Summary Report for Special Services Agreement TAL-NAPC20180912-001

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Statement of Work

To research, document ICSBEP for experimental information on spectral indices and reaction rates; 2. To retrieve, modify and create MCNP6 inputs deck that correspond to the above cases; 3. To perform simulations of the experiment with MCNP6, to output the results, using the 660 Cullen group structure and to provide the results for TENDL-2017 and ENDF/B-VIII.O in a report.

Introduction

A review of the ICSBEP and IRPhEP Handbooks as well as other sources (references 1 – 19) determined that reaction rate (spectral index) or pin power data are available for a variety of critical experiments. The experiments for which MCNP6© input and output files have been developed are noted in the following Table.

Table 1: A List of ICSBEP and IRPhEP Benchmarks with Reaction Rate Data

ICSBEP or IRPhEP Identifier	Comment
HEU-MET-FAST-001	Godiva. CAUTION: The ICSBEP Handbook description is for the original (spherical, or Godiva-I) assembly which ceased operation in 1954, but the experimental data are said to come from a 1959 measurement. The 1959 "Godiva" assembly, Godiva-II, was a cylindrical assembly with a dome top. Further research is needed to determine the applicable model for these data.
HEU-MET-FAST-028	Flattop-25. A spherical HEU core surrounded by a spherical ^{nat}U reflector. Most of the experimental reaction rate data come from measurements near the core center.
IEU-MET-FAST-007	Big-10. A large cylindrical assembly consisting of uranium metal plates of various enrichments. Measurements were made in the center of a large 10% enriched region.
Pu-MET-FAST-001	Jezebel. A bare spherical mostly ^{239}Pu (~5 atom % ^{240}Pu) core. Reaction rate measurements were made near the core center.
Pu-MET-FAST-002	"dirty" Jezebel. A bare spherical, mostly ^{239}Pu core (^{240}Pu content is ~ 20 atom %). Reaction rate measurements were made near the core center.
Pu-MET-FAST-006	Flattop-Pu. A spherical ^{239}Pu core surrounded by a spherical ^{nat}U reflector. Most of the experimental reaction rate data come from measurements near the core center.
Pu-MET-FAST-008	THOR. A spherical mostly ^{239}Pu core (~5 atom % ^{240}Pu) surrounded by a cylindrical thorium reflector.

Table 1: A List of ICSBEP and IRPhEP Benchmarks with Reaction Rate Data

ICSBEP or IRPhEP Identifier	Comment
LEU-COMP-THERM-008	Mid-plane pin power distribution measurements were made in the central 15x15 region of a large (~4400 rods) Babcock & Wilcox reactor lattice. This evaluation includes 17 critical configurations with varying water hole and poison rod alignments. Twelve configurations included pin power measurements. These data are provided in Appendix B to the evaluation.
DIMPLE-LWR-EXP-002 (LEU-COMP-THERM-055)	Mid-plane pin power distributions. Data are provided for two configurations, designated as S06A and S06B. Although a full 3D description of these configurations is provided in the ICSBEP Handbook, when analyzing pin power data the IRPhEP evaluator recommends using a 2D model employing octant symmetry.
U233-MET-FAST-001	Jezebel-23. A spherical, bare, ^{233}U critical assembly. Reaction rate measurements were made near the core center.
U233-MET-FAST-006	Flattop-23. A spherical ^{233}U core surrounded by a spherical ^{nat}U reflector. Reaction rate measurements were made near the core center.
FUND-IPPE-FR-MULT-RRR-001	Cross section ratio data for a variety of foils irradiated near the center mid-plane of IPPE's Pu metal BR-1 core.

MCNP6© input decks have been developed, using the recommended information provided by the respective evaluators in Section 3 of the various ICSBEP and IRPhEP reports. f4 and/or *f4 tallies (described below and in Appendix B) have been added to these decks to allow calculation of reaction rates (which when divided by the ^{235}U(n,f) or ^{239}Pu(n,f) rate, as appropriate for the reported data, provides a spectral index), pin power by individual fuel rod and the average reaction rate energy. In addition to the reaction rate or pin power tally which is integrated over the problem energy range, multigroup flux spectra were also calculated. Results for the "Culham-660" group structure, the "SAND-725" group structure as well as for a very dense (1000 equi-lethargy energy points per decade) energy mesh are provided. For the bare LANL assemblies these spectra were calculated within a small sphere (radius=0.25 cm) at the core center. For Flattop-25 and Flattop-Pu the flux spectra were also calculated in successive 0.5 cm thick shells, extending from the core center through the outer reflector. For the BR-1 core the flux region was a 1 cm tall cylinder at the core mid-plane center location.

