MCNP-4B Validation for the DFS System at SRS

by

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1.0 INTRODUCTION

ANSI/ANS Standard 8.1¹ requires that computer codes and methods used to determine limits for criticality safety be validated against experiments. This document provides the current work to date on the validation of the WSRC certified^{9, 10} MCNP-4B code, and is the last stage of the WSRC Validation Plan³ that was drafted to guide the validation effort.

1.1 WSRC MCNP-4B Validation

Given the fact that MCNP-4B has been validated on the WSMS DEC Alpha machines in the Centennial Complex, it was desirable to determine if such validation could be used to efficiently document the SRS MCNP-4B validation on their RS/6000 workstations. For this, a representative sample of input files from each of the major fissile types and forms were run under the SRS certified MCNP-4B code and subsequently compared to their WSMS counterpart. The results of these comparisons demonstrate that the two platforms provide statistically similar k_{eff} and uncertainty values without the introduction of a bias. This gives sufficient certification that the validation for MCNP-4B under the WSMS system is directly compatible as the MCNP-4B validation for the WSRC system. Table 1 in Appendix B shows the results of this comparison. Based on this comparison, it is appropriate to use the bias and bias uncertainties generated by the WSMS workstation when evaluating corresponding cases generated by the WSRC system.

The input files for the SRS MCNP-4B validation experiments can be found in the */raid1/packages/crit/Validation/Mcnp4b* directory on the WSMS DEC Alpha workstation platform, while the output files are saved on a compact disk held by the owner of the WSRC MCNP-4B Certification Notebook⁹. The remainder of this document (with the exception of Appendix B, and formatting such as page numbering) is identical to the WSMS MCNP-4B validation document, authored by N. J. Jordan and M. N. Eakin.

1.2 WSMS MCNP-4B Validation

This validation utilized the MCNP-4B control sequence, with the ENDF/B-V cross section library, running on the WSMS Digital Equipment Alpha Processors (DEC Alpha) UNIX workstation cluster under the Network File System (NFS). The values of bias and bias uncertainty are presented for uranium and plutonium systems. For each fissile system, the area of applicability of the validation is presented, followed by a brief description of the benchmarks that was used in the determination of the bias. Following this is a discussion of the bias and bias uncertainty and the limitations of the validation. This document does not present values of k_{safe} ⁴, as these are system dependent. The limits presented in this document encompass the bias, the uncertainty due to reported experimental parameters, the statistical uncertainties in the calculation of the experiments, and the uncertainty associated with geometrical or modeling uncertainties in the computational method.

When used with a margin for Area of Applicability, and an appropriate subcritical margin, the value of k_{safe} for a particular application can be determined⁴.

Table 1.A presents a quick reference guide for the complete list to date (as of 5/19/99) of technical reports and calculation notes.

Table 1.A Technical Report and Calculation Note List.

<u>Experiments</u>		<u>Tech Report / Calc Note</u>	<u>Originator</u>
<i>PU-MET-FAST</i>	001-006, 008-011, 016-017, 022-023, 037	Contained within this document.	-
<i>PU-SOL-THERM</i>	001-007, 009-012	Contained within this document.	-
<i>HEU-MET-FAST</i>	001-004, 007, 012, 013 021-024, 026, 033-035	WSMS-CRT-98-0063	G. Kessler
<i>IEU-MET-FAST</i>	005, 006	WSMS-CRT-98-0063	G. Kessler
<i>HEU-MET-THERM</i>	006	Contained within this document.	
<i>HEU-SOL-THERM</i>	001-003, 007-012	WSMS-CRT-98-0070	G. Kessler
<i>HEU-COMP-THERM</i>	011-014	WSMS-CRT-98-0070	G. Kessler
<i>LEU-COMP-THERM</i>	001, 002, 010, 017	N-CLC-H-00314	T. G. Williamson

Section 2 provides an overview of the calculational methods used in computing the k_{eff} values for the critical benchmarks and the MCNP-4B analytical sequence. Section 3 provides an overview of the methodology used in the validation and in the generation of the bias and uncertainty. Sections 4 and 5 provide detailed discussions of bias and bias uncertainty for each fissile material. Appendix A provides the calculated k_{eff} and statistical deviation as well as validation parameters for each critical experiment. The input files are not included in this compilation. For input files and a more detailed description of the experiments and statistical analyses, refer to the individual calculation notes and/or to the International Handbook of Evaluated Criticality Safety Benchmark Experiments⁵. The input/output files for the systems compiled in this validation document can be found in the */raid1/packages/crit/Validation/Mcnp4b* directory.

2.0 CALCULATION METHODOLOGY

MCNP- 4B is a general-purpose, continuous-energy (or multi-group), generalized geometry, neutral particle and electron Monte Carlo transport code developed at the Los Alamos National Laboratory. The code is applicable in two modes: criticality and external source modes (the source mode is primarily for shielding evaluations). Monte Carlo can be used to calculate the system multiplication factors (k_{eff}), the energy spectrum

for neutrons and photons, and the reaction rate distribution. This validation incorporates the criticality mode to calculate k_{eff} .

3.0 BIAS AND UNCERTAINTY METHODOLOGY

The methods used in this document to determine the value of bias and bias uncertainty for a particular area of applicability are given in Chapter 6 of the Criticality Methods Manual⁴. In Chapter 6, the bias methodology is subdivided into different approaches depending on the amount of data and its characteristics. In this report, the upper subcritical limit and lower tolerance limit are used.

The upper subcritical limit (USL) is determined from a non-parametric analysis of a non-normal distribution of data. The USL is a limit determined from the smallest observed value in which a certain fraction of the true population of data is expected to lie above for some degree of confidence. A lower tolerance limit (LTL), on the other hand, assumes that the distribution of the data is normal, and thus a single value of k_{eff} can be determined, above which a specified percent of the data will fall with some confidence. A LTL cannot be extrapolated, and thus is only valid within the range of the experimental data. A LTL is typically used when a good fit (or correlation) cannot be found between an independent parameter and the calculated k_{eff} values.

For all reported LTL values in this report, a confidence and population level have been set at 95 percent. Thus the LTL's represent values that 95 percent of the population will lie above with 95 percent confidence. For USL's, the percent of the of the population that will lie above with 95 percent confidence will be determined by the number of data points. Table 1.B contains a summary of the biases for each set of experiments.

Table 1.B Summary of limits for each system.

<u>EXPERIMENT (# OF CASES)</u>	<u>TYPE OF LIMIT</u>	<u>LIMIT VALUE</u>	<u>PAGE</u>
<i>PU-MET-FAST (51)</i>	Lower Tolerance Limit	0.990	13
<i>PU-SOL-THERM (91)</i>	Upper Subcritical Limit	0.994	32
<i>HEU-MET-FAST & IEU-MET-FAST (130)</i>	Upper Subcritical Limit	0.984	51
<i>HEU-MET-THERM (14)</i>	Lower Tolerance Limit	0.976	53
<i>HEU-SOL-THERM 1-3,7-12(85)</i>	Lower Tolerance Limit	0.994 ^A	63
<i>LEU-COMP-THERM & LEU-SOL-THERM (71)</i>	Lower Tolerance Limit	0.986	69

^A See system description (Section 5.3.2) and bias and uncertainties (Section 5.3.3).

4.0 PLUTONIUM SYSTEMS

4.1 Plutonium Metal

4.1.1 Area of Applicability

This section presents the MCNP validation analysis for plutonium metal systems. The result from this analysis is a lower tolerance limit (LTL) for the MCNP code system with the ENDF/B-V cross section library. The MCNP user should employ the F-4 flux tally to obtain the average energy to assure that the evaluated system is contained within the applicable neutron spectrum. Key areas of applicability for these experiments include:

1. Fuel:	Plutonium Metal System
2. Moderation:	H/Pu-239: ~0.0
3. Pu-240 Content:	1.8 – 20.1 Wt % Pu-240 ^B
4. Moderating Material:	None or Slight (Polymer Mock Explosive)
5. Reflecting Material:	Bare, Thorium, Beryllium, Graphite, Tungsten, Gallium, Polyethylene, Aluminum, Uranium, or Hydrogenous
6. Geometry:	Single Spheres and Cylindrical Arrays
7. Neutron Spectrum ^C :	Fast; 2.5 keV – 1.8 MeV
AEG: 4.22-10.04

4.1.2 System Description

4.1.2.1 Single Unit Plutonium Spheres

Ten experiments, extracted from the International Handbook of Evaluated Criticality Safety Benchmark Experiments, have been evaluated and documented. These experiments utilized spheres of plutonium metal with different compositions and reflectors. A summary of the experimental parameters is provided in Table 2.

^B See limitations (Sect. 4.1.4).

^C The neutron spectrum represents the average energy of the neutrons causing fission.

Table 2. Pu Metal Sphere Experiment Critical Parameters.

Benchmark Descriptor	Fuel Alloy	Pu Isotopic Composition (wt %)				Sphere Radius (cm)	Reflector & Thickness (cm)
		239	240	241	242		
PU-MET-FAST-001 ⁵	98.98 % δ -phase Pu, 1.02 % Ga	95.2	4.5	0.3	0.0	6.3849	None
PU-MET-FAST-002 ⁵	98.99 % δ -phase Pu, 1.01 % Ga	76.4	20.1	3.1	0.4	6.6595	None
PU-MET-FAST-005 ⁵	99.00 % δ -phase Pu, 1.00 % Ga	94.77	4.92	0.31	0.0	5.0419	W, 4.699
PU-MET-FAST-006 ⁵	98.90 % δ -phase Pu, 1.10 % Ga	93.8	4.80	0.30	0.0	4.5332	U, 19.6088
PU-MET-FAST-008 ⁵	98.99 % δ -phase Pu, 1.01 % Ga	94.55	5.15	0.30	0.0	5.310	Th, 24.57
PU-MET-FAST-009 ⁵	99.00 % δ -phase Pu, 1.00 % Ga	94.8	4.90	0.30	0.0	5.5118	Al, 7.9248
PU-MET-FAST-010 ⁵	99.00 % δ -phase Pu, 1.00 % Ga	94.79	4.90	0.31	0.0	5.0419	U, 4.699
PU-MET-FAST-011 ⁵	100 % δ -phase Pu, 0 % Ga	94.48	5.20	0.30	0.02	4.1217	H ₂ O, 25.40
PU-MET-FAST-022 ⁵	98.00 % δ -phase Pu, 1.00 % Ga	98.2	1.8	0.00	0.0	6.67 (Hollow)	None
PU-MET-FAST-023 ⁵	Varied by layer	98.2	1.8	0.00	0.0	Layered	Graphite, 2.35

4.1.2.2 Arrays of Plutonium Metal Cylinders

Three sets of benchmark experiments have been evaluated. Experimental arrays were constructed from canned plutonium metal cylinders. Alpha phase plutonium with the composition specified in Table 3 was used for these experiments. Specific details on the experiments are provided in the following sections.

Table 3. Plutonium Isotopic Composition, Arrays of Cylinders.

Benchmark Descriptor	Isotopic Composition (Wt %)			
	239	240	241	242
PU-MET-FAST-003 ⁵ , 004 ⁵ , and 017 ⁵	93.56	5.97	0.46	0.01

4.1.2.2.1 *Unmoderated Button Array*

Four experiments involving arrays of plutonium metal cylinders were evaluated. Plutonium cylinders were contained within aluminum cans with steel lids. Square pitched arrays were constructed using single (3 kg) and double (6 kg) parts. Spacing between arrays was maintained by use of aluminum support tubes and spacers fastened to an experimental table by means of a support shoe. Benchmark specifications for these experiments did not include an experimental room. A summary of the experimental parameters for these experiments is provided in Table 4.

Table 4. Reported Parameters for PU-MET-FAST-003.

Experiment Descriptor	Array & Unit Size	Vertical CTC ^D Spacing (cm)	Horizontal CTC ^D Spacing (cm)	Reflector
101	2x2x2 3 kg Cyl.	5.40	7.30	None
102	2x2x2 3 kg Cyl.	5.74	7.64	Polyethylene
103	3x3x3 3 kg Cyl.	7.71	9.60	None
105	2x2x1 6 kg Cyl.	N/A	7.59	None

4.1.2.2.2 *Unmoderated Cylinders Array*

Nine experiments involving three-dimensional arrays of plutonium metal cylinders were evaluated. These experiments are similar to the experiments described in section 4.1.2.2.1 with the exceptions noted in the following paragraph.

Square pitched arrays were constructed using single and double parts. Spacing between arrays was maintained by use of aluminum support tubes and spacers fastened to an experimental table by means of a support shoe. A summary of the experimental parameters for these experiments is provided in Table 5.

^D Center-to-center spacing measured from centers of double and single parts.

Table 5. Reported Parameters for PU-MET-FAST-004.

Experiment Descriptor	Array & Unit Size	Vertical CTC Spacing (cm)	Horizontal CTC Spacing (cm)	Reflector
207	4x4x4, bare 3 kg	7.86±0.01	12.51±0.01	None
208	4x4x4, bare 6kg	17.12±0.02	17.28±0.01	None
209	4x4x4, bare 6 kg	32.12±0.02	13.09±0.01	None
210	4x4x4, bare 6 kg	47.12±0.02	11.93±0.01	None
211	4x4x4, bare 6kg	22.12±0.02	15.23±0.01	None
212	4x4x4, bare 6 kg	13.12±0.02	20.19±0.02	None
213	4x4x1, bare 6 kg	N/A	10.91±0.02	None
214	3x3x3, bare 6 kg	13.68±0.02	14.51±0.03	None
215	2x2x2, bare 6 kg	11.98±0.02	9.76±0.03	None

4.1.2.2.3 Moderated Cylinders Array

Five experiments involving three-dimensional arrays of moderated plutonium metal cylinders were evaluated. These experiments were conducted using the same support apparatus as the experiments in section 4.1.2.2.1. Moderator jackets and end disks were added to the outside of the support tube and above or below heat sinks, respectively. These disks were made of a mock explosive material. A polymer material consisting primarily of carbon, hydrogen, and oxygen was used for the mock explosive moderator disks. Three sizes of moderator jackets and end disks were used. The dimensions of these moderator pieces are provided in Table 6.

Table 6. Moderator Dimensions For PU-MET-FAST-017.

Case #	Thickness (cm)	Jacket Height (cm)
201	1.2707	13.493
202	2.5487	16.049
203	3.8163	18.5842
204	1.2707	8.3964
205	2.5487	10.9524

4.1.2.3 Flooded Arrays of Plutonium Metal Cylinders (Phases I & II)

Two sets of benchmark experiments have been evaluated. A total of thirty-eight experiments were extracted from the International Handbook of Evaluated Criticality Safety Benchmark Experiments. Experimental arrays constructed from plutonium metal cylinders were flooded with water. Alpha phase plutonium in varying compositions was used for these experiments. Details on the experiments are provided in the following sections.

4.1.2.3.1 Flooded Array of Cylinders (Phase I)

Thirteen experiments involving water reflected arrays of plutonium metal cylinders were conducted at the Rocky Flats Critical Mass Laboratory (CML). Plutonium metal cylinders were assembled into a 3x3x3 array and flooded with water. For each of the thirteen experiments, horizontal and vertical spacings were chosen and water was added until the array was critical. However, three of the measurements remained subcritical on full reflection and are not considered acceptable benchmark experiments. Four of the remaining ten experiments were repeated measurements and were not considered valid. Five out of the remaining six experiments were evaluated and considered valid as benchmark experiments. Plutonium cylinders were contained within aluminum cans with steel lids. Square pitched arrays were constructed using twenty-seven 3-kg plutonium metal parts. Spacing between arrays was maintained by the use of aluminum support tubes and spacers. Specific details on the benchmark specifications for these experiments can be found in Reference 7. A summary of the experimental parameters for these experiments is provided in Table 7.

Table 7. Reported Parameters for PU-MET-FAST-016⁵ (CTC Spacing and Critical Water Heights).

Benchmark Case #	Experiment Number	Lateral Spacing $\Delta X = \Delta Y$ (cm)	Vertical Spacing ΔZ (cm)	Water Height (cm)
2	2	12.70	12.75	58.40
3	3	12.90	12.75	60.60
4	6-9	13.00	12.75	62.78
5	10	13.05	12.75	65.80
6	13	12.80	13.10	65.60

Table 8 lists the atom densities for the plutonium isotopes.

Table 8. Atom Densities for Plutonium Metal.

Isotope	Atoms/barn-cm
Pu-239	4.6054×10^{-2}
Pu-240	2.9264×10^{-3}
Pu-241	9.9882×10^{-5}
Pu-242	4.8613×10^{-6}
Am-241	1.2467×10^{-4}

4.1.2.3.2 *Flooded Array of Cylinders (Phase II)*

Sixteen experiments were conducted at the Rocky Flats Critical Mass Laboratory (CML) and used for this evaluation. These experiments (PU-MET-FAST-037⁵) are similar to the experiments described in section 4.1.2.3.1. The plutonium cans were placed on aluminum trays instead of inside aluminum sleeves. Plutonium cylinders were assembled into 2x2xN arrays (N is the height in number of cylinders; 2, 3, 4, or 5) and flooded with water. The horizontal and vertical spacing varied between the experiments. The arrays were assembled and water was added until the critical water height could be determined. These sixteen experiments are considered valid for use as benchmark experiments.

4.1.3 Bias and Uncertainty

A computational bias is determined by statistically analyzing the (normalized) calculated k_{eff} values from the benchmark experiments. In accordance to Reference 4, a Shapiro-Wilk test is performed to determine if the data are normally distributed. The data was proven to have a normal distribution. The plot of the k_{eff} values versus the average energy group is shown in Figure 1.

Figure 1. k_{eff} versus Average Energy Group.

The linear correlation coefficient, R^2 , determines how closely the dependent values fit the least squares regression of the data. A value of one signifies an exact match; compared to zero if there is no correlation. For this data set, there is little correlation between the data and the linear fit. An attempt to fit this data to the curves specified in Reference 4 also failed. Therefore, a lower tolerance limit was calculated using all 49 experimental cases and Equation 1 below.

$$\text{LTL} = k_{\text{eff}} - U \cdot S_p \quad (1)$$

where k_{eff} is the weighted mean k_{eff} value
 S_p is the pooled variance, and
 U is the one-sided lower tolerance factor

A single-sided lower tolerance limit for the plutonium metal systems is 0.990.

Table 9 summarizes the results of the statistical analysis for this data set.

Table 9. Results from Statistical Analysis.

	All 49 Experiments (WEIGHTED DATA)
One-sided Lower Tolerance Factor (U)	2.092*
Sqrt of Pooled Variance (Sp)	5.279E-03
Variance About the Mean (S²)	2.037E-05
Average Uncertainty (σ^2)	7.503E-06
Average k_{eff}	1.0015
Lower Tolerance Limit	0.990

* This is the tolerance factor for 45 data points; therefore, it is conservative for this data set.

4.1.4 Limitations

The evaluated experiments utilized the following reflector types: aluminum, beryllium, uranium, graphite, gallium, tungsten, polyethylene, water, and thorium. Thus, the results obtained from this analysis are applicable only to plutonium reflected by these reflector types with the average energy of the fissioning neutrons from 2.5 keV to 1.8 MeV using MCNP 4B running on the WSMS DEC Alpha workstation. Many of these reflector types had only a single experimental point, so care should be taken when evaluating systems with those reflectors, due to the scarcity of data. These results are not applicable to thermal systems, or systems containing significant interstitial moderation (i.e., H/Pu-239 ratio $\neq 0$).

The data used in this validation covers a broad spectrum of materials with various Pu-240 contents. The Pu-240 content ranged from 1.8-20.1%. There was one experiment with Pu-240 content of 20.1% and two experiments with Pu-240 content of 1.8%. The majority of the experiments, however, had Pu-240 content near 5 %. Therefore, a subcritical margin as low as 0.02 may be appropriate for those experiments having Pu-240 content near 5 %. The use of this bias with cases having Pu-240 content significantly different from 5 % requires the use of the area of applicability margin (AOA)⁴.

4.2 Plutonium Solutions

4.2.1 Area of Applicability

This section presents the MCNP validation analysis for plutonium nitrate solution systems. The result from this analysis is an upper subcritical limit for the MCNP code system with the ENDF/B-V cross section library. The MCNP user should employ the F-4 flux tally to obtain the average energy to assure that the evaluated system is contained within the applicable neutron spectrum. Key areas of applicability for these experiments include:

1. Fuel:	Plutonium Nitrate ($\text{Pu}(\text{NO}_3)_4$) Solution
2. Moderation:	H/Pu-239: 300 to 1200
3. Pu-240 Content:	0.54 – 18.91 wt % Pu-240 ^E
4. Moderating Material:	Hydrogenous Material
5. Reflecting Material:	Bare or Water Reflected
6. Geometry:	Single Spheres or Slabs
7. Neutron Spectrum ^F :	Thermal; 0.062 – 0.30 eV

4.2.2 System Description

Ninety-six critical experiments involving unreflected and water reflected spheres, slabs, and also cylinders were extracted from the International Handbook Of Evaluated Criticality Benchmark Experiments for this evaluation. The experimental configurations for these experiments are described in the following sections.

4.2.2.1 Unreflected Spheres

4.2.2.1.1 Unreflected 16 Inch Diameter Spheres

Five of the experiments utilized a single unreflected 16-inch diameter sphere of plutonium nitrate ($\text{Pu}(\text{NO}_3)_4$) solution. The isotopic distribution of the plutonium is given in Table 10. The plutonium used in these experiments was 95.83 wt % Pu-239 and 4.17 wt % Pu-240.

^E See limitations (Sect. 4.2.4).

^F The neutron spectrum represents the average energy of the neutrons causing fission.

Table 10. Pu Isotopic Distribution for PU-SOL-THERM-011⁵.

Isotope	Wt %, 16" Spheres	Wt %, 18" Spheres
²³⁹ Pu	95.83	95.80
²⁴⁰ Pu	4.17	4.20

The geometry data are given in Table 11.

Table 11. Geometry Data for PU-SOL-THERM-011.

Parameter	16" Sphere Dimension s, cm	18" Sphere Dimension s, cm
Solution Outer Radius	20.1206	22.6974
Sphere Outer Radius	20.2476	22.8244
Cadmium Outer Radius	N/A	22.8752

A summary of the reported experimental parameters is provided in Table 12.

Table 12. Reported 16-Inch Sphere Experiment Parameters (Fuel Material Atom Densities (atoms/barn-cm) for PU-SOL-THERM-011, 16" Cases).

Case →	16-1	16-2	16-3	16-4	16-5
H	6.4544E-02	6.4357E-02	6.3652E-02	6.2803E-02	6.0233E-02
O	3.4983E-02	3.5017E-02	3.5976E-02	3.5964E-02	3.7178E-02
N	1.0140E-03	1.0625E-03	1.5831E-03	1.7482E-03	2.7369E-03
Pu-239	8.4397E-05	8.7439E-05	9.2050E-05	9.2122E-05	1.0484E-04
Pu-240	3.6572E-06	3.7890E-06	3.9888E-06	3.9919E-06	4.5432E-06
Fe	1.1215E-06	1.2940E-06	1.3371E-06	1.9194E-06	1.9302E-06

4.2.2.1.2 Unreflected 18 Inch Diameter Spheres

Seven of the experiments utilized a single unreflected 18-inch diameter sphere of plutonium nitrate ($\text{Pu}(\text{NO}_3)_4$) solution. A thin cadmium shell (0.02 inches thick) was placed on the outside of the spherical reactor tank. A summary of the reported experimental parameters is provided in Table 13. The plutonium used in these experiments was 95.8 wt % Pu-239 and 4.2 wt % Pu-240.

Table 13. Reported 18-Inch Sphere Experiment Parameters (Fuel Material Atom Densities (atoms/barn-cm) for PU-SOL-THERM-011, 18" Cases).

Case→	18-1	18-2	18-3	18-4	18-5	18-6	18-7
H	6.5147E-02	6.4659E-02	6.4569E-02	6.3220E-02	6.3180E-02	6.0264E-02	6.3701E-02
O	3.4534E-02	3.4820E-02	3.5018E-02	3.5333E-02	3.6553E-02	3.7209E-02	3.5021E-02
N	7.3930E-04	9.4957E-04	1.0468E-03	1.4414E-03	1.9343E-03	2.7753E-03	1.2199E-03
Pu-239	5.3938E-05	5.6159E-05	5.5748E-05	5.7486E-05	6.0816E-05	6.6343E-05	5.7776E-05
Pu-240	2.3549E-06	2.4518E-06	2.4339E-06	2.5097E-06	2.6552E-06	2.8964E-06	2.5224E-06
Fe	1.2940E-06	1.3587E-06	1.4557E-06	1.3263E-06	1.4773E-06	1.5204E-06	4.1947E-07

4.2.2.1.3 Unreflected 48-Inch Diameter Sphere

This validation contains three experiments consisting of bare, type 1100 aluminum spheres filled with highly enriched (97.386% Pu-239) plutonium nitrate solutions. The plutonium concentration in the solution is varied (9.457 to 10.020 g/l), as is the height of solution in the spherical tank. The H/Pu-239 ratio varied between 2648.2 and 2802.8. The isotopic distribution of the plutonium is given in Table 14.

Table 14. Pu Isotopic Distribution for PU-SOL-THERM-009⁵.

Isotope	Weight Percent
²³⁸ Pu	0.004
²³⁹ Pu	97.386
²⁴⁰ Pu	2.521
²⁴¹ Pu	0.075
²⁴² Pu	0.014

The geometry data are given in Table 15. In addition, the heights of the solution above the midline of the spherical tank are 15.9558 and 45.3705 cm, respectively, for cases 1 and 2. In case 3, the tank was completely full.

Table 15. Geometry Data for PU-SOL-THERM-009.

Parameter	Dimension (cm)
Solution Outer Radius	60.964
Tank Outer Radius	61.734

The material data for the plutonium solution given in PU-SOL-THERM-009/Table 4 of Reference 5 are used to calculate the weight fractions for the isotopes in the solution, for input into MCNP. Note that two classes of material specifications are provided: one modeling the impurities and one ignoring the impurities. In the validations performed in this document, the impurities are disregarded, since Reference 5 indicates that they have a very small reactivity effect ($\Delta k = \sim 0.0003$). This effect is included in the experimental k_{eff} 's. The resulting weight fractions are given in Table 16, and are consistent with the atom densities presented in PU-SOL-THERM-009/Table 6 of Reference 5.

Table 16. Fuel Material Weight Fractions for PU-SOL-THERM-009.

Case	ρ (g/cc)	^{238}Pu	^{239}Pu	^{240}Pu	^{241}Pu	^{242}Pu	N	H	O
1	1.055	3.7991E-07	9.2494E-03	2.3944E-04	7.1232E-06	1.3297E-06	1.6830E-02	1.0343E-01	8.7027E-01
2	1.053	3.6236E-07	8.8221E-03	2.2837E-04	6.7942E-06	1.2682E-06	1.6755E-02	1.0352E-01	8.7071E-01
3	1.053	3.5924E-07	8.7462E-03	2.2641E-04	6.7358E-06	1.2573E-06	1.6804E-02	1.0351E-01	8.7071E-01

4.2.2.2 Water Reflected Spheres

4.2.2.2.1 Water Reflected 11.5-Inch Diameter Sphere

This validation contains six experiments consisting of water reflected, type 304L stainless steel spheres partially filled with highly enriched (95.011% Pu-239) plutonium nitrate solutions. The plutonium concentration in the solution is varied (73.0 to 268.7 g/l), as is the height of solution in the spherical tank. The H/Pu-239 ratio varied between 91.2 and 371.3. The isotopic distribution of the plutonium is given in Table 17.

Table 17. Pu Isotopic Distribution for PU-SOL-THERM-001⁵.

Isotope	Weight Percent
²³⁸ Pu	0.006
²³⁹ Pu	95.011
²⁴⁰ Pu	4.668
²⁴¹ Pu	0.305
²⁴² Pu	0.009

The geometry data are given in Table 18. In addition, the heights of the solution above the midline of the spherical tank are 12.9807, 13.3995, 12.9091, 13.2170, 13.2170, and 13.0555 cm for the six cases respectively.

Table 18. Geometry Data for PU-SOL-THERM-001.

Parameter	Dimension (cm)
Solution Outer Radius	14.5603
Tank Outer Radius	14.6848
Reflector Outside Radius	34.6848

The material data for the plutonium solution given in PU-SOL-THERM-001/Table 2 of Reference 5 are used to create weight fractions for the fuel solution constituents for input into MCNP. The resulting weight fractions are given in Table 19, and are consistent with the atom densities presented in PU-SOL-THERM-001/Table 6 of Reference 5.

Table 19. Fuel Material Weight Fractions for PU-SOL-THERM-001.

Case	ρ (g/cc)	²³⁸ Pu	²³⁹ Pu	²⁴⁰ Pu	²⁴¹ Pu	²⁴² Pu	N	H	O
1	1.130	3.8761E-06	6.1379E-02	3.0156E-03	1.9704E-04	5.8142E-06	1.7612E-02	9.6101E-02	8.2169E-01
2	1.219	4.7252E-06	7.4824E-02	3.6762E-03	2.4020E-04	7.0878E-06	3.7637E-02	8.5664E-02	7.9793E-01
3	1.270	5.6220E-06	8.9026E-02	4.3740E-03	2.8579E-04	8.4331E-06	4.4005E-02	8.1023E-02	7.8128E-01
4	1.293	6.1253E-06	9.6995E-02	4.7655E-03	3.1137E-04	9.1879E-06	4.8831E-02	7.7878E-02	7.7122E-01
5	1.307	6.4269E-06	1.0177E-01	5.0002E-03	3.2670E-04	9.6404E-06	4.8671E-02	7.7309E-02	7.6692E-01
6	1.484	1.0864E-05	1.7203E-01	8.4521E-03	5.5225E-04	1.6296E-05	5.2806E-02	6.6142E-02	6.9999E-01

4.2.2.2.2 *Water Reflected 11.5-Inch Diameter Spheres Partly Filled*

This validation contains 11 experiments consisting of water reflected, type 304L stainless steel spheres partially filled with plutonium nitrate solutions with 95.011% Pu-239. As described in Reference 5, however, only eight of these are considered acceptable for validation purposes (cases 1, 4, and 11 are eliminated). The plutonium concentration in the solution is varied (93.5 to 232.0 g/l), as is the height of solution in the spherical tank. The H/Pu-239 ratio varied between 109.6 and 285.0. The isotopic distribution of the plutonium is given in Table 20.

Table 20. Pu Isotopic Distribution for PU-SOL-THERM-007⁵.

Isotope	Weight Percent
²³⁸ Pu	0.006
²³⁹ Pu	95.011
²⁴⁰ Pu	4.668
²⁴¹ Pu	0.305
²⁴² Pu	0.009

The geometry data are given in Table 21. In addition, the heights of the solution above the midline of the spherical tank are 10.8373, 10.8373, 10.9741, 10.6720, 10.9741, 10.9051, 10.4503, and 10.8373 cm for the eight cases respectively.

Table 21. Geometry Data for PU-SOL-THERM-007.

Parameter	Dimension (cm)
Solution Outer Radius	14.5603
Tank Outer Radius	14.6848
Reflector Outside Radius	34.6848

The material data for the fuel solution given in PU-SOL-THERM-007/Table 2 of Reference 5 are used to calculate the weight fractions for the isotopes in the fissile solution for input into MCNP. The resulting weight fractions are given in Table 22, and are consistent with the atom densities presented in PU-SOL-THERM-007/Table 5 of Reference 5.

Table 22. Fuel Material Weight Fractions for PU-SOL-THERM-007.

Case	ρ (g/cc)	^{238}Pu	^{239}Pu	^{240}Pu	^{241}Pu	^{242}Pu	N	H	O
2	1.409	9.8793E-06	1.5644E-01	7.6861E-03	5.0220E-04	1.4819E-05	4.3448E-02	7.2261E-02	7.1964E-01
3	1.386	9.5671E-06	1.5150E-01	7.4432E-03	4.8633E-04	1.4351E-05	4.3729E-02	7.2800E-02	7.2402E-01
5	1.180	5.0949E-06	8.0679E-02	3.9638E-03	2.5899E-04	7.6424E-06	2.3451E-02	9.1005E-02	8.0063E-01
6	1.180	5.1610E-06	8.1726E-02	4.0153E-03	2.6235E-04	7.7415E-06	2.4791E-02	9.0286E-02	7.9891E-01
7	1.179	5.0941E-06	8.0667E-02	3.9632E-03	2.5895E-04	7.6412E-06	2.4889E-02	9.0385E-02	7.9983E-01
8	1.179	5.1705E-06	8.1875E-02	4.0226E-03	2.6283E-04	7.7557E-06	2.7207E-02	8.9224E-02	7.9740E-01
9	1.184	5.1486E-06	8.1530E-02	4.0056E-03	2.6172E-04	7.7230E-06	2.7207E-02	8.9270E-02	7.9772E-01
10	1.165	4.8155E-06	7.6253E-02	3.7464E-03	2.4479E-04	7.2232E-06	2.3365E-02	9.1633E-02	8.0475E-01

4.2.2.2.3 Water Reflected 12-Inch Diameter Spheres

Seven experiments consisting of water reflected, type 347 stainless steel spheres filled with plutonium nitrate solutions (96.88 wt % Pu-239) were evaluated. The plutonium concentration in the solution is varied from 49.84 to 77.09 g/l. The H/Pu-239 ratio varied between 309 and 524. The isotopic distribution of the plutonium is given in Table 23.

Table 23. Pu Isotopic Distribution for PU-SOL-THERM-002⁵.

Isotope	Wt %
^{239}Pu	96.88
^{240}Pu	3.12

The geometry data are given in Table 24.

Table 24. Geometry Data for PU-SOL-THERM-002.

Parameter	Dimension (cm)
Solution Outer Radius	15.3399
Sphere Outer Radius	15.4669
Reflector Outside Radius	45.4669

The material data for the fuel solutions given in PU-SOL-THERM-002/Table 3 of Reference 5 was used to calculate atom density values for the fuel solution constituents for input into MCNP. The calculated values were identical to those presented in PU-SOL-THERM-002/Table 5 of Reference 5 and are reproduced below as Table 25.

Table 25. Fuel Material Atom Densities (atoms/barn-cm) for PU-SOL-THERM-002.

Case	Pu-239	Pu-240	N	H	O	Fe
1	1.2164E-04	3.9010E-06	1.3452E-03	6.3772E-02	3.5500E-02	2.0380E-06
2	1.2549E-04	4.0246E-06	1.5831E-03	6.3356E-02	3.5895E-02	2.9330E-06
3	1.3689E-04	4.3902E-06	2.0104E-03	6.1779E-02	3.6198E-02	2.6419E-06
4	1.4555E-04	4.6680E-06	2.3018E-03	6.1211E-02	3.6660E-02	2.0704E-06
5	1.5456E-04	4.9568E-06	2.6223E-03	6.0707E-02	3.7228E-02	2.1243E-06
6	1.7111E-04	5.4875E-06	3.1274E-03	5.8902E-02	3.7623E-02	2.3507E-06
7	1.8814E-04	6.0338E-06	3.4867E-03	5.8109E-02	3.8160E-02	2.5556E-06

Also included in the MCNP models are water for the reflector and type 347 stainless steel for the sphere material. Water is modeled as a combination of hydrogen and oxygen with atom fractions of 2 and 1, respectively, and a density of 0.99651 g/cc. The material composition of type 347 stainless steel is taken from Reference 5 and is reproduced as Table 26. The density is assumed to be 7.92 g/cc.

Table 26. Type 347 Stainless Steel Weight Fractions.

Element	Weight Fraction
Fe	0.685
Cr	0.180
Ni	0.105
Mn	0.020
Si	0.010

4.2.2.2.4 *Water Reflected 13-Inch Diameter Spheres*

This validation contains eight experiments consisting of water reflected, type 347 stainless steel or type 2S aluminum spheres filled with highly enriched (96.88 to 98.24% Pu-239) plutonium nitrate solutions. The plutonium concentration in the solution is varied (33.32 to 44.09 g/l), with the tanks completely full. The H/Pu-239 ratio varied between 562.8 and 788.0. The isotopic distributions of the plutonium are given in Table 27.

Table 27. Pu Isotopic Distribution for PU-SOL-THERM-003⁵.

Isotope	Weight Percent (Cases 1-2)	Weight Percent (Cases 3-8)
²³⁹ Pu	98.24	96.88
²⁴⁰ Pu	1.76	3.12

The geometry data are given in Table 28. The steel tank is used in cases 1 through 6, while the aluminum tank is used in cases 7 and 8.

Table 28. Geometry Data for PU-SOL-THERM-003.

Parameter	Steel Tank Dimension (cm)	Aluminum Tank Dimension (cm)
Solution Outer Radius	16.5156	16.2487
Tank Outer Radius	16.6426	16.3777
Reflector Outside Radius	46.6426	46.3777

The material data for the plutonium solution given in PU-SOL-THERM-003/Table 3 of Reference 5 are used to calculate the weight fractions for the isotopes in the solution, for input into MCNP. The resulting weight fractions are given in Table 29, and are consistent with the atom densities presented in PU-SOL-THERM-003/Table 5 of Reference 5.

Table 29. Fuel Material Weight Fractions for PU-SOL-THERM-003.

Case	ρ (g/cc)	²³⁹ Pu	²⁴⁰ Pu	N	H	O	Fe
1	1.0853	3.0161E-02	5.4034E-04	1.8046E-02	1.0020E-01	8.5094E-01	1.1425E-04
2	1.1009	3.0626E-02	5.4867E-04	2.3905E-02	9.7614E-02	8.4720E-01	1.0628E-04
3	1.1107	3.2648E-02	1.0514E-03	2.6440E-02	9.6201E-02	8.4356E-01	9.2734E-05
4	1.1279	3.2743E-02	1.0545E-03	3.1244E-02	9.4113E-02	8.4072E-01	1.2501E-04
5	1.1548	3.4103E-02	1.0983E-03	4.0101E-02	9.0103E-02	8.3438E-01	2.2255E-04
6	1.1908	3.5870E-02	1.1552E-03	5.1125E-02	8.5116E-02	8.2651E-01	2.2338E-04
7	1.0910	3.1950E-02	1.0289E-03	1.9277E-02	9.9382E-02	8.4826E-01	1.0449E-04
8	1.1106	3.2110E-02	1.0341E-03	2.5425E-02	9.6707E-02	8.4461E-01	1.1525E-04

4.2.2.2.5 Water Reflected 14-Inch Diameter Spheres

This validation contains 13 experiments consisting of water reflected, type 347 stainless steel spheres filled with plutonium nitrate solutions (96.57 to 99.46% Pu-239). The plutonium concentration in the solution is varied from 26.27 to 39.38 g/l. The H/Pu-239 ratio is varied between 592 and 987. The isotopic distributions of the plutonium are given in Table 30.

Table 30. Pu Isotopic Distribution for PU-SOL-THERM-004⁵.

Isotope	Wt % (Cases 1-4)	Wt % (Case 5)	Wt % (Cases 6-12)	Wt % (Case 13)
²³⁹ Pu	99.46	98.24	96.88	96.57
²⁴⁰ Pu	0.54	1.76	3.12	3.43

The geometry data are given in Table 31.

Table 31. Geometry Data for PU-SOL-THERM-004.

Parameter	Dimension (cm)
Solution Outer Radius	17.7865
Sphere Outer Radius	17.9135
Reflector Outside Radius	47.9135

The material data for the fuel solution given in PU-SOL-THERM-004/Table 3 of Reference 5 are used to calculate atom density values for the fuel solution constituents for input into MCNP. The calculated values were identical to those presented in PU-SOL-THERM-004/Table 5 of Reference 5 and are reproduced below as Table 32.

Table 32. Fuel Material Atom Densities (atoms/barn-cm) for PU-SOL-THERM-004.

Case	Pu-239	Pu-240	N	H	O	Fe
1	6.5821E-05	3.5587E-07	7.5562E-04	6.4964E-02	3.4503E-02	1.5636E-06
2	6.5921E-05	3.5641E-07	1.0392E-03	6.4397E-02	3.4929E-02	1.6067E-06
3	6.8151E-05	3.6847E-07	1.3354E-03	6.3697E-02	3.5324E-02	1.6822E-06
4	7.0381E-05	3.8053E-07	1.8211E-03	6.2562E-02	3.5975E-02	1.7684E-06
5	6.8256E-05	1.2177E-06	1.0635E-03	6.4299E-02	3.4947E-02	1.0136E-06
6	6.9800E-05	2.2385E-06	8.4885E-04	6.4732E-02	3.4632E-02	1.1862E-06
7	7.2167E-05	2.3144E-06	1.0635E-03	6.4353E-02	3.4984E-02	1.3803E-06
8	7.3095E-05	2.3442E-06	1.3889E-03	6.3518E-02	3.5382E-02	1.2185E-06
9	7.7122E-05	2.4733E-06	2.0202E-03	6.2101E-02	3.6260E-02	1.2940E-06
10	8.6298E-05	2.7676E-06	3.0060E-03	5.9494E-02	3.7440E-02	1.5636E-06
11	9.6109E-05	3.0823E-06	3.9626E-03	5.6870E-02	3.8540E-02	1.5851E-06
12	7.1850E-05	2.3043E-06	1.1169E-03	6.4144E-02	3.5013E-02	1.2185E-06
13	7.1207E-05	2.5186E-06	1.0810E-03	6.4304E-02	3.5002E-02	1.5096E-06

Also included in the MCNP models are water for the reflector, and type 347 stainless steel for the sphere material. Water is modeled as a combination of hydrogen and oxygen with atom fractions of 2 and 1, respectively, and a density of 0.99651 g/cc. The material composition of type 347 stainless steel is taken from Reference 3. The density is assumed to be 7.92 g/cc.

4.2.2.2.6 *Water Reflected 14-Inch Diameter Spheres with 4.05% and 4.40% ²⁴⁰Pu*

This validation contains nine experiments consisting of water reflected, type 347 stainless steel spheres filled with highly enriched (95.6 to 95.95% Pu-239) plutonium nitrate solutions. The plutonium concentration in the solution is varied (29.65 to 40.91 g/l), with the tanks completely full. The H/Pu-239 ratio varied between 580.6 and 902.8. The isotopic distributions of the plutonium are given in Table 33.

Table 33. Pu Isotopic Distribution for PU-SOL-THERM-005⁵.

Isotope	Weight Percent (Cases 1-7)	Weight Percent (Cases 8-9)
²³⁹ Pu	95.95	95.60
²⁴⁰ Pu	4.05	4.40

The geometry data is given in Table 34.

Table 34. Geometry Data for PU-SOL-THERM-005.

Parameter	Dimension (cm)
Solution Outer Radius	17.7865
Tank Outer Radius	17.9135
Reflector Outside Radius	47.9135

The material data for the plutonium solution given in PU-SOL-THERM-005/Table 3 of Reference 5 are used to calculate the weight fractions for the isotopes in the solution, for input into MCNP. The resulting weight fractions are given in Table 35, and are consistent with the atom densities presented in PU-SOL-THERM-005/Table 5 of Reference 5.

Table 35. Fuel Material Weight Fractions for PU-SOL-THERM-005.

Case	ρ (g/cc)	²³⁹ Pu	²⁴⁰ Pu	N	H	O	Fe
1	1.0777	2.6398E-02	1.1142E-03	1.8339E-02	1.0048E-01	8.5355E-01	1.1877E-04
2	1.0967	2.6719E-02	1.1278E-03	2.4573E-02	9.7752E-02	8.4976E-01	7.2034E-05
3	1.1117	2.7127E-02	1.1450E-03	2.9830E-02	9.5430E-02	8.4639E-01	7.7359E-05
4	1.1496	2.7994E-02	1.1816E-03	4.1403E-02	9.0321E-02	8.3901E-01	8.4377E-05
5	1.1826	2.9241E-02	1.2342E-03	5.2033E-02	8.5569E-02	8.3183E-01	8.7942E-05
6	1.2172	3.0341E-02	1.2807E-03	6.2209E-02	8.1032E-02	8.2503E-01	1.0352E-04
7	1.2405	3.1643E-02	1.3356E-03	7.0091E-02	7.7460E-02	8.1937E-01	1.0157E-04
8	1.1019	2.6531E-02	1.2211E-03	2.5933E-02	9.7174E-02	8.4904E-01	9.8013E-05
9	1.1205	2.7174E-02	1.2507E-03	3.1853E-02	9.4536E-02	8.4510E-01	9.1031E-05

4.2.2.2.7 Water Reflected 15-Inch Diameter Spheres

This validation contains three experiments consisting of water reflected, type 347 stainless steel spheres filled with plutonium nitrate solutions (96.88 % Pu-239). The plutonium concentration in the solution is varied from 24.80 to 26.97 g/l. The H/Pu-239 ratio varied between 940 and 1061. The isotopic distributions of the plutonium are given in Table 36.

Table 36. Pu Isotopic Distribution for PU-SOL-THERM-006⁵.

Isotope	Wt %
---------	------

²³⁹ Pu	96.88
²⁴⁰ Pu	3.12

The geometry data are given in Table 37.

Table 37. Geometry Data for PU-SOL-THERM-006.

Parameter	Dimension (cm)
Solution Outer Radius	19.0416
Sphere Outer Radius	19.1686
Reflector Outside Radius	49.1686

The material data for the fuel solution given in PU-SOL-THERM-006/Table 3 of Reference 5 are used to calculate atom density values for the fuel solution constituents for input into MCNP. The calculated values were identical to those presented in PU-SOL-THERM-006/Table 5 of Reference 5 and are reproduced below as Table 38.

Table 38. Fuel Material Atom Densities (atoms/barn-cm) for PU-SOL-THERM-006.

Case	Pu-239	Pu-240	N	H	O	Fe
1	6.0526E-05	1.9411E-06	1.1266E-03	6.4225E-02	3.5054E-02	9.4892E-07
2	6.2381E-05	2.0006E-06	1.4277E-03	6.3492E-02	3.5444E-02	1.0136E-06
3	6.5822E-05	2.1109E-06	2.0590E-03	6.1880E-02	3.6223E-02	1.0352E-06

Also included in the MCNP models are water for the reflector and type 347 stainless steel for the tank material. Water is modeled as a combination of hydrogen and oxygen with atom fractions of 2 and 1, respectively, and a density of 0.99651 g/cc. The material composition of type 347 stainless steel is taken from Reference 5. The density is assumed to be 7.92 g/cc.

4.2.2.3 Water Reflected 9-, 10-, 11-, and 12-Inch Diameter Cylinders

This validation contains 14 experiments consisting of water reflected, type 347 stainless steel cylinders filled with plutonium nitrate solutions at 97.10 to 97.15% Pu-239. The plutonium concentration in the solution is varied (31.14 to 99.09 g/l), the diameter of the cylindrical tanks are varied (9 to 12 in), and the critical solution heights are varied (8.80 to 17.55 in). The H/Pu-239 ratio varied between 266.9 and 849.7. The isotopic distributions of the plutonium are given in Table 39.

Table 39. Pu Isotopic Distribution for PU-SOL-THERM-010⁵.

Isotope	Weight Percent (Cases 1-8)	Weight Percent (Cases 9-14)
²³⁹ Pu	97.15	97.10
²⁴⁰ Pu	2.85	2.90

The type 347 stainless steel tanks are 0.1575 cm thick. Immediately above the critical liquid surface in the tanks, a tamper is positioned to provide reflection. The tamper is a type 347 stainless steel cylinder (with no top) containing a 30.48 cm height of water. An empty, type 347 stainless steel tube runs through the middle of the tamper with inner and outer radii of 1.0465 and 1.3335 cm, respectively. The tank itself extends 97.9488 cm above the inner surface of the floor of the tank. Above the tamper, the tank is empty. Surrounding the tank and this empty region radially is at least 30 cm of water, providing infinite reflection. An identical amount of water is present below the tank, as well. Geometry data on critical heights, tank radii, and tamper radii are presented in Table 40.

Table 40. Geometry Data for PU-SOL-THERM-010.

Case	Critical Height (cm)	Tamper		Tank	
		IR (cm)	OR (cm)	IR (cm)	OR (cm)
1	30.7086	11.1419	11.2994	11.4264	11.5839
2	35.4076	11.1419	11.2994	11.4264	11.5839
3	44.5770	11.1419	11.2994	11.4264	11.5839
4	25.6032	13.6839	13.8414	13.9684	14.2910 ^G
5	28.1686	13.6839	13.8414	13.9684	14.2910 ^G
6	27.0764	13.6839	13.8414	13.9684	14.1259
7	32.6390	13.6839	13.8414	13.9684	14.1259
8	43.0022	13.6839	13.8414	13.9684	14.1259
9	22.8092	13.6839	13.8414	13.9684	14.1259
10	25.9588	13.6839	13.8414	13.9684	14.1259
11	22.3520	14.9545	15.1120	15.2390	15.3965
12	25.2476	14.9545	15.1120	15.2390	15.3965

^G In these two experiments, a 0.065" layer of stainless steel is placed around the cylindrical tank. The ends of the tank are not affected.

13	28.4734	14.9545	15.1120	15.2390	15.3965
14	33.4264	14.9545	15.1120	15.2390	15.3965

The material data for the fuel solution given in PU-SOL-THERM-010/Table 3 of Reference 5 are used to create weight fractions for the fuel solution constituents for input into MCNP. The resulting weight fractions are given in Table 41, and are equivalent to the atom densities presented in PU-SOL-THERM-010/Table 5 of Reference 5.

Table 41. Fuel Material Weight Fractions for PU-SOL-THERM-010.

Case	ρ (g/cc)	^{239}Pu	^{240}Pu	N	H	O	Fe
1	1.1997	8.0242E-02	2.3540E-03	2.5702E-02	9.0291E-02	8.0109E-01	3.1508E-04
2	1.1592	6.1951E-02	1.8174E-03	2.4476E-02	9.3222E-02	8.1833E-01	1.9928E-04
3	1.1329	4.6761E-02	1.3718E-03	2.3888E-02	9.5456E-02	8.3229E-01	2.2685E-04
4	1.1329	4.6676E-02	1.3693E-03	2.3928E-02	9.5450E-02	8.3235E-01	2.2685E-04
5	1.1202	4.0943E-02	1.2011E-03	2.3594E-02	9.6341E-02	8.3768E-01	2.4549E-04
6	1.1202	4.0943E-02	1.2011E-03	2.3594E-02	9.6341E-02	8.3768E-01	2.4549E-04
7	1.1604	3.4937E-02	1.0249E-03	4.1854E-02	8.9250E-02	8.3271E-01	2.1975E-04
8	1.2022	2.9819E-02	8.7477E-04	5.6371E-02	8.3656E-02	8.2906E-01	2.1877E-04
9	1.1483	5.4110E-02	1.6160E-03	2.3823E-02	9.4517E-02	8.2567E-01	2.5951E-04
10	1.1360	4.1866E-02	1.2504E-03	2.7641E-02	9.4476E-02	8.3456E-01	2.0951E-04
11	1.1260	4.2039E-02	1.2556E-03	2.3332E-02	9.6313E-02	8.3686E-01	1.9805E-04
12	1.1152	3.6822E-02	1.0997E-03	2.5644E-02	9.6002E-02	8.4028E-01	1.5603E-04
13	1.1077	3.2013E-02	9.5611E-04	2.1841E-02	9.8272E-02	8.4677E-01	1.4535E-04
14	1.1028	2.7418E-02	8.1888E-04	2.3352E-02	9.8222E-02	8.5005E-01	1.3874E-04

4.2.2.4 Reflected Slabs of Plutonium Nitrate ($\text{Pu}(\text{NO}_3)_4$) Solutions

Thirteen experiments were conducted in a stainless steel slab tank with a 130-cm square base. Critical solution heights were determined for various plutonium nitrate solution compositions. The tank was either fully reflected by water on all six sides or reflected by water on only five sides. The plutonium concentration ranged in this experiment from 13.2 to 105 g/l. The H/Pu-239 ratio varied between 309.08 and 2573.31. The isotopic distributions of the plutonium are given in Table 42.

Table 42. Pu Isotopic Distribution for PU-SOL-THERM-012⁵.

Isotope	Wt %
^{239}Pu	74.20
^{240}Pu	18.88

The geometrical data are listed below:

- 1) The tank, 130 x 130 x 100 cm inside dimensions, 0.5 cm wall thickness,
- 2) The water around the tank, in reflected configurations (calculations indicate that a 25 cm thickness is enough),
- 3) The Lucoflex box:
 - floating on the nitrate solution, full of water, in cases of full water reflection positioned at the top (80 cm between the bottom of the tank and the lower Lucoflex face):
 - empty in cases of water reflection on five sides
 - empty or full of water in cases of no close water reflection
- 4) The steel pool wall and concrete room wall, ceiling, and floor (calculations indicate that a 50-cm thickness for the concrete is enough) for configurations without close water reflection. The pool is centered in the room.

The fuel material densities are given in Table 43.

Table 43. Fuel Material Atom Densities (atoms/barn-cm) for PU-SOL-THERM-012.

Case	Pu-239	Pu-240	N	H	O	Fe
1	3.68825E-05	9.34548E-06	1.41344E-03	6.34983E-02	3.53933E-02	4.96028E-06
2	3.31381E-05	8.39670E-06	1.38481E-03	6.36291E-02	3.53758E-02	4.42112E-06
3	3.12659E-05	7.92231E-06	1.38532E-03	6.36398E-02	3.53767E-02	4.09762E-06
4	2.75215E-05	6.97353E-06	1.37017E-03	6.36186E-02	3.53176E-02	3.88196E-06
5	2.47132E-05	6.26195E-06	1.37165E-03	6.35948E-02	3.53011E-02	3.55846E-06
6	1.96582E-04	4.98109E-05	2.51393E-03	6.07598E-02	3.72502E-02	2.48014E-05
7	1.57266E-04	3.98488E-05	2.07086E-03	6.19361E-02	3.66145E-02	2.02724E-05
8	9.86655E-05	2.50004E-05	1.78497E-03	6.24015E-02	3.59564E-02	1.21850E-05
9	5.97235E-05	1.51330E-05	1.56626E-03	6.29542E-02	3.55707E-02	7.54825E-06
10	5.03624E-05	1.27611E-05	1.52854E-03	6.30426E-02	3.54927E-02	6.36209E-06
11	4.06270E-05	1.02943E-05	1.41749E-03	6.36500E-02	3.54903E-02	5.39161E-06
12	3.68825E-05	9.34548E-06	1.41344E-03	6.34983E-02	3.53933E-02	4.96028E-06
13	2.47132E-05	6.26195E-06	1.37165E-03	6.35948E-02	3.53011E-02	3.55846E-06

4.2.3 Bias and Uncertainty

Table 44 gives a summary of the evaluated experiments and the associated average k_{eff} from each set.

Table 44. Computed k_{eff} Values for Plutonium Solutions.

Experiment	Description	Avg k_{eff}
PU-SOL-THERM-001	11.5" Water-reflected Spheres	1.0107
PU-SOL-THERM-002	12" Water-reflected Spheres	1.0113
PU-SOL-THERM-003	13" Water-reflected Spheres	1.0117
PU-SOL-THERM-004	14" Water-reflected Spheres	1.0094
PU-SOL-THERM-005	15" Water-reflected Spheres of 4.05% and 4.40% ^{240}Pu	1.0105
PU-SOL-THERM-006	15" Water-reflected Spheres	1.0092
PU-SOL-THERM-007	11.5" Water-reflected partially-filled spheres	1.0070
PU-SOL-THERM-009	48" Unreflected Spheres	1.0224
PU-SOL-THERM-010	9, 10, 11, and 12" Water-reflected Cylinders	1.0160
PU-SOL-THERM-011	16" Unreflected Spheres	1.0200
PU-SOL-THERM-011	18" Unreflected Spheres	1.0050
PU-SOL-THERM-012	Pu slabs-reflected	1.0130

The 48-inch spheres calculate significantly higher results than the other experiments. Slab experiments approaching the H/Pu-239 ratios represented by the spheres calculate lower, but their higher Pu-240 content may cloud the comparison. The 48-inch results were used in this validation; however, caution should be used when using bias results with H/Pu-239 greater than 2000 until the number of data points in this region has been increased.

The handbook⁵ recommends not using the 16-inch spheres for validation if the resulting k_{eff} 's are higher than the results of similar experiments. The average values for these cases are approximately 1.5 % higher than the average of the 18-inch cases. Therefore, the results from the 16-inch spheres are not included in the bias calculations.

Some of the 18-inch cadmium reflected spheres calculate values lower than the results from the other experiments. The average k_{eff} of 1.0050 for these spheres is 0.0072 lower than the average k_{eff} for the rest of the experiments. This result does not appear to be the result of the cadmium shell around the spheres. Removal of the shell from the experimental models results in a statistically insignificant change in the k_{eff} . These

experiments were retained because their net effect would be to reduce the positive bias (conservative). The inclusion of the cadmium reflected spheres in this validation should not be considered an adequate test of the cadmium cross sections (i.e., its presence is not statistically significant).

A computational bias is determined by statistically analyzing the calculated k_{eff} values from the benchmark experiments. In accordance to Reference 4, a Chi-square test is performed to determine if the data are normally distributed. This distribution is determined to be non-normal. The plot of the k_{eff} values versus the H/Pu ratio is shown in Figure 2.

Figure 2. K_{eff} versus H/Pu Ratio.

A non-parametric upper subcritical limit was calculated due to the non-normal distribution of the data and the poor fit of the trendline to the data series ($R^2 = 0.0957$). An attempt to fit this data to the curves specified in Reference 4 also failed. With a data set of 91, there is a 99.1% confidence that 95% of the data lies above the smallest value as suggested by Equation 2.

$$\beta = 1 - (q)^n \quad (2)$$

where q = desired population fraction (normally 0.95)
 n = number of data samples

The non-parametric margin for this level of confidence is 0.0 (see section 2.9.1 of Reference 4). Therefore, the upper subcritical limit can be calculated from Equation 3 as follows:

$$k_{\text{limit}} = \text{smallest } k_{\text{eff}} \text{ value} - \text{bias uncertainty} - \text{non-parametric margin} \quad (3)$$

$$= 1.0000 - \sqrt{(0.0052)^2 + (0.0012)^2} - 0.0 = 0.9947$$

(Note: 1.0 is the maximum acceptable smallest value for k_{eff} ; i.e., positive bias is not allowed)

The upper subcritical limit for the plutonium solution systems is 0.994.

4.2.4 Limitations

The data used in this validation covers a broad spectrum of materials with various Pu-240 contents. The Pu-240 content ranged from 0.54-18.91%, with the majority of the experiments having Pu-240 content of 2.5-4.7 %. Thirteen experiments had a Pu-240 content near 19%.

The upper subcritical limit developed is applicable to unreflected and water reflected systems of plutonium nitrate solutions as evaluated on the WSMS DEC Alpha workstation. These results are not applicable to plutonium metal systems or to plutonium solution systems with significant non-water reflectors. Use of these results with systems containing different reflectors requires additional analysis and justification.

Use of the results with H/Pu-239 ratios above 2000 is strongly cautioned and requires the use of an area of applicability margin (AOA)⁴. The results in this region are based on two sets of experiments that span a range of 1.4 % of k_{eff} . Additional analysis and justification are recommended prior to using the results from this region.

5.0 URANIUM SYSTEMS

5.1 Uranium Metal (Fast)⁶

5.1.1 Area of Applicability

This section presents the MCNP validation analysis for reflected and unreflected highly enriched uranium metal systems. The result from this analysis is an upper subcritical limit for the MCNP code system with the ENDF/B-V cross section library. The MCNP user should employ the F-4 flux tally to obtain the average energy to assure that the evaluated system is contained within the applicable neutron spectrum. Key areas of applicability for these experiments include:

1. Fuel:	Highly enriched uranium metal
2. Moderation:	H/U-235: ~ 0
3. Enrichment:	~37% U-235 for IEU, ~90-97% U-235 for HEU
4. Moderating Material:	Polyethylene, Plexiglas, Teflon, Ti, Al, and steel
5. Reflector Material:	Bare, water, U-238, Polyethylene, Paraffin, Lucite, Tungsten Carbide, Steel, Al, or Tuballoy
6. Geometry:	Single spherical units, arrays of cylinders, slabs, pseudo-spheres, cylinders, parallelepipeds
7. Neutron Spectrum ^H :	Intermediate-Fast; 2.0 eV – 1.5 MeV
AEG: 4.84-15.81

5.1.2 System Description

One hundred and thirty uranium metal critical experiments were extracted from the International Handbook of Evaluated Criticality Benchmark Experiments for this evaluation. The experiments were divided into two categories: single unit systems, and array systems. The single unit systems used in this report include two experiments from HEU-MET-FAST-001⁵, six from HEU-MET-FAST-002⁵, eleven from HEU-MET-FAST-003⁵, one from HEU-MET-FAST-004⁵, and forty-three from HEU-MET-FAST-007⁵. Also included are thirteen single unit systems from Russian experiments. The array systems consist of 22 experiments from HEU-MET-FAST-023⁵ and 32 from HEU-MET-FAST-026⁵. The experimental configurations for these experiments are described in the following sections.

5.1.2.1 Single Unit Systems

The single unit experiment sets contain five different configuration systems. Four experiment sets (HEU-MET-FAST-001, -002, -003, and -004) were performed at Los Alamos National Laboratory (LANL). The next experiment set (HEU-MET-FAST-007)

^H The neutron spectrum represents the average energy of the neutrons causing fission.

was performed at the Oak Ridge National Laboratory (ORNL). The last experimental sets (HEU-MET-FAST-012^s, -013^s, -021^s, -022^s, -024^s, -033^s, -034^s, -035^s, and IEU-MET-FAST-005^s and -006^s) were performed at the Russian Federal Nuclear Institutes of Technical Physics (VNIITF and VNIIEF).

5.1.2.1.1 *Unreflected HEU Spheres*

Two experiments involved unreflected uranium spheres. The first, referred to as Godiva, was performed with a bare uranium sphere. The second experiment was a Shell Model involving layers of uranium with gaps of air. Both experiments consisted of two identical sets of nested oralloy hemispheres. In this setup, a 0.015-inch-thick diaphragm of stainless steel supported the upper hemisphere, while the lower hemisphere rested on a thin-wall aluminum cylinder. A summary of the experimental parameters for these experiments is provided in Table 47.

Table 47. Reported Parameters for HEU-MET-FAST-001.

Benchmark Descriptor	Composition	U Isotopic Composition (wt %)			Sphere Radius (cm)
		234	235	238	
Godiva	HEU	1.02	93.71	5.27	8.7407
Shell Model:					
Shell 1	HEU	1.02	93.26	5.72	1.0216
Shell 2	Air gap	-	-	-	1.0541
Shell 3	HEU	1.02	93.90	5.08	6.2809
Shell 4	Air gap	-	-	-	6.2937
Shell 5	HEU	1.02	93.95	5.03	7.7525
Shell 6	Air gap	-	-	-	7.7620
Shell 7	HEU	1.02	93.58	5.40	8.2527
Shell 8	Air gap	-	-	-	8.2610
Shell 9	HEU	1.02	93.89	5.09	8.7062
Shell 10	HEU	1.02	93.86	5.12	8.7499

5.1.2.1.2 *Natural Uranium-Reflected Pseudosphere, Pseudocylinder, and Parallelepipeds*

Six experiments involving tuballoy-reflected critical assemblies were run on the Topsy machine. This set of oralloy assemblies includes a pseudosphere, a pseudocylinder, and four parallelepipeds. The density of oralloy in all six assemblies is 18.75 g/cm³, and it is composed of 93.5 wt % U-235, 1.02 wt % U-234, and 5.48 wt % U-238. The tuballoy reflector has a density of 18.90 g/cm³, and is composed of 0.0055 at % U-234, 0.72 at % U-235, and 99.2745 at % U-238. A summary of the experimental parameters for these experiments is provided in Table 48.

Table 48. Reported Parameters for HEU-MET-FAST-002.

Configuration	Region	Width (cm)	Depth (cm)	Height (cm)	Radius (cm)	Material
Sphere	1	-	-	-	6.0509	Oralloy
	2	-	-	-	26.3709	Tuballoy
Cylinder	1	-	-	11.43	5.1706	Oralloy
	2	-	-	52.07 ¹	25.4906	Tuballoy
4x4x3.66 Inch Parallelepiped	1	10.16	10.16	9.3	-	Oralloy
	2	50.80	50.80	49.94	-	Tuballoy
5x5x2.53 Inch Parallelepiped	1	12.70	12.70	6.415	-	Oralloy
	2	53.34	53.34	47.0550	-	Tuballoy
3x3x7.56 Inch Parallelepiped	1	7.62	7.62	19.1970	-	Oralloy
	2	48.26	48.26	59.8370	-	Tuballoy
3x3.5x6 Inch Parallelepiped	1	7.62	8.89	15.2344	-	Oralloy
	2	48.26	49.53	55.8744	-	Tuballoy

Table 49 lists the atom densities for the different isotopes.

Table 49. Atom Densities.

Material	Isotope	Concentration (atoms/barn-cm)
Oralloy	²³⁴ U	4.9210×10^{-4}
	²³⁵ U	4.4917×10^{-2}
	²³⁸ U	2.5993×10^{-3}
Tuballoy	²³⁴ U	2.6299×10^{-6}
	²³⁵ U	3.4428×10^{-4}
	²³⁸ U	4.7470×10^{-2}

¹ 20.32 cm above and below region 1.

5.1.2.1.3 Unmoderated, Reflected HEU Spheres

Twelve experiments, taken from HEU-MET-FAST-003, involved unmoderated, reflected spherical assemblies. The setup included seven spherical oralloy assemblies reflected by tuballoy, four spherical oralloy assemblies reflected by tungsten carbide, and one spherical oralloy assembly reflected by nickel. The density of the oralloy was 18.75 g/cm³, with constituents of 1.02 wt % U-234, 93.5 wt % U-235, and 5.48 wt % U-238. The density of the tuballoy was 18.90 g/cm³. Tables 50 and 51 contain the isotopic abundance for the uranium and tungsten reflectors.

Table 50. Isotopic Abundance (at %) for Uranium Reflector.

Isotope	Abundance (at %)
²³⁴ U	0.0055
²³⁵ U	0.72
²³⁸ U	99.2745

Table 51. Isotopic Abundance (at %) for Tungsten Reflector.

Isotope	Abundance (at %)
¹⁸⁰ W	0.12
¹⁸² W	26.3
¹⁸³ W	14.28
¹⁸⁴ W	30.7
¹⁸⁶ W	28.6

A summary of the experimental parameters for these experiments is provided in Table 52. Region 1 refers to the spherical oralloy, while region 2 denotes the reflector.

Table 52. Reported Parameters for HEU-MET-FAST-003.

Reflector Thickness (in.)	Region	Outer Radius (cm.)	Material
2.0	1	6.7820	Oralloy
	2	11.8620	Tuballoy
3.0	1	6.4423	Oralloy
	2	14.0623	Tuballoy
4.0	1	6.2851	Oralloy
	2	16.4451	Tuballoy
5.0	1	6.1535	Oralloy
	2	18.8535	Tuballoy
7.0	1	6.0740	Oralloy
	2	23.8540	Tuballoy
8.0	1	6.0509	Oralloy
	2	26.3709	Tuballoy
11.0	1	6.0276	Oralloy
	2	33.9676	Tuballoy
1.9	1	6.6020	Oralloy
	2	11.4280	Tungsten Carbide
2.9	1	6.2527	Oralloy
	2	13.6187	Tungsten Carbide
4.5	1	6.0509	Oralloy
	2	17.4809	Tungsten Carbide
6.5	1	6.0159	Oralloy
	2	22.5259	Tungsten Carbide
8.0	1	6.4627	Oralloy
	2	26.7827	Nickel

Table 53 gives the atom densities for the four different reflectors.

Table 53. Atom Densities.

Material	Isotope	Concentration (atoms/barn-cm)
Oralloy	^{234}U	4.9210×10^{-4}
	^{235}U	4.4917×10^{-2}
	^{238}U	2.5993×10^{-3}
Tuballoy	^{234}U	2.6299×10^{-6}
	^{235}U	3.4428×10^{-4}
	^{238}U	4.7470×10^{-2}
Tungsten Carbide (WC)	^{182}W	1.2697×10^{-2}
	^{183}W	6.8626×10^{-3}
	^{184}W	1.4754×10^{-2}
	^{18}W	1.3744×10^{-2}
Nickel	C	4.8057×10^{-2}
	Ni	9.1322×10^{-2}

Seven experiments containing unmoderated, reflected spheres were also performed at the Russian facilities. A description of each is listed below in Table 54.

Table 54. Description of Russian Experiments.

Handbook I.D.	Experiment Description
HEU-MET-FAST-012	This experiment, conducted at the Russian Federal Nuclear Center Institute of Technical Physics (VNIITF), was a two-unit assembly consisting of twelve spherical layers of highly enriched uranium and an aluminum reflector. The bottom reflector has one shell; the reflector on the top hemisphere has three shells. In the experiment, top part of the assembly rested on a steel diaphragm while the lower part was raised into a critical configuration.
HEU-MET-FAST-013	This experiment, conducted at VNIITF, was a two-unit assembly consisting of nine spherical layers of highly enriched uranium and a four-layer aluminum reflector. The top part of the assembly rested on a steel diaphragm, while the lower part was raised into a critical configuration.
HEU-MET-FAST-021	This experiment, conducted at VNIIEF, was a two-unit assembly consisted of seven spherical layers of highly enriched uranium with a central cavity and steel reflector. The upper unit consisted of a hemispherical steel shell resting on a steel diaphragm, and the movable lower unit incorporated the remainder of the core and reflector.

Table 54. Description of Russian Experiments (continued).

Handbook I.D.	Experiment Description
HEU-MET-FAST-022	This experiment, conducted at VNIIEF, consisted of two units: an upper unit composed of a hemispherical shell of highly enriched uranium and three hemispherical shells of the Duralumin reflector, and a movable lower unit containing the remainder of the core and reflector. An aluminum diaphragm supported the upper unit.
HEU-MET-FAST-024	This experiment, performed at VNIITF, was a two-unit assembly consisting of ten spherical layers of highly enriched uranium, a single-layer steel reflector, and a three-layer polyethylene reflector.
IEU-MET-FAST-005	This critical experiment, conducted at VNIIEF, consisted of two units: an upper unit comprised of three hemispherical shells of steel reflector on a steel diaphragm, and the movable lower unit containing the remainder of the core and reflector.
IEU-MET-FAST-006	This critical experiment, conducted at VNIIEF, consisted of two units: an upper unit comprised of five hemispherical shells of Duralumin reflector on a steel diaphragm, and the movable lower unit containing the remainder of the core and reflector.

Table 55 gives the material composition and dimensions for the evaluated experiments.

Table 55. Uranium Metal System Compositions and Dimensions.

Handbook I.D.	Core Material Composition and Density (wt %, g/cc)	Uranium Isotopic Composition (wt %)	Core Material	Core Radius (cm)	Reflector Material	Reflector Thickness (cm)
HEU-MET-FAST-012	U=99.2626 C=0.0428 Fe=0.0698 W=0.0211 Cu=0.4226 Ni=0.1811 Density=17.9924	^{234}U =1.1369 ^{235}U =89.5982 ^{236}U =0.1931 ^{238}U =9.0772	Uranium Metal	9.15	Aluminum	Top=2.85 Bottom=1.7
HEU-MET-FAST-013	U=99.2538 C=0.0443 Fe=0.0698 W=0.0211 Cu=0.4277 Ni=0.1833 Density=17.9924	^{234}U =1.1362 ^{235}U =89.6324 ^{236}U =0.1941 ^{238}U =9.0730	Uranium Metal	8.38	steel	3.65
HEU-MET-FAST-021 (average values used in the simplified benchmark model)	U=99.6921 C=0.1185 Fe=0.098 W=0.0914 Density=18.38	^{234}U =1.1045 ^{235}U =89.49 ^{238}U =9.4064	Uranium Metal	7.55	steel	9.7
HEU-MET-FAST-022 (average values used in the simplified benchmark model)	U=99.7072 C=.1137 Fe=.0933 W=.0858 Density=18.4	^{234}U =1.104 ^{235}U =89.4927 ^{238}U =9.403	Uranium Metal	8.35	Duralumin	3.9
HEU-MET-FAST-024	U=99.2144 C=0.0447 Fe=0.0733 W=0.0210 Cu=0.4525 Ni=0.1939 Density=18.0044	^{234}U =1.1298 ^{235}U =89.5252 ^{236}U =0.1970 ^{238}U =9.0502	Uranium Metal	7.55	Steel and CH ₂	0.8 and 9.65, respectively
IEU-MET-FAST-005 (average values used in the simplified benchmark model)	U=99.5429 C=.0703 Fe=.062 W=.0178 Cu=.1535 Ni=.1535 Density=18.42	^{234}U =.3287 ^{235}U =36.5129 ^{238}U =63.1575	Uranium Metal	13.25	steel	8.25
IEU-MET-FAST-006 (average values used in the simplified benchmark model)	U=99.5435 C=.0702 Fe=.0621 W=.0178 Cu=.1532 Ni=.1532 Density=18.43	^{234}U =.3288 ^{235}U =36.5122 ^{238}U =63.1586	Uranium Metal	13.25	Duralumin	11.75

5.1.2.1.4 Water-Reflected HEU Sphere

One experiment involved a water-reflected uranium sphere consisting of two hemispheres of highly enriched uranium. The hemispheres were joined together using a small pin of enriched uranium to form a near-uniform sphere with a radius of 6.5537 cm. The sphere was placed on a plexiglas stand inside a cylindrical aluminum tank. Input files were used to perform calculations for both, one-dimensional and three dimensional, idealizations of the system. The one-dimensional experimental procedure omits the plexiglas stand, and uses a spherical water reflector that preserves the volume of the actual cylindrical reflector. The 1-D idealization was not included in the validation, as there were no experimental results with which to compare it against. The geometrical dimensions and materials and the isotopic concentrations are shown in Tables 56 and 57, respectively.

Table 56. Geometrical Dimensions and Material for HEU-MET-FAST-004.

Item	Hemisphere 1	Hemisphere 2	Pin
Net Mass (kg)	11.335	11.336	0.013
Uranium Mass (kg)	11.328	11.331	0.013
²³³ U (wt %)	<0.01	<0.01	<0.01
²³⁴ U (wt %)	1.17	1.05	1.04
²³⁵ U (wt %)	97.67	97.68	97.67
²³⁶ U (wt %)	0.20	0.20	0.21
²³⁸ U (wt %)	0.95	1.06	1.07

Table 57. Isotopic Concentrations for HEU-MET-FAST-004.

Material	Isotope	Atom Density (atoms/barn-cm)
HEU	²³⁴ U	5.3678×10^{-4}
	²³⁵ U	4.7033×10^{-2}
	²³⁶ U	9.5896×10^{-5}
	²³⁸ U	4.7782×10^{-4}
Plexiglas	¹ H	5.7745×10^{-2}
	¹² C	3.6090×10^{-2}
	¹⁶ O	1.4435×10^{-2}
Water	¹ H	6.6807×10^{-2}
	¹⁶ O	3.3403×10^{-2}

5.1.2.1.5 *Moderated, Reflected and Unreflected HEU Slabs*

Forty-three of the experiments involved moderated slabs of highly enriched uranium metal (1.07 wt % U-234, 93.15 wt % U-235, 0.68 wt % U-236, and 5.10 wt % U-238). The unreflected experiments consisted of uranium metal slabs interleaved with polyethylene, Plexiglas, or Teflon. Some of the experiments being moderated by polyethylene also had a six-inch polyethylene reflector. Densities of the three moderator types are shown in Table 58.

Table 58. Densities of Moderators in HEU-MET-FAST-007.

Moderator	Density (g/cm³)
Polyethylene (CH ₂)	0.92
Plexiglas (C ₅ O ₂ H ₈)	1.18
Teflon (CF ₂)	2.17

The experiments were performed on the Split Table Apparatus, which consists of two cast iron bench plates, one stationary and one moveable. Table 59 contains the parameters for these forty-three experiments.

Table 59. Experimental Parameters for HEU-MET-FAST-007.

Case Number	Height (cm)	Material (kg)		Number of Cells	Cell Layer Thickness (cm)		Basic Assembly Features
		Uranium	Plastic		Uranium	Plastic	
1	8.722	104.001	-	1	4.3610	-	Unreflected, Polyethylene Moderated, Base Dimensions 25.4 x 25.4 cm
2	9.545	99.660	0.7142	4	1.04144	0.30340	
3	9.771	97.756	0.9384	3	1.36267	0.53176	
4	9.898	95.929	1.1177	5	0.80032	0.37908	
5	10.251	93.975	1.4073	7	0.56137	0.34174	
6	10.401	92.089	1.6070	3	1.27965	0.90778	
7	10.401	92.089	1.6090	6	0.63962	0.45432	
8	10.424	92.055	1.6083	8	0.48077	0.34146	
9	10.427	92.021	1.6183	4	0.96169	0.68328	
10	11.689	76.687	3.0944	5	0.64219	1.05342	
11	12.921	64.300	4.4132	8	0.33717	0.94076	
12	13.007	61.444	4.5931	8	0.32268	0.98056	
13	13.000	61.444	4.5931	4	0.64497	1.95998	
14	13.165	61.444	4.6831	8	0.32277	1.00006	
15	12.715	61.333	4.4733	4	0.64024	1.89830	
16	12.758	61.333	4.4953	4	0.64050	1.90856	
17	14.211	46.058	6.0803	6	0.32152	1.72550	
18	14.328	46.058	6.1478	6	0.32156	1.74488	
19	12.355	74.095	-	1	6.1775	-	Unreflected, Polyethylene Moderated, Base Dimensions 12.7 x 25.4 cm
20	15.730	71.721	1.1121	5	1.19605	0.75392	
21	15.931	71.721	1.1699	5	1.19640	0.79334	
22	16.132	71.721	1.2277	5	1.19675	0.83278	
23	17.750	68.879	1.8390	4	1.43819	1.56098	
24	17.915	68.879	1.8852	4	1.43886	1.60094	
25	19.759	66.959	2.5234	5	1.11882	1.71404	
26	19.964	66.959	2.5812	5	1.11935	1.75414	
27	10.140	99.712	1.3717	4	1.04059	0.45372	Unreflected, Plexiglas Moderated, Base Dimensions 25.4 x 25.4 cm
28	10.996	95.921	2.2778	5	0.79891	0.60130	
29	11.831	92.063	3.1701	6	0.63780	0.69628	
30	14.514	76.692	6.1834	5	0.63719	1.62832	
31	18.395	61.403	10.0897	8	0.31899	1.66134	Unreflected, Teflon Moderated, Base Dimensions 25.4 x 25.4 cm
32	11.908	109.189	3.881	6	0.75962	0.46534	
33	14.709	114.991	6.963	6	0.80546	0.84060	
34	17.770	120.709	10.460	6	0.84775	1.26612	
35	5.362	31.771	-	1	2.681	-	Polyethylene Reflected and Moderated, Base Dimensions 12.7 x 25.4 cm
36	6.307	30.664	0.3553	4	0.63837	0.30056	
37	7.120	28.728	0.6716	6	0.40219	0.38222	
38	7.351	28.646	0.7410	12	0.20074	0.21108	
39	7.427	28.646	0.7640	12	0.19982	0.21666	
40	7.242	28.641	0.7240	5	0.47836	0.49158	
41	8.674	22.968	1.4141	6	0.32105	0.80356	
42	8.809	22.968	1.4488	6	0.32165	0.82482	
43	10.688	15.712	2.3558	11	0.12003	0.73160	

5.1.2.2 Multiple Unit Systems

Six critical experiments were evaluated at the Russian experimental facility VNIITF in 1986. These experiments consisted of uranium metal in hemicylinders comprised of alternating materials. In 1962 and 1963 a set of detailed criticality experiments utilizing highly enriched uranium metal cylinders was conducted at the Oak Ridge Critical Experimental Facility (CEF). Critical arrays of uranium metal cylinders were constructed on a split table apparatus. The surface-to-surface spacing (STS) between the units were measured as a function of the number of units and the thickness of a paraffin reflector. These experiments are referred to as Tinkertoy experiments. HEU-MET-FAST-023 (Tinkertoy 1) provides a detailed description of the experimental configuration for 22 evaluated benchmark experiments developed from these experiments. HEU-MET-FAST-026 (Tinkertoy 2) provides a detailed description of the experimental configuration for 32 evaluated benchmark experiments developed from these experiments. Table 60 contains the material composition for both experiments.

Table 60. Uranium Metal Composition (18.76 g/cm³).

Isotope	Wt %
U-234	1.0
U-235	93.2
U-236	0.2
U-238	5.6

Details on the benchmark specifications used in validation model development are provided in the following paragraphs.

5.1.2.2.1 *Hemicylinders*

Six critical experiments involving hemicylinders of uranium metal were performed at the Russian facilities. Tables 61 and 62 provide the experimental descriptions and dimensions, respectively.

Table 61. Description of Russian Experiments.

Handbook I.D.	Experiment Description
HEU-MET-FAST-033	These two critical experiments, conducted at VNIITF, consisted of two hemicylinders of alternating HEU, steel, and polyethylene disks separated by a gap that yielded a critical configuration. The top hemicylinder rested on a steel diaphragm supported by a Duralumin tripod and the movable bottom half rested in a Duralumin cone.
HEU-MET-FAST-034	These three critical experiments, conducted at VNIITF, consisted of two hemicylinders of alternating HEU, polyethylene, and either steel, titanium, or aluminum disks separated by a gap that yielded a critical configuration. The top hemicylinder rested on a steel diaphragm supported by a Duralumin tripod and the movable bottom half rested in a Duralumin cone.
HEU-MET-FAST-036	This critical experiment, conducted at VNIITF, consisted of two hemicylinders of alternating HEU, polyethylene, and titanium disks, separated by a gap that yielded a critical configuration, and reflected on all sides by polyethylene. The top hemicylinder rested on a steel diaphragm and the movable bottom half rested on a steel disk.

Table 62. Uranium Metal System Compositions and Dimensions.

Handbook I.D.	Core Material Composition and Density (wt %, g/cc)	Uranium Isotopic Composition (wt %)	Core Material	Core Radius (cm)	Reflector Material	Reflector Thickness (cm)
HEU-MET-FAST-033	U=99.9896 C=.008 Fe=.009 W=.0015 Density=18.5892	²³⁴ U=1.18 ²³⁵ U=95.95 ²³⁸ U=2.84	Uranium Metal with CH ₂ and steel	9.995	None	N/A
HEU-MET-FAST-034	U=99.9815 C=.008 Fe=.009 W=.021 Density=18.5887	²³⁴ U=1.18 ²³⁵ U=95.96 ²³⁸ U=2.84	Uranium Metal with CH ₂ and Al, Ti, and steel	9.995	none	N/A
HEU-MET-FAST-036	U=99.9815 C=.008 Fe=.009 W=.021 Density=18.5887	²³⁴ U=1.1798 ²³⁵ U=95.9603 ²³⁸ U=2.8395	Uranium Metal with CH ₂ and Ti	9.995	CH ₂	Bottom=9.94 Top=9.94 Side=9.393

5.1.2.2.2 *Tinkertoy 1*

Arrays were built using cylinders of uranium metal with paraffin blocks set up as reflector walls. Two stainless steel rods passed through each cylinder and through the paraffin to support and space the units in the array. The benchmark dimensions are given in Table 63.

Table 63. Benchmark Array Dimensions for HEU-MET-FAST-023.

Case #	Array	Cylinder Diameter, D (cm)	Cylinder Height, H (cm)	Cylinder Spacing, STS ¹ (cm)	Reflector Thickness, RTH (cm)
2	2x2x2	11.506	5.382	0.229	1.3
3	2x2x2	11.506	5.382	1.981	3.8
4	2x2x2	11.506	5.382	3.416	7.6
5	2x2x2	11.506	5.382	3.696	15.2
6	3x3x3	11.509	5.382	2.007	0.0
7	3x3x3	11.509	5.382	2.992	1.3
8	3x3x3	11.509	5.382	5.872	3.8
9	3x3x3	11.509	5.382	8.258	7.6
10	3x3x3	11.509	5.382	8.689	15.2
12	2x2x2	9.116	8.641	0.602	1.3
13	2x2x2	9.116	8.641	2.362	3.8
14	2x2x2	9.116	8.641	3.97	7.6
15	2x2x2	9.116	8.641	4.308	15.2
16	3x3x3	9.116	8.641	2.436	0.0
17	3x3x3	9.116	8.641	3.426	1.3
18	3x3x3	9.116	8.641	6.579	3.8
19	3x3x3	9.116	8.641	9.017	7.6
20	3x3x3	9.116	8.641	9.434	15.2
21	4x4x4	11.481	5.382	3.952	0.0
22	4x4x4	11.481	5.382	12.36	15.2
28	3x3x3	11.506	5.382	1.349	0.0
29	3x3x5	11.494	5.382	3.442	0.0

Several arbitrary materials were used in the validation models. Arbitrary materials for the 0.88 g/cm³ and 0.93 g/cm³ paraffin were modeled as compounds (C₂₅H₅₂) with the appropriate density (0.88 g/cm³ for 1.3 cm thick paraffin and 0.93 g/cm³ for all other paraffin thickness).

¹ Surface-to-Surface spacing of uranium units in vertical and horizontal directions.

5.1.2.2.3 Tinkertoy 2

These experiments were performed using cylinders in four mass groups and with different height-to-diameter ratios. The experiments reported include cylinders with approximate masses of 15, 20, and 25 kg. Table 64 lists the experimental array parameters.

Table 64. Benchmark Array Parameters for HEU-MET-FAST-026.

Case #	Array	Cylinder Diameter, D (cm)	Cylinder Height, H (cm)	Cylinder Spacing, STS ^k (cm)	Reflector Thickness, RTH (cm)
1	2x2x2	11.494	8.077	0.902	0
2	2x2x2	11.494	8.077	1.905	1.3
3	2x2x2	11.494	8.077	4.961	3.8
4	2x2x2	11.494	8.077	7.391	7.6
5	2x2x2	11.494	8.077	7.823	15.2
6	3x3x3	11.490	8.077	4.204	0
7	3x3x3	11.490	8.077	5.677	1.3
8	3x3x3	11.490	8.077	10.190	3.8
9	3x3x3	11.490	8.077	13.693	7.6
10	3x3x3	11.490	8.077	14.194	15.2
11	2x2x2	11.464	10.765	2.217	0
12	2x2x2	11.506	10.765	2.248	0
13	2x2x2	11.506	10.765	3.678	1.3
14	2x2x2	11.506	10.765	5.710	2.5
15	2x2x2	11.506	10.765	8.207	3.8
16	2x2x2	11.506	10.765	11.509	7.6
17	2x2x2	11.506	10.765	11.986	15.2
18	3x3x3	11.484	10.765	6.363	0
19	3x3x3	11.484	10.765	8.574	1.3
20	3x3x3	11.484	10.765	14.764	3.8
21	3x3x3	11.484	10.765	18.720	7.6
22	3x3x3	11.484	10.765	19.147	15.2
23	2x2x2	11.509	13.459	3.543	0
24	2x2x2	11.509	13.459	5.423	1.3
25	2x2x2	11.509	13.459	11.532	3.8
26	2x2x2	11.509	13.459	15.697	7.6
27	2x2x2	11.509	13.459	16.378	15.2
28	3x3x3	11.486	13.459	8.494	0
29	3x3x3	11.486	13.459	11.323	1.3
30	3x3x3	11.486	13.459	19.606	3.8
31	3x3x3	11.486	13.459	24.498	7.6
32	3x3x3	11.486	13.459	24.991	15.2

^k Surface-to-Surface spacing of uranium units in vertical and horizontal directions.

5.1.3 Bias and Uncertainty

The distribution of the data for the fast uranium experiments was determined to be non-normal. Figure 3 provides a plot of the calculated k_{eff} values versus the average energy groups.

Figure 3. K_{eff} versus Average Energy Group.

A non-parametric upper subcritical limit was calculated due to the non-normal distribution of the data and the poor fit of the trendline to the data series ($R^2 = 0.0512$). An attempt to fit this data to the curves specified in Reference 4 also failed. With a data set of 128, there is a 99.8% confidence that 95% of the data lies above the smallest value (see Equation 2 on page 33).

The non-parametric margin for this level of confidence is 0.0 (see section 2.9.1 of Reference 4). Therefore, the upper subcritical limit can be calculated from Equation 3 on page 34.

$$= 0.9863 - \sqrt{(0.0012)^2 + (0.0010)^2} - 0.0 = 0.9847$$

The upper subcritical limit for the uranium metal systems is 0.984.

5.1.4 Limitations

These results were obtained using MCNP version 4B running on the WSMS DEC Alpha Workstation. They are applicable to bare and reflected highly enriched uranium metal systems with the average energy of the fissioning neutrons from 2.0 eV to 1.5 MeV. The results cover an intermediate to fast average fission energy range and are not applicable to systems containing significant interstitial moderation (i.e., H/U-235 ratio $\neq$ 0) or those for which the average energy group is in the thermal range.

As can be seen in the tables in this section, the majority of the evaluated experiments have U-238 content near 5 %. A subcritical margin as low as 0.02 may be appropriate for those experiments. Use of this bias with cases having U-238 significantly different from 5 % requires use of the area of applicability margin (AOA)⁴.

5.2 Research Reactor Fuel

5.2.1 Area of Applicability

This section presents the MCNP validation analysis for the SPERT-D fuel element experiment (HEU-MET-THERM-006⁵). It is important to note that the plates and water gaps in the SPERT-D fuel element were modeled explicitly in all experiments. The results of this analysis present a weighted (including statistical and experimental uncertainties), single-sided lower tolerance limit. The MCNP user should employ the F-4 flux tally to obtain the average energy to assure that the evaluated system is contained within the applicable neutron spectrum. Key areas of applicability for these experiments include:

1. Fuel:	MTR type fuel (uranium-aluminum alloy)
2. Moderation:	H/U-235 ~ 140 (fully flooded fuel assembly)
3. Enrichment:	High (93.5 wt % U-235)
4. Moderating Material:	Water
5. Reflector Material:	Water
6. Geometry:	Lattices of SPERT-D fuel elements
7. Neutron Spectrum ^L :	Thermal; 0.069 – 0.146 eV
AEG: (18 energy bin structure)12.89-13.31

5.2.2 System Description

Twenty-three critical experiments involving lattices of SPERT-D fuel elements were performed at the Oak Ridge National Laboratory (ORNL). The SPERT-D fuel element consists of a 3-inch square aluminum container, 0.062 inches thick and 27.625 inches long. The container holds a maximum of 22 fuel plates; each plate containing an average of 13.93 grams of U-235. The fuel is a uranium-aluminum alloy with 23.8 wt % uranium and the isotopic mixture contains 93.17 wt % of U-235. Fourteen of the twenty-three experiments were deemed acceptable for validation purposes.

5.2.3 Bias and Uncertainty

The Shapiro-Wilk⁴ test is used to determine if the distribution is normal. This test assumes that the data are normally distributed and calculates the test statistic for normality. If the value of the test statistic falls under a critical value, the distribution of the data is not normal. We applied the Shapiro-Wilk test to 13 out of the 14 data points. For these experiments, the data is determined to be normal from the evaluation of this test. One data point was considered an outlier due to its magnitude and therefore was excluded in the normalcy test calculation. Figure 4 provides a plot of the k_{eff} values versus the average energy group.

^L The neutron spectrum represents the average energy of the neutrons causing fission.

HEU-MET-THERM

Figure 4. K_{eff} versus Average Energy Group.

Due to the undesirable fit of the data to the independent variable, a lower tolerance limit was determined for the data set using Equation 1 on page 13. For the lower tolerance limit calculation, all 14 data points were taken into account.

A single-sided lower tolerance limit of 0.976 is calculated for the 14 thermal uranium experiments.

Table 65 lists the results from the statistical analysis of the 14 data points.

Table 65. Results from Statistical Analysis.

	All 14 Experiments (WEIGHTED DATA)
One-sided Lower Tolerance Factor (U)	2.614
Sqrt of Pooled Variance (Sp)	9.901E-03
Variance About the Mean (S²)	7.989E-05
Average Uncertainty (σ²)	1.814E-05
Average k_{eff}	1.0026
Lower Tolerance Limit	0.976

5.2.4 Limitations

Although the parameters of the benchmark experiments do not completely envelop MIT type fuel, the applicability parameters are considered sufficient for analysis of MIT type fuel in flooded conditions. Use of this bias with cases extended outside the area of applicability listed in section 5.2.1 requires the use of an area of applicability margin (AOA). A subcritical margin of 0.05 is to be used unless there is justification to use a smaller safety margin.

5.3 Uranium Solution⁷

5.3.1 Area of Applicability

This section presents the MCNP validation analysis for reflected and unreflected highly enriched uranium solutions. The result from this analysis is a lower tolerance limit for the MCNP-4B code system with the ENDF/B-V cross section library. The MCNP user should employ the F-4 flux tally to obtain the average energy to assure that the evaluated system is contained within the applicable neutron spectrum. Key areas of applicability for these experiments include:

1. Fuel:	Highly enriched uranium solutions
2. Moderation:	H/U-235: ~50-1300
3. Enrichment:	High, 80-92.3 wt % U-235 ^M
4. Moderating Material:	Water
5. Reflecting Material:	Concrete, Plexiglas, Water or None (with Al or Steel Containers or Sleeves)
6. Geometry:	Single Unit Spheres, Cylinders, and Arrays of Cylinders
7. Neutron Spectrum ^N :	Thermal; 0.051 – 0.68 eV
AEG: 21.47-24.99

5.3.2 System Description

In support of this validation, seventy-four critical uranyl nitrate experiments involving bare and concrete or Plexiglas reflected single cylinders or arrays of cylinders were extracted from the International Handbook of Evaluated Criticality Benchmark Experiments. In addition, eleven critical uranium oxyfluoride experiments involving single water reflected spheres were extracted from draft reports issued in Reference 5.

5.3.2.1 Single Unit Unreflected Cylinders of Uranyl Nitrate

Ten of the experiments utilized single bare cylinders of uranyl nitrate. A summary of the experimental parameters from Reference 5 is provided in Table 66. The isotopic composition of the uranium used in the experiments is provided in Table 67.

^M See limitations (Sect. 5.3.4)

^N The neutron spectrum represents the average energy of the neutrons causing fission.

Table 66. Reported Single Unit Cylinder Parameters (HEU-SOL-THERM-001⁵).

Experiment Descriptor	Tank Composition	Critical Height (cm)	Inner Diameter (cm)	Uranium Concentration (g/l)	Molarity (Excess Nitric Acid – moles/L)	Solution Density (g/cm ³)
1	304 SS	31.20	27.92	145.68	0.294	1.2038
2	304 SS	28.93	27.92	346.73	0.542	1.4800
3	6061 Al	33.55	28.01	142.92	0.283	1.2007
4	6061 Al	30.91	28.01	357.71	0.549	1.4951
5	6061 Al	39.48	33.01	54.89	0.105	1.0758
6	6061 Al	36.67	33.01	59.65	0.114	1.0825
7	6061 Al	23.96	33.01	137.40	0.287	1.1923
8	6061 Al	23.67	33.01	145.68	0.294	1.2038
9	6061 Al	22.53	33.01	357.71	0.549	1.4951
10	6061 Al	20.48	50.69	63.95	0.111	1.0883

Table 67. Uranium Isotopic Composition.

Isotope	Wt %
²³⁴ U	1.022
²³⁵ U	93.172
²³⁶ U	0.434
²³⁸ U	5.372

5.3.2.2 Single Unit Concrete-Reflected Cylinders of Uranyl Nitrate

Fourteen of the experiments utilized single concrete-reflected cylinders of uranyl nitrate. A summary of the experimental parameters from Reference 5 is provided in Table 68. The isotopic composition of the uranium present matches the composition of that found in Table 67. The composition of the concrete used in the experimental models is provided in Table 69. Cylinder position was varied within a ~10-inch-thick concrete box. The inside dimensions of this box formed a rough cube (122 cm per side).

Table 68. Reported Single Unit Cylinder Parameters (HEU-SOL-THERM-002⁵).

Experiment Descriptor	Tank Composition	Critical Height (cm)	Inner Diameter (cm)	Uranium Concentration (g/l)	Molarity (Excess Nitric Acid – moles/L)	Solution Density (g/cm ³)
1	304 SS	29.79	27.92	144.38	0.272	1.2023
2	304 SS	24.19	27.92	144.38	0.272	1.2023
3	304 SS	27.23	27.92	334.77	0.521	1.4636
4	304 SS	21.79	27.92	334.77	0.521	1.4636
5	6061 Al	31.37	28.01	144.38	0.272	1.2023

6	6061 Al	24.70	28.01	144.38	0.272	1.2023
7	6061 Al	28.60	28.01	334.77	0.521	1.4636
8	6061 Al	22.33	28.01	334.77	0.521	1.4636
9	6061 Al	34.10	33.01	59.65	0.114	1.0825
10	6061 Al	27.27	33.01	59.65	0.114	1.0825
11	6061 Al	22.85	33.01	144.38	0.272	1.2023
12	6061 Al	18.24	33.01	144.38	0.272	1.2023
13	6061 Al	21.50	33.01	334.77	0.521	1.4636
14	6061 Al	16.78	33.01	334.77	0.521	1.4636

Table 69. Concrete Composition ($\rho = 2.321 \text{ g/cm}^3$).

Isotope	Wt %
H	0.75
K	1.37
Si	15.50
S	0.19
Na	0.63
Ti	0.1
Ca	23.0
C	5.52
N	0.02
O	48.49
Mg	1.25
Al	2.17
Fe	1.01

5.3.2.3 Single Unit Plexiglas-Reflected Cylinders of Uranyl Nitrate

Nineteen of the experiments utilized single Plexiglas-reflected cylinders of uranyl nitrate. A summary of the experimental parameters from Reference 5 is provided in Table 70. The isotopic composition of the uranium present matches the composition of that found in Table 67. The composition of the Plexiglas used in the experimental models is

provided in Table 71. Cylinder position was varied within ~ 8-inch-thick Plexiglas box. The inside dimensions of this box formed a rough cube (122 cm per side).

Table 70. Reported Single Unit Cylinder Parameters (HEU-SOL-THERM-003⁵).

Experiment Descriptor	Tank Composition	Critical Height (cm)	Inner Diameter (cm)	Uranium Concentration (g/l)	Molarity (Excess Nitric Acid – moles/L)	Solution Density (g/cm ³)
1	304 SS	50.52	27.93	60.32	0.113	1.0837
2	304 SS	67.48	27.93	60.32	0.113	1.0837
3	304 SS	29.71	27.92	147.66	0.271	1.2069
4	304 SS	25.03	27.92	147.66	0.271	1.2069
5	304 SS	27.60	27.92	345.33	0.534	1.4779
6	304 SS	22.75	27.92	345.33	0.534	1.4779
7	6061 Al	51.67	27.88	60.32	0.133	1.0837
8	6061 Al	31.26	28.01	147.66	0.271	1.2069
9	6061 Al	25.26	28.01	147.66	0.271	1.2069
10	6061 Al	28.84	28.01	345.33	0.534	1.4779
11	6061 Al	22.87	28.01	345.33	0.534	1.4779
12	6061 Al	34.33	33.01	60.32	0.113	1.0837
13	6061 Al	27.70	33.01	60.32	0.113	1.0837
14	6061 Al	31.75	33.01	60.32	0.113	1.0837
15	6061 Al	25.10	33.01	66.33	0.120	1.0920
16	6061 Al	22.78	33.01	147.66	0.271	1.2069
17	6061 Al	18.49	33.01	147.66	0.271	1.2069
18	6061 Al	21.67	33.01	345.33	0.534	1.4779
19	6061 Al	17.20	33.01	345.33	0.534	1.4779

Table 71. Plexiglas Composition, wt % (ρ side panels = 1.1863 g/cm³, ρ top and bottom panels = 1.286 g/cm³).

Element	Top and Bottom Panels (Fire Retardant)	Four Side Panels (Non-Fire Retardant)
Hydrogen	7.18	8.03
Carbon	52.68	59.72
Nitrogen	0.10	Not measured
Oxygen	29.4	32.14
Phosphorous	1.54	Not measured
Chlorine	1.63	Not measured
Bromine	6.5	Not measured
Ash	0.71	Not measured

5.3.2.4 Concrete-Reflected Arrays of Uranyl Nitrate Cylinders

Seventeen of the experiments utilized concrete-reflected arrays of uranyl cylinders. A summary of the experimental parameters from Reference 5 is provided in Table 72. Arrays of various sizes were placed with a ~10 inch-thick concrete box that was used for the experiments. The inside dimensions of this box formed a rough cube (122 cm per side). The isotopic composition of the uranium matches the composition contained in Table 67. The composition of the concrete used in the experimental models is provided above in Table 69.

Table 72. Reported Concrete-Reflected Array Parameters (HEU-SOL-THERM-007⁵).

Experiment Descriptor (array size)	Tank Composition	Critical Height (cm)	Inner Diameter (cm)	Uranium Concentration (g/l)	Molarity (Excess Nitric Acid – moles/L)	Solution Density (g/cm ³)
1(4x4x1)	6061 Al	28.63	21.12	67.28	0.128	1.0934
2(4x4x1)	6061 Al	17.24	21.12	369.96	0.598	1.5120
3(4x4x1)	6061 Al	27.15	21.12	67.28	0.128	1.0934
4(4x4x1)	6061 Al	17.13	21.12	364.11	0.584	1.5054
5(2x2x1)	6061 Al	60.70	21.12	76.09	0.137	1.1057
6(2x2x1)	6061 Al	29.49	21.12	360.37	0.585	1.4995
7(2x2x1)	6061 Al	62.34	21.12	76.09	0.137	1.1057
8(2x2x1)	6061 Al	31.11	21.12	364.11	0.584	1.5054
9(2x2x1)	6061 Al	57.88	21.12	80.72	0.143	1.1122
10(4x4x1)	6061 Al	57.34	16.12	83.49	0.151	1.1164
11(4x4x1)	6061 Al	32.32	16.12	360.37	0.585	1.4995
12(4x4x1)	6061 Al	51.21	16.12	83.49	0.151	1.1164
13(4x4x1)	6061 Al	31.82	16.12	359.55	0.578	1.4984
14(2x4x1)	6061 Al	51.45	16.12	359.55	0.578	1.4984
15(2x3x1)	6061 Al	65.49	16.12	359.55	0.578	1.4984
16(2x2x1)	6061 Al	101.45	16.12	359.55	0.578	1.4984
17(2x2x1)	6061 Al	104.04	16.12	359.55	0.578	1.4984

5.3.2.5 Plexiglas-Reflected Arrays of Uranyl Nitrate Cylinders

Fourteen of the experiments utilized single Plexiglas-reflected cylinders of uranyl nitrate. A summary of the experimental parameters from Reference 5 is provided in Table 73. The isotopic composition of the uranium matches the composition of that contained in Table 67. The composition of the Plexiglas used in the experimental models is identical to that provided in Table 71. Arrays of various sizes were placed with a ~8 inch-thick Plexiglas box that was used for the experiments. The inside dimensions of this box formed a rough cube (122 cm per side).

Table 73. Reported Plexiglas-Reflected Array Parameters (HEU-SOL-THERM-008⁵).

Experiment Descriptor (array size)	Tank Composition	Critical Height (cm)	Inner Diameter (cm)	Uranium Concentration (g/l)	Molarity (Excess Nitric Acid – moles/L)	Solution Density (g/cm ³)
1(4x4x1)	6061 Al	34.82	21.12	60.32	0.113	1.0837
2(4x4x1)	6061 Al	19.27	21.12	355.94	0.494	1.4925
3(4x4x1)	6061 Al	31.76	21.12	60.32	0.113	1.0837
4(4x4x1)	6061 Al	18.82	21.12	355.94	0.494	1.4925
5(2x2x1)	6061 Al	110.20	21.12	60.32	0.113	1.0837
6(2x2x1)	6061 Al	31.93	21.12	355.94	0.494	1.4925
7(2x2x1)	6061 Al	102.29	21.12	60.32	0.113	1.0837
8(2x2x1)	6061 Al	33.20	21.12	355.94	0.494	1.4925
9(4x4x1)	6061 Al	105.85	16.12	60.32	0.113	1.0837
10(4x4x1)	6061 Al	38.10	16.12	355.94	0.494	1.4925
11(4x4x1)	6061 Al	78.40	16.12	60.32	0.113	1.0837
12(4x4x1)	6061 Al	35.56	16.12	355.94	0.494	1.4925
13(2x3x1)	6061 Al	95.20	16.12	355.94	0.494	1.4925
14(2x3x1)	6061 Al	89.78	16.12	355.94	0.494	1.4925

5.3.2.6 Uranium Oxyfluoride (UO₂F₂) Solution Experiments

These experiments utilized single water-reflected spheres of uranium oxyfluoride. A summary of the experimental parameters is provided in Table 74. The isotopic composition of the uranium is provided in Table 75. For all cases the spheres were reflected by at least 15 cm of water.

Table 74. Reported UO₂F₂ Experiment Parameters.

Descriptor	Solution Density (g/cc)	Uranium Concentration (g/l)	H/U-235	Radius (cm)	²³⁵ U Mass (kg)
HEU-SOL-THERM-009⁵					
1	1.79495	696	36	11.5177	4.15
2	1.62055	543	47	11.4695	3.20
3	1.40045	349	76	11.5177	2.08
4	1.23955	213	126	11.8442	1.37
HEU-SOL-THERM-011⁵					
1	1.0597	53	523	15.9572	0.84
2	1.0596	52	533	15.9569	0.83
HEU-SOL-THERM-012⁵					
1	1.0265	22	1272	27.9244	1.87
HEU-SOL-THERM-010⁵					
1	1.1159	102	270	13.2123	0.92
2	1.1136	104	264	13.2187	0.94
3	1.1015	109	246	13.2359	0.99
4	1.096	112	239	13.2418	1.01

Table 75. Uranium Isotopic Composition.

Isotope	wt % (HEU-SOL-THERM-009,-011, -012)	wt % (HEU-SOL-THERM-010)
U-234	0.98	1.1
U-235	93.18	93.13
U-236	0.50	0.50
U-238	5.34	5.27

5.3.3 Bias and Uncertainty

Figure 5 provides a plot of the calculated k_{eff} values versus the AEG for this group.

Figure 5. K_{eff} versus Average Energy Group.

The data was determined to be normal by the Chi-squared test as outlined in Reference 4. The poor coefficient of fit for the linear regression proves that no trend can be established in the data. An attempt to fit this data to the curves specified in Reference 4 also failed. Therefore, a lower tolerance limit was calculated using Equation 1 on page 13.

A single-sided lower tolerance limit of 0.994 was calculated for the 85 experiments.

Table 76 summarizes the results from the statistical analysis for this group.

Table 76. Results from Statistical Analysis.

	All 85 Experiments (WEIGHTED DATA)
One-sided Lower Tolerance Factor (U)	2.065
Sqrt of Pooled Variance (Sp)	5.597E-03
Variance About the Mean (S²)	1.904E-05
Average Uncertainty (σ^2)	1.228E-05
Average k_{eff}	1.0060
Lower Tolerance Limit	0.994

5.3.4 Limitations

The material data of the experiments used in this evaluation are limited in two fashions. First, the experimental data are limited to a small range of uranium enrichment. The majority of the experiments are enriched to ~93 %, while six experiments had an enrichment of 80%. Second, the reflector materials are limited to Plexiglas, water, and concrete. The lower tolerance limits developed in this evaluation are applicable to those reflectors and enrichments mentioned. Further justification is necessary if other reflectors or uranium enrichments are to be used.

Care should be used to determine the importance of concrete or Plexiglas to the system being modeled. Concrete and Plexiglas compositions vary. For the concrete, water and iron content can have significant effect on calculated k_{eff} values. Using different MCNP standard concrete compositions can cause variations of up to 0.005 in k_{eff} . For Plexiglas, many older chemical analyses did not measure chlorine, which can also have a major effect.

5.4 Uranium Compounds (Low Enrichment)⁸

5.4.1 Area of Applicability

This section presents the MCNP validation analysis for the low enriched uranium fuel experiments. The results of this analysis present a weighted, (including statistical and experimental uncertainties) single-sided lower tolerance limit for the MCNP-4B code system with the ENDF/B-V cross section libraries. The MCNP user should employ the F-4 flux tally to obtain the average energy to assure that the evaluated system is contained within the applicable neutron spectrum. Key areas of applicability for these experiments include:

1. Fuel:	Uranium
2. Moderation:	H/U-235: 100-1400
3. Enrichment:	Low (2-10 wt % U-235)
4. Moderating Material:	Water
5. Reflecting Material:	Steel, Lead, Water or None
6. Geometry:	Thin Rod Lattices, Spheres and Cylinders
$22 < 4 V/S < 80$
7. Neutron Spectrum ^o :	Thermal; 0.051 – 0.34 eV
AEG: 21.84-23.61

5.4.2 System Description

In support of this validation, seventy-one low enriched uranium fuel experiments were marked as acceptable and extracted from the International Handbook of Evaluated Criticality Benchmark Experiments. This validation consisted of low enriched compounds and solutions and is detailed further in the following paragraphs.

5.4.2.1 UO₂ Rods at 2.35 % and 4.31 % U-235

These critical experiments (described in LEU-COMP-THERM-001⁵, 002⁵, 010⁵ and 017⁵) are a series of measurements performed at Pacific Northwest Laboratory (PNL) in the late sixties. They consist of UO₂ rod lattices at various pitches, various separations between lattice blocks, and with different reflectors. From the four evaluations 51 measurements were chosen. These include measurements with water, steel and lead reflectors and at lattice pitches of 1.684, 1.892, 2.032, and 2.54 cm. The fuel rods were a nominal 1.27 cm diameter and 92 cm long and arranged in relatively large arrays, e.g. 13x8 to 25x18. LEU-COMP-THERM-017⁵ has 29 benchmark experiments but only 19 are included in

^o The neutron spectrum represents the average energy of the neutrons causing fission.

this validation. The other 10 experiments had uranium reflectors and consequently, were not considered for this validation.

5.4.2.2 UO_2F_2 Solutions at 5 %

Four measurements with UO_2F_2 solutions are reported in LEU-SOL-THERM-001⁵ and 002⁵. One experiment in LEU-SOL-THERM-001, SHEBA-II at Los Alamos National Lab, consists of an isolated stainless steel cylinder with an empty central steel thimble. The three measurements in LEU-SOL-THERM-002 were done at Oak Ridge National Laboratory and include two water-reflected spheres and one bare sphere.

5.4.2.3 Uranium Nitrate Solutions at 10 %

The evaluations LEU-SOL-THERM-003⁵ and 004⁵ describe experiments with uranium nitrate solutions at a nominal enrichment of 10 % U-235. In LEU-SOL-THERM-003 there are nine measurements made in bare spherical geometry at the Solution Critical Facility of the Institute of Physics and Power Engineering in Obninsk Russia. The evaluation of LEU-SOL-THERM-004 contains descriptions of seven experiments in water-reflected cylinders performed with the Static Experimental Critical Facility (STACY) at the Nuclear Fuel Cycle Safety Engineering Research Facility in the Tokai Research Establishment