international community for data testing recent evaluated nuclear data files such as ENDF/B-VII.0 and later, JEFF-3.x, JENDL-4.x, CENDL-3.x and so forth.

Another USDOE/NEA cooperative effort has been the International Reactor Physics Evaluation Project (IRPhEP) and its associated Handbook. The benchmark descriptions here are necessarily more complex than the ICSBEP benchmarks, but it represents an additional information source for expanded data testing beyond the calculation of criticality.

Finally, there is a compilation of shielding benchmarks known as "SINBAD". Recently there has been a renewed interest in this area, with the creation of an NEA Working Party for Evaluation Cooperation (WPEC) Sub-group devoted to reviewing the available shielding benchmark data in order to develop uniform benchmark specifications and assess the underlying uncertainty in these data. This database includes over 100 experiments of relevance to the reactor shielding, fusion blanket neutronics and accelerator shielding communities.

In light of the above summary the reader might be tempted ask ... "Do we really need any further compilations of experimental measurements for testing our nuclear data files?". And as any nuclear data tester will readily say, the answer is "Yes! There never can be too much data". The more data the technical community has for testing the greater will be one's confidence in the underlying accuracy of today's cross section databases, and the greater is our knowledge of where deficiencies remain. This latter point ... "knowing what we don't know" ... cannot be over-emphasized and a continued expansion of our benchmark databases is the best way to learn both the strengths and weaknesses of the underlying basic nuclear data.

And so, what follows is a brief summary of what the IAEA's TRS-480 (initially published in 2015 with a second edition in the Summer 2020) has to offer to the nuclear data testing community:

# (i) ATI TRIGA Nuclear Reactor (Austria) Technical Report Series No. 480 – Second Edition

The Training Research and Isotope Production, General Atomics (TRIGA) reactor is a pool type reactor using 104-type TRIGA fuel elements. These fuel elements are comprised of U-Zr-H1.65. The uranium is approximately 19.8 weight percent <sup>235</sup>U. This core originally used highly-enriched uranium fuel but was converted to the current fuel configuration in 2012.

Experimental data are in the form of gamma spectroscopy along the vertical axis of selected fuel elements to determine the type and amount of individual fission products.

In a separate measurement, uranium and thorium foils were irradiated and subsequently gamma scanned to evaluate the amount of major and minor actinides and fission products.

# (ii) ETRR-2 Nuclear Reactor (Egypt) Technical Report Series No. 480 – First Edition

The Egypt Test and Research Reactor Number 2 (ETRR-2) is an open pool type reactor, cooled and moderated by light water and reflected by beryllium. The fuel is a Materials Testing Reactor plate type with  $U_3O_8$  fuel meat (~19.8% enriched in <sup>235</sup>U).

Neutronics measurements of interest include (i) criticality, (ii) flux profile, (iii) control rod worth, and (iv) reactivity coefficients.

(iii) IEA-R1 Nuclear Reactor (Brazil) Technical Report Series No. 480 – First Edition The IEA-R1 is an open pool type reactor, cooled and moderated by light water and reflected by graphite and beryllium. The fuel elements are ~20% enriched uranium in the form of  $U_3O_8$ -Al and  $U_3Si_2$ -Al.

The benchmark experiments provided in this Technical Report are focused on thermalhydraulics and therefore currently are of limited interest for nuclear data testing.

# (iv) INR TRIGA 14 MW Nuclear Reactor (Romania) Technical Report Series No. 480 – Second Edition

This reactor is currently fueled with low-enriched uranium (LEU) but was originally fueled with highly enriched uranium (HEU). This conversion took place in 2006. The criticality benchmark defined here is for the initial, HEU-fueled, configuration. A second benchmark involving the burnup of a  $UO_2$  test sample is also defined.

# (v) IRR-1 Nuclear Reactor (Israel) Technical Report Series No. 480 – Second Edition

The Israel Research Reactor is a pool type reactor cooled and moderated by light water. The reactor core is composed MTR assemblies with ~93% enriched uranium fuel. Graphite (primarily) and light water serve as reflectors.

Benchmark measurements of (i) criticality, (ii) fuel depletion, (iii) <sup>137</sup>Cs distribution, and (iv) core follow.