<u>MCNP Running Strategy and File Summary</u>

For each benchmark up to six MCNP6© "kcode" jobs were executed. The first two jobs were run for 50 million and 250 million active neutron histories respectively, employing 5100 cycles (100 warmup cycles and 5000 active cycles) with either 10,000 or 50,000 neutrons per cycle. The remaining jobs were run with 40 warmup cycles and 2,500,000 neutrons per cycle. These jobs were stopped/continued after 440, 2040, 4040 and 10040 cycles, for a total of 1 billion, 5 billion, 10 billion and 25 billion active histories, respectively. Jobs for at least 1 billion histories were run for all benchmarks. Appendix A provides a brief description of how to continue a previously completed MCNP6© job for additional histories.

Reaction rate and multigroup flux tallies are available for each job. In addition, the average energy for these tallies was determined. In MCNP6© this may be determined in one of two ways. For a given f4 tally we also specify an identical *f4 tally. Division of the *f4 tally result by the f4 tally result yields the average energy for that reaction. Alternately for a given f4 tally a second identical f4 tally is defined with the addition of "de" and "df" cards that define an f(E)=E function. Again, division of the second tally result by the initial tally result yields the average energy for that reaction. The equivalence of these techniques was confirmed with a test job containing both f4 and *f4 tally cards. Identical average energies were obtained.

In some cases the measured reaction rate involves formation of a daughter reaction product in an isomeric state, or perhaps a fraction of the reaction goes to a long-lived isomer (or long-lived or stable ground state) and so that fraction of the reaction may not be measured. Fortunately the evaluated nuclear data file, either from ENDF/B-VIII.0 or (more often) TENDL-2017, contains the necessary information to account for this. File 3 in any evaluation provides reaction cross section information, often regardless of daughter product's final state while the corresponding information provided in File 9 or File 10 can be used to determine the split between a daughter nuclide's isomeric and ground states. When necessary we have extracted the appropriate energy dependent fraction and used the previously described "de" and "df" cards to modify the reaction rate tally to account for this. An example of this is provided in Appendix B.

All input and output files have been uploaded to the server location provided by the IAEA (Sublet). A summary list of these files is provided in the following Table.

Table II: MCNP Output File Summary

Benchmark ID	Cross Section Source	MCNP© Output File Summary
HEU-MET-FAST-001 (Godiva)	ENDF/B-VIII.0 TENDL-2017	Output files with central region multigroup flux and specific reaction rate tallies are available for both cross section data sets for 50M, 250M, 1B, 5B and 10B histories. CAUTION: The bare, spherical (Godiva I) model has been used for these calculations. Input files through 1B are also provided with jobs for greater neutron histories continued using the technique described in Appendix A. This comment applies to all of the benchmarks described in this Table.

Table II: MCNP Output File Summary

Benchmark ID	Cross Section Source	MCNP© Output File Summary
HEU-MET-FAST-028 (Flattop-25)	ENDF/B-VIII.0 TENDL-2017	Input and output files exist with central region only multigroup flux and specific reaction rate tallies for both cross section data sets for 50M, 250M, 1B and 5B histories. In addition, multigroup flux tallies for both cross section data sets are available at 50M, 250M and 1B histories at a series of 0.5cm thick radial shells from the core center to the outer reflector boundary.
IEU-MET-FAST-007 (Big-10)	ENDF/B-VIII.0 TENDL-2017	Input and output files with central region multigroup flux and specific reaction rate tallies are available for both cross section data sets for 50M, 250M and 1B histories.
Pu-MET-FAST-001 (Jezebel)	ENDF/B-VIII.0 TENDL-2017	Input and output files with central region multigroup flux and specific reaction rate tallies are available for both cross section data sets for 50M, 250M, 1B, 5B, 10B and 25B histories.
Pu-MET-FAST-002 ("dirty" Jezebel)	ENDF/B-VIII.0 TENDL-2017	Input and output files with central region multigroup flux and specific reaction rate tallies are available for both cross section data sets for 50M, 250M, 1B, 5B and 10B histories.
Pu-MET-FAST-006 (Flattop-Pu)	ENDF/B-VIII.0 TENDL-2017	Input and output files exist with central region only multigroup flux and specific reaction rate tallies for both cross section data sets for 50M, 250M, 1B and 5B histories. In addition, multigroup flux tallies for both cross section data sets are available at 50M, 250M and 1B histories at a series of 0.5cm thick radial shells from the core center to the outer reflector boundary.
Pu-MET-FAST-008 (THOR)	ENDF/B-VIII.0 TENDL-2017	Input and output files with central region multigroup flux and specific reaction rate tallies are available for both cross section data sets for 50M, 250M and 1B histories.

Table II: MCNP Output File Summary

Benchmark ID	Cross Section Source	MCNP© Output File Summary
LEU-COMP-THERM-008 (cases 2 – 9, 11, 16 & 17)	ENDF/B-VIII.0 TENDL-2017	Input and output files with central cluster mid-plane pin power distributions are available for both cross section data sets for 50M, 250M and 1B histories. The model assumes quarter core symmetry and the "mid-plane" is defined as an axial region extending ±8.17 cm from the axial mid-point of the fuel stack. The 16.34 cm tall region represents 10% of the total fuel stack length. Reactivity calculations are also available for the remaining cases that lack pin power data. Also reactivity calculations using either a water only thermal scattering kernel or both water and uo_2 thermal scattering kernels are provided.
DIMPLE-LWR-EXP-002 (LEU-COMP-THERM-055)	ENDF/B-VIII.0 TENDL-2017	Input and output files with pin power distributions were performed for both cross section data sets at 50M, 250M and 1B histories for the "S06A" and "S06B" configurations. The model is 2D and employs octant symmetry, as recommended by the evaluator.
U233-MET-FAST-001 (Jezebel-23)	ENDF/B-VIII.0 TENDL-2017	Input and output files with central region multigroup flux and specific reaction rate tallies are available for both cross section data sets for 50M, 250M, 1B, 5B, 10B and 25B histories.
U233-MET-FAST-006 (Flattop-23)	ENDF/B-VIII.0 TENDL-2017	Input and output files with central region multigroup flux and specific reaction rate tallies are available for both cross section data sets for 50M, 250M, 1B, 5B, 10B and 25B histories.
FUND-IPPE-FR-MULT-RRR-001	ENDF/B-VIII.0 TENDL-2017	Input and output files with central region multigroup flux and specific reaction rate tallies are available for both cross section data sets for 50M, 250M, 1B, 5B and 10B histories.

Concluding Thoughts

Monte Carlo jobs that attempt to calculate reaction rates typically require many more histories than a simple criticality k_{eff} calculation. The question that is never easy to answer is how much is "many more"? For many years LANL has typically run 50 million histories when reporting calculated k_{eff} results to the technical community. This number typically yields a k_{eff} result with a 5 to 25 pcm uncertainty. And based upon casual conversations with others I would say that 25 million to 100 million histories represents a typical job size at the present time. On the other hand, reaction rate calculations are often performed with 5 to 50 times as many histories. That said there has not been a systematic study as to what represents the best practice. The intent in providing results for a variety of neutron histories here is to allow the issue of "how many more" to be studied.

For simple assemblies, such as the bare Godiva, Jezebel and Jezebel-23 spheres it is likely that the answer has converged with a modest increase over the 50M history k_{eff} job and so the advantage of running further histories is to reduce the stochastic uncertainty. More complex assemblies (e.g., reactor lattices) may require even more histories than in the output files provided to date. These jobs can be run for as many additional histories as institutional computing resources permit. Using mcnp's "continue" capability is an easy way to extend an existing job for additional histories. A sample input deck and instructions on executing this option are provided in the Appendix A.

The "scope of work" for this contract specified that benchmarks from the ICSBEP Handbook be reviewed, and that has been the principal focus of this effort. In one instance we have shifted from the ICSBEP LEU-COMP-THERM-055 benchmark to the identical IRPhEP DIMPLE-LWR-EXP-002 benchmark (in order to take advantage of the pin power data described in the latter evaluation). Nevertheless it is this author's opinion that the IRPhEP Handbook is an underutilized resource that likely contains much additional data that will be useful to future CoNDERC efforts.

References

Note: All references cited below (excluding the ICSBEP and IRPhEP Handbooks) are available in electronic form. The ICSBEP and IRPhEP Handbooks are available from the Nuclear Energy Agency, either online or on DVD.

1. M.B.Chadwick *et al*, "The CIELO Collaboration: Neutron Reactions on 1H, 16O, 235,238U and 239Pu," Nucl. Data Sheets 118(2014)1.
2. D.A.Brown *et al*, "ENDF/B-VIII.0: The 8th Major Release of the Nuclear Reaction Data Library with CIELO-Project Cross Sections, New Standards and Thermal Scattering Data," Nucl. Data Sheets 148(2018)1.

3. M.B.Chadwick *et al*, "ENDF/B-VII.1 Nuclear Data Library for Science and Technology: Cross Sections, Covariances, Fission Product Yields and Decay Data," Nucl. Data Sheets 112(2011)2887.
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7. S.C.Frankle, "Spectral Measurements in Critical Assemblies: MCNP Specifications and Calculated Results," LA-13675, December 1999.
8. CSEWG, "Cross Section Evaluation Working Group Benchmark Specifications (revised September 1991)," BNL-19302 (also ENDF-202).
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10. L.B.Engle, G.E.Hansen & H.C.Paxton, “Reactivity Contributions of Various Materials in Topsy, Godiva and Jezebel, Nucl.Sci.Eng. 8, 543-569 (1960).
11. P.I.Amundson *et al*, “An International Comparison of Fission Detector Standards,” in Proceedings of an International Conference on Fast Critical Experiments and the Analysis, October 1666. Argonne National Laboratory report ANL-7320, p. 679-687.
12. R.E.MacFarlane *et al*, “Data Testing of ENDF/B-V Revision 2” in Applied Nuclear Science Research and Development Semiannual Progress Report, October 1,1983 – May31, 1984. LA-10288-PR, p. 42-45. NOTE: Progress Reports are rarely cited as a primary source and where these data have been reported in many of the preceding references they are generally cited as “R.E.MacFarlane, private communication”.
13. G.E.Hansen, “Status of Computational and Experimental Correlations for Los Alamos Fast-Neutron Critical Assemblies” in Proceedings of the Seminar on the Physics of Fast and Intermediate Reactors, Vol I, p. 445 (SM 18/53), Vienna 1962.
14. G.E.Hansen and H.C.Paxton, “A Critical Assembly of Uranium Enriched to 10% in Uranium-235,” Nucl.Sci.Eng. 72, 230-236 (1979).
15. G.E.Hansen and H.C.Paxton, “THOR, A Thorium-Reflected Plutonium-Metal Critical Assembly,” Nucl.Sci.Eng. 71, 287-293 (1979).
16. D.M.Gilliam and J.A.Grundl, “Dosimetry Results for Big Ten and Related Benchmarks,” LA-UR-79-2685 (Submitted to the Third ASTM-Euratom Symposium in Reactor Dosimetry, Italy, 1979).
17. M.N.Baldwin and M.E.Stern, “Physics Verification Program Part III, Task 4 Summary Report,” BAW-3647-20, March 1971.
18. J.D.Bess (editor), “International Handbook of Evaluated Criticality Safety Benchmark Experiments”, NEA No. 7360 (2018). NOTE: New and revised benchmark information are published on an annual or every other year basis. The 2018 edition of the Handbook is the latest available as this report is written but the individual benchmark evaluations

that are used in this report were developed many years earlier. The specific benchmark revision and evaluation data are typically noted in comments embedded in the specific MCNP© input deck. Also note that reaction rate data are rarely included in ICSBEP evaluations and so must be obtained from other sources, such as the preceding references in this section.

19. J.D.Bess (editor), "International Handbook of Evaluated Reactor Physics Benchmark Experiments," NEA No. 7361 (2018). NOTE: New and revised benchmark information are published on an annual or every other year basis. The 2018 edition of the Handbook is the latest available as this report is written but individual benchmark evaluations may have been developed many years earlier. The specific benchmark revision and evaluation data are typically noted in comments embedded in the specific MCNP© input deck.

Appendix A

Sample “continue” input for MCNP6©

The boxed text that follows constitutes a complete input deck to “continue” an MCNP6© job. In addition to this sample deck a “runtpe” file from the job that ran the initial 440 iterations is assumed to be available and in response to this input the job will continue until cycle 2040. Simple modifications to this input deck allow further continuation to 4040 cycles, 10040 cycles and 40040 cycles. For these further continuation jobs it is always the “runtpe” file from the immediately preceding job that is also required. Also, note the value for “mrkp”. Many legacy “kcode” input cards omit specifying this parameter and simply accept its default value. This variable defines the maximum number of active cycles to include when calculating tallies and their uncertainty. MCNP6©’s default value for this variable is 6500 cycles and so we define this larger value to assure that all active cycles contribute to final tally calculations regardless of which kcode card is made active. Use of default values for the kcode input card variables not explicitly described is acceptable.

```
  continue
c
c
c nsrck is number of histories per cycle
c   ikz = warmup cycles to skip
c   kct = total number of cycles to run
c  mrkp = maximum cycle number to include in MCTAL and RUNTPE files
c
c kcode   nsrck rkk ikz  kct  msrk,knrm  mrkp kc8
c
c kcode 2500000 1.0  40 40040 2j    40100 $2,500,000x40,000=100B hist
c kcode 2500000 1.0  40 10040 2j    40100 $2,500,000x10,000= 25B hist
c kcode 2500000 1.0  40  4040 2j    40100 $2,500,000x 4,000= 10B hist
  kcode 2500000 1.0  40  2040 2j    40100 $2,500,000x 2,000=  5B hist
c kcode 2500000 1.0  40   440 2j    40100 $2,500,000x   400=  1B hist
c kcode   50000 1.0 100  5100 2j    40100 $   50,000x 5,000=250M hist
c kcode   10000 1.0 100  5100 2j    40100 $   10,000x 5,000= 50M hist
```

As utilized by this author, the MCNP6© command line to execute the continuation job is

```
mcnp620 c tasks 4 i=continue.inp
```

where the “c” keyword specifies a continuation job, the “tasks 4” keyword and number option specifies use of 4 cpu’s and “i=continue.inp” specifies the input file to be used by MCNP6© for the continuation. “mcnp620” is the filename for the mcnp, version 6.2.0, executable as stored on the author’s computer.

Appendix B

Sample f4 tally definition with “de” and “df” input cards

f4 tally cards for the $^{241}Am(n,\gamma)^{242g}Am$ reaction, as used in the MCNP6© Flattop-25 model, are shown below.

```
c
c - 241Am(n,g) with e80 (mf9/mt102) ratio data for capture to 242gAm.
c   - these ratio data are unchanged from e71 and e70.
c   - a separate factor is applied offline to account for the beta
c     decay branch to 242Cm.
 fc164 241Am(n,g) ---> 242gAm
  f164:n 1
 fs164 -11
 fm164 (1 931            (102))  $241Am(n,g)
 de164 LIN
       1.00E-11     3.69E-7     1.00E-3     1.00E-1     6.00E-1
       1.00E+0      2.00E+0     4.00E+0     30.0E+0
 df164 LIN
       0.9          0.9         0.8667      0.842       0.81533
       0.74382      0.5703      0.52        0.52
```

Points to note about these cards include

- Use of the fs164 card in conjunction with f164. F164 specifies the tally to occur in cell 1 which is the core while fs164 applies a further restriction that the tally only accrue for collisions occurring within surface 11 (which defines a sphere whose radius is 0.25 cm located at the core center).
- Card fm164 specifies reaction 102 (the (n,γ) reaction) for material 931. Not shown is card m931 which specifies the ^{241}Am ZAID.
- Card de164 specifies a list of energies (in MeV) and further specifies use of linear-linear interpolation.
- Card df164 specifies a list of function values at the de164 energies. Again linear-linear interpolation is specified.

These cards, without the de164 and df164 input would provide the tally for the $^{241}Am(n,\gamma)$ reaction without consideration of the ^{242}Am nuclide’s final state. However we know the compound nucleus decays into either the long-lived ^{242m}Am isomer or the much shorter lived ^{242g}Am ground state which subsequently β-decays to ^{242}Cm (~82.7% of the time). It is the β-decay that is measured and so the pure capture reaction rate tally must be modified to account for both the energy-dependent ^{242g}Am versus ^{242m}Am production ratio as well as the subsequent β-decay branching fraction.

The β-decay branch fraction is easily accounted for in post-MCNP6© analyses, but the ^{242g}Am ratio must be accounted for on a collision-by-collision basis during the MCNP6© simulation. That is the role of the de164 and df164 cards. The specific data on these cards comes from the information tabulated in File 9 of the ^{242}Am(n,γ) ENDF/B-VIII.0 evaluation. The tally fraction for a given collision is modified by the df164 card value, allowing the pure capture tally to be reduced so that only the tally fraction leading to ^{242g}Am is calculated.

Having such data in File 9 is particularly useful as it is already in the fractional form suitable for direct use on “df#4” cards. Similar information is sometimes provided in the evaluation’s File 10. In this case what is provided are the cross sections for creation of the isomer(s) and the ground state. These data are moved into a spreadsheet where the desired ratio values are calculated for use in the MCNP6© job.

As a final caution the reader is reminded that ENDF evaluations use “eV” for the energy unit while all versions of MCNP© uses “MeV”. The 1.e+6 factor is easy to apply, but also easy to forget, when entering data on the “de#4” input card. MCNP© assumes a unity function value for collisions occurring at energies outside the range specified on the “de#4” card.