# (vi) JSI TRIGA Mark II Nuclear Reactor (Slovenia) Technical Report Series No. 480 – Second Edition

The Jozef Stefan Institute (JSI) TRIGA Mark II reactor also appears in the International Criticality Safety Benchmark Evaluation Project's Handbook (LEU-COMP-THERM-003). Benchmark problem data are available for (i) flux distributions, (ii) material activation (bare as well as cadmium and boron nitride covered samples), and (iii) neutron spectrum filters.

The benchmark data from this facility are likely to be most readily available given the Agency's continuing close association between recently retired NDS staff member Andrej Trkov who is now affiliated with the JSI.

(vii) McMaster Nuclear Reactor (Canada) Technical Report Series No. 480 – First Edition The McMaster Nuclear Reactor (MNR) is an open pool type reactor, cooled and moderated by light reactor and reflected by light water, lead and graphite. The fuel elements are MTR plate type with  $U_3Si_2$  fuel meat and aluminum cladding.

Neutronic benchmark problems are defined for (i) criticality, (ii) flux profile, (iii) control rod worth, and (iv) reactivity coefficients.

# (viii) MINERVE Nuclear Reactor (France) Technical Report Series No. 480 – First Edition

MINERVE is an experimental, pool-type, reactor containing a highly-enriched uranium "driver" zone surrounding a central cavity. The central cavity can accommodate a test lattice within a watertight volume. A thick graphite reflector surrounds the core.

Neutronic benchmarks include (i) criticality, (ii) flux profiles, and (iii) control rod worths.

# (ix) Syrian Miniature Neutron Source Reactor, MNSR (Syria) Technical Report Series No. 480 – First Edition

MNSR is a small, pool-type, reactor using highly-enriched uranium fuel (UAl<sub>4</sub>). Light water serves as moderator, coolant and shield. Beryllium is also present as a reflector material.

Neutron benchmark experiments include (i) flux profiles, (ii) control rod worths, (iii) reactivity coefficients, and (iv) kinetic parameters.

# (x) OPAL Nuclear Reactor (Austrialia) Technical Report Series No. 480 – First Edition. Updated and new benchmarks added in the Second Edition

The Open-Pool Austrialian lightwater reactor (OPAL) uses low-enriched uranium (U<sub>3</sub>Si<sub>2</sub>) platetype fuel assemblies with light-water moderation and coolant and heavy-water reflection.

Neutronic benchmark experiments include (i) criticality, (ii) flux profiles, (iii) control rod worth, (iv) reactivity coefficients, (v) kinetic parameters, and (vi) burnup.

# (xi) Indonesian RSG-GAS Reactor Technical Report Series No. 480 – First Edition

The Reaktor Serba Guna G. A. Siwabessy (RGS-GAS) is an open pool-type reactor.

The benchmark experiments provided in this Technical Report are focused on thermalhydraulics and therefore currently are of limited interest for nuclear data testing.

# (xii) SAFARI-1 Nuclear Reactor (South Africa) Technical Report Series No. 480 – Second Edition

SAFARI is an open pool-type reactor. It originally utilized HEU fuel but was converted to LEU  $(U_3Si_2 MTR plate type)$  fuel in 2008-2009. Only LEU fuel data are provided and so the benchmarks defined here are for core operations after 2009.

The neutronic benchmark experiments mostly involve multi-cycle measurements. They include (i) reactivity, (ii) Cu wire activation, (iii) control rod worth, and (iv) core follow and depletion.

# (xiii) SPERT-III Nuclear Reactor (USA) Technical Report Series No. 480 – First Edition

The Special Power Excursion Reactor Test III (SPERT-III) reactor is a pressurized water reactor facility. The core utilizes low-enriched uranium-dioxide (UO<sub>2</sub>) fuel pins and is moderated, cooled and reflected by light water.

The neutronic benchmark experiments include (i) criticality, (ii) flux profile, (iii) control rod worth, (iv) reactivity coefficients, and (v) kinetics parameters.

Note that the facility description here says "SPERT III Core E". There is also a "SPERT III" benchmark in the ICSBEP Handbook, but that evaluation, HEU-COMP-THERM-022, describes a core using HEU-O<sub>2</sub> plate type fuel and so bears no resemblance to the TRS-480 benchmark described here.

# (xiv) SPERT-IV D-12/25 (Canada) Technical Report Series No. 480 – First Edition

The SPERT-IV D-12/25 reactor was an open pool type reactor using highly-enriched uranium  $(UO_2)$  MTR plate-type fuel with light water moderation, cooling and reflection. These specifications, including a 5 x 5 assembly configuration are similar to that given in the ICSBEP HEU-COMP-THERM-022 evaluation, but the active fuel height in HCT22 is significantly taller than that in this TRS-480 report.

The neutronic benchmark experiments include (i) criticality, (ii) flux profile, (iii) control rod worth, (iv) reactivity coefficients, and (v) kinetics parameters.

# (xv) TRR-1/M1 Nuclear Reactor (Thailand) Technical Report Series No. 480 – Second Edition

The Thai Research Reactor, Mod 1 (TRR-1/M1) is a TRIGA Mark III reactor, designed and manufactured by General Atomics.

The benchmark is a multi-cycle depletion case, including (i) criticality, (ii) fuel depletion and (iii) multi-cycle core follow.

# Appendix C

# MCNP6© Reactor Lattice "kcode" Calculations with Light Water and Uranium Fuel Thermal Scattering Kernels

## IAEA Contract TAL-NAPC20200423-003 September 2020

In this Appendix we discuss the impact on criticality calculations for low-enriched uranium fuel reactor lattice models include or omit u-uo<sub>2</sub> and o-uo<sub>2</sub> thermal scattering kernels.

MCNP6© kcode calculations were performed for several benchmark series, including KRITZ-LWR-RESR-002 and -003 from the International Reactor Physics Evaluation Project's "International Handbook of Evaluated Reactor Physics Benchmark Experiments", as well as cases 1, 5 and 12 of the LEU-COMP-THERM-005 evaluation, cases 1 through 10 of the LEU-COMP-THERM-007 evaluation and select cases (2 - 9, 11, 16 & 17) of the LEU-COMP-THERM-008 evaluation. The LEU-COMP-THERM (LCT) benchmarks are from the International Criticality Safety Benchmark Evaluation Project's "International Handbook of Evaluated Criticality Safety Benchmark Experiments".

The KRITZ calculations were performed at both room temperature and at elevated (248°C for -002 and 243°C for -003) while the LCT5, LCT7 and LCT8 calculations are at room temperature only. The room temperature calculations used ACE files derived from ENDF/B-VIII.0 (e80) that were produced by the MCNP Nuclear Data Team at Los Alamos. Those files are freely available at <u>https://nucleardata.lanl.gov/ACE/Production/Lib80x.html</u>. The elevated temperature KRITZ jobs used temperature appropriate cross sections produced by the author with a local version of the NJOY code, plus the LANL produced light water, u-uo<sub>2</sub> and o-uo<sub>2</sub> ENDF/B-VIII.0 derived thermal kernel ACE files at the nearest temperature.

The MCNP kcode calculations were run for 250 million active neutron histories using 50,000 histories/cycle, 50 warmup cycles and 5,000 active cycles. Results for the KRITZ assemblies are given in the following Table

Assembly ID	k <sub>calc</sub> (h-h <sub>2</sub> o only)	$k_{calc}$ (h-h <sub>2</sub> o, u- uo <sub>2</sub> and o-uo <sub>2</sub> )	Δk <sub>calc</sub> , pcm	EALF (h- h <sub>2</sub> o only), eV
KRITZ-LWR-RESR-002, 19C	0.99785(4)	0.99809(4)	24(6)	0.346
KRITZ-LWR-RESR-002, 248C	0.99637(4)	0.99648(4)	11(6)	0.560
KRITZ-LWR-RESR-003, 22C	1.00044(4)	1.00056(4)	12(6)	0.212

KRITZ-LWR-RESR-003,	1 00007(4)	1 00028(4)	21(0)	0.257
243C	1.00007(4)	1.00028(4)	21(6)	0.357

For many years it has been a "rule-of-thumb" that when a critical system is dominated by water moderation, as occurs in typical reactor lattice geometries, the only important thermal scattering kernel to include in one's model is for hydrogen bound in water. These results suggest if the eigenvalue calculation is done with a statistical precision of 5 to 10 pcm or so there is a statistically significant increase in calculated eigenvalues when the uranium (actually only <sup>238</sup>U)-in-fuel and oxygen-in-fuel kernels are included. Since many legacy kcode calculations were run for a few tens of millions of neutron histories, or fewer, they would have had much larger  $k_{calc}$  uncertainties, and so are insensitive to this difference.

Similar results are obtained for the room temperature LCT5, LCT7 and LCT8 kcode calculations, as shown in the following Table. Once again calculated eigenvalues that include the fuel thermal scattering kernels are slightly larger. Most of the differences are statistically significant for these 250 million active neutron history jobs, but once again the differences are relatively small and as stated above, for legacy calculations with much fewer histories and correspondingly larger k<sub>calc</sub> uncertainties there is minimal bias caused by omitting these kernels.

Assembly ID	k <sub>calc</sub> (h-h <sub>2</sub> o only)	$k_{calc}$ (h-h <sub>2</sub> o, u-uo <sub>2</sub> and o-uo <sub>2</sub> )	Δk <sub>calc</sub> , pcm	EALF (h- h <sub>2</sub> o only), eV
LEU-COMP-THERM-005				
Case 1	1.00226(5)	1.00240(5)	14(7)	0.153
Case 5	1.00307(5)	1.00310(5)	3(7)	0.654
Case 12	1.00486(5)	1.00486(5)	0(7)	3.181
LEU-COMP-THERM-007				
Case 1	0.99665(5)	0.99694(5)	29(7)	0.246
Case 2	0.99881(5)	0.99905(5)	24(7)	0.112
Case 3	0.99801(4)	0.99832(4)	31(6)	0.073
Case 4	0.99857(4)	0.99901(4)	44(6)	0.062
Case 5	0.99603(5)	0.99619(5)	16(7)	0.270
Case 6	0.99868(5)	0.99906(5)	38(7)	0.113
Case 7	0.99874(4)	0.99916(5)	42(7)	0.073
Case 8	0.99733(5)	0.99760(5)	27(7)	0.254
Case 9	0.99818(5)	0.99850(5)	32(7)	0.113
Case 10	0.99889(4)	0.99926(4)	37(6)	0.073
LEU-COMP-THERM-008				
Case 2	1.00090(4)	1.00104(4)	14(6)	0.248
Case 3	1.00153(4)	1.00158(4)	5(6)	0.248
Case 4	1.00064(4)	1.00074(4)	10(6)	0.248
Case 5	1.00031(4)	1.00040(4)	9(6)	0.248
Case 6	1.00058(4)	1.00075(4)	17(6)	0.248

Case 7	0.99995(4)	1.00006(4)	11(6)	0.248
Case 8	0.99933(4)	0.99963(4)	30(6)	0.246
Case 9	0.99958(4)	0.99980(4)	22(6)	0.245
Case 11	1.00130(4)	1.00142(4)	12(6)	0.256
Case 16	1.00058(4)	1.00070(4)	12(6)	0.230
Case 17	0.99967(4)	0.99968(4)	1(6)	0.201

One attribute these systems have in common is they are under-moderated or perhaps nearly optimally-moderated. In an effort to further assess the impact of including the fuel system scattering kernels in an over-moderated system two artificial problems were developed. In the first case a 51 x 51 rod lattice with 5 w/o<sup>235</sup>U in UO<sub>2</sub> was defined. The fuel rod radius was 0.475 cm and the lattice pitch was an abnormally large 3.376 cm. The second problem reduced the fuel content to 3 w/o<sup>235</sup>U, which required a larger lattice – now 61 x 61 with a 2.800 cm pitch. The k<sub>calc</sub> uncertainty was further reduced by running one billion active neutron histories for models at were light-water moderated only versus both light-water and fuel moderation. Once again the addition of fuel system scattering kernels led to an increased k<sub>calc</sub>, but now the increase was in the 50 to 60 pcm range while the calculated eigenvalue uncertainty was about 2 pcm. This suggests that the increase in calculated eigenvalue with inclusion of fuel system scattering kernels becomes larger with higher degrees of moderation, as for these artificial problems we observe nearly 95% thermal fission whereas for the benchmark problems presented previously typically exhibit 80% to near 90% thermal fission.

A feature of these over-moderated systems is their low Energy of Average Lethargy Causing Fission (EALF), around 0.05 eV. In contrast the only case where no difference in  $k_{calc}$  was seen was for LCT5.12, an extremely undermoderated system whose EALF was over 3 eV. This suggests that there may be a dependence in the  $k_{calc}$  bias as a function of EALF, but additional studies are warranted to better characterize this dependence. Also, it is important to remember that thermal scattering kernels are only applied over a limited energy range. For h-h<sub>2</sub>o that range is up to 10 eV while the fuel system kernels only extend to 5 eV. Hence for these higher EALF configurations the presence or absence of the additional kernel becomes less important as a significant contribution to the total eigenvalue comes from interactions at energies beyond the thermal kernel energy range. Hence the lack of a  $k_{calc}$  difference for LCT5.12 whose EALF is over 3 eV may be due in part to a lack of fuel system thermal scattering kernel data above 5 eV.

In conclusion, as ongoing and future Monte Carlo eigenvalue calculations occur to ever increasing degrees of precision, it becomes necessary to question some of our long-standing assumptions as to what model features remain insignificant. In this study we conclude that if the Monte Carlo precision is sufficiently great that the eigenvalue uncertainty is less than about 5 to 10 pcm in a reactor lattice calculation, there is likely a need to include more than just the hydrogen bound in water thermal scattering kernel in order to avoid a small (tens of pcm) bias in the final calculated result. Also, there is slight evidence to suggest when omitting fuel system scattering kernels, the k<sub>calc</sub> bias increases with decreasing EALF.

#### Appendix D

# Replicate Monte Carlo Eigenvalue and Reaction Rate Calculations

# IAEA Contract TAL-NAPC20200423-003 September 2020

In this Appendix we discuss the results of replicate MCNP6© kcode calculations as it relates to the accuracy of MCNP's reported eigenvalue and select reaction rate uncertainties. To be clear, as used here the term "uncertainty" refers to one standard deviation, either as calculated by MCNP for a specific datum, or as determined from the variation in that datum from N independent MCNP jobs (N is typically 20 for the results presented in this Appendix).

The following calculations were performed using the PU-MET-FAST-001 (Jezebel, revison 4 simple model) benchmark. A series of 20 independent jobs were run, each consisting of one million histories per cycle with fifty warmup cycles and 1000 active cycles, for one billion active neutron histories per job.

MCNP's reported eigenvalue uncertainty is 2 pcm for each of these twenty jobs. The 20 calculated eigenvalues,  $k_{calc}$ , are shown in the following Figure, and are seen to vary from a minimum of 1.000669 to a maximum of 1.000725. Note that for the calculated eigenvalue we use MCNP's "k(col/abs/tk ln) combined average" value that appears in Print Table 175 and which is printed to six significant digits rather than the 5 significant digit value provided in the Summary Table (and also printed to the terminal).



The estimated standard deviation for this population of 20  $k_{calc}$  values is 1.8 pcm, a value in excellent agreement with MCNP's reported individual kcode eigenvalue uncertainty.

Central region reaction rates were also calculated for a number of reactions, including  $^{235}$ U(n,f),  $^{239}$ Pu(n,f),  $^{238}$ U(n, $\gamma$ ),  $^{238}$ U(n,f), and  $^{238}$ U(n,2n). The  $^{235}$ U(n,f) reaction rate was chosen as this value is often used in ratio to other reaction rates, with the ratio commonly referred to as a "spectral index". The  $^{239}$ Pu(n,f) and  $^{238}$ U(n, $\gamma$ ) results are for cross sections that are continuous over the entire problem energy range while the  $^{238}$ U(n,f) and  $^{238}$ U(n,2n) results are for threshold reactions of increasing average energy; namely ~3.3 MeV and ~8.5 MeV, respectively.

The job-to-job variation for the <sup>235</sup>U(n,f), <sup>239</sup>Pu(n,f), and <sup>238</sup>U(n,f) reactions is illustrated in the following figure. With significant cross sections that span the problem energy space these reactions are frequently sampled and so the ordinate scale is very small, only extending for several tenths of a percent.



We show these values as a ratio to the 20-job average so that numbers whose absolute values differ significantly are shown in a single plot. It is interesting to note that for most cases the results are correlated, in that if a given reaction tally exceeds its 20-job average the other reaction tallies also exceed their average value. This should manifest itself in a large difference in the calculated spectral index uncertainty as calculated using the assumed independent reaction rate uncertainties calculated by MCNP versus the uncertainty determined from the variation in the 20 independent jobs. For example, the reaction tallies for <sup>239</sup>Pu(n,f) and <sup>235</sup>U(n,f) from the first job are 1.44203e-2  $\pm$  0.08% and 1.01025e-2  $\pm$  0.08%, respectively, leading to a spectral index of 1.427  $\pm$  0.11%. However, if we calculate the spectral index as the average of 20 independent <sup>239</sup>Pu(n,f) and <sup>235</sup>U(n,f) tallies and use the distribution of those 20 spectral index estimates to assess the uncertainty we obtain 1.42721  $\pm$  0.00012, or an uncertainty of less than 0.01%. Note that this is the uncertainty in the N (in this case 20) sample population, not the uncertainty in the average which would be further reduced by a sqrt(N-1) factor.

If we repeat this exercise for the  $^{238}$ U(n, $\gamma$ ) spectral index, the computed spectral index from a single MCNP job is 0.06433 ± 0.13%, whereas the average spectral index from 20 jobs is 0.06435 and the uncertainty of the 20 sample population is ~0.05%. Once again, a value significantly less than that obtained directly from MCNP.

However, this does not mean that the MCNP reaction rate tally uncertainty is always significantly over-estimated.

There are many instances where the reaction rate tally, and resulting spectral index, involves a threshold reaction whose cross section only resides over a portion of the problem energy space. This is often the case when dealing with (n,2n) or charged particle (p,d,t,<sup>3</sup>He and  $\alpha$ ) emission reactions whose cross sections are only non-zero in the high energy tail of the assembly spectrum. The following figure expands the previous Figure by adding reaction rate tally ratios for the <sup>238</sup>U(n,2n) and <sup>63</sup>Cu(n,2n) reactions whose average energies are ~8.5 Mev and ~14.0 MeV, respectively.



At these higher energies the degree of sampling is significantly reduced, resulting in a much greater job-to-job variation in the tally result. As a consequence, the ordinate scale has been expanded by over an order of magnitude compared to the previous figure. This greater job-to-job variation exhibits itself is less correlation among the different reaction rate tallies, which has a significant impact when comparing the spectral index uncertainty derived from MCNP's tally uncertainties versus the reaction rate population uncertainties derived from the 20-job sample. We repeat the same exercise as above, but now for the  ${}^{63}$ Cu(n,2n)/ ${}^{235}$ U(n,f) spectral index. For a single (job 1 of 20) job, the reaction rate tallies are 1.01557e-6 ± 4.26% and 1.01025e-2 ± 0.08%, resulting in a  ${}^{63}$ Cu(n,2n)/ ${}^{235}$ U(n,f) spectral index of 1.01e-4 ± 4.26%, whereas working from the 20 individual job reaction rate tallies the computed spectral index is

1.01e-4  $\pm$  3.44%. In this case the spectral index uncertainty derived from the individual MCNP reaction rates is little changed from that derived from the 20-job population. This is in stark contrast to the spectral index uncertainty for reactions whose cross sections span the entire energy space where differences of a factor of 2 and up to an order of magnitude difference was observed.

Finally, a series of 20 independent kcode jobs were run for the LEU-COMP-THERM-008, case 17 benchmark. This is a Babcock & Wilcox low-enriched (~2.5 w/o<sup>235</sup>U in UO<sub>2</sub>) rod lattice benchmark. The core consists of 4457 fuel rods and 504 water holes, each defined within a square 1.64 cm unit cell. The water holes are located within a central 45 x 45 rod array and the overall core geometry exhibits  $1/8^{th}$  (octant) symmetry; a feature incorporated in the MCNP6© model. In addition to criticality, pin power data are available at select locations within the central 45 x 45 region, and so the MCNP model includes fission tallies for all unit cells within this octant symmetric geometry. The kcode jobs were run for 250 million active neutron histories using 50,000 histories/cycle with 50 warmup cycles and 5,000 active cycles.

Pin power, represented by the <sup>235</sup>U(n,f) reaction rate tally, was calculated for a 20 cm axial region centered at the fuel meat midplane. While there is a natural variation in individual pin power uncertainties, the individual tally uncertainties are in the 0.3% range for each of these 250 million history MCNP jobs. Another estimate of the pin power tally uncertainty comes from the job-to-job tally variation for these 20 independent Monte Carlo calculations. This variation also produces a 0.3% or so uncertainty estimate, indicating that MCNP's uncertainty estimate is reliable.

In summary, we conclude that when calculating uncertainties, MCNP's estimates for criticality and individual reaction rates are reliable. However, when computing ratio quantities (i.e., spectral indices), the assumption of independent uncertainty estimates for the respective tallies being ratioed can be suspect, and can easily lead to an overestimate in the MCNP computed uncertainty on that ratio. This is particularly true for spectral index uncertainties involving cross sections that span the problem energy range and whose individual tally estimates are highly correlated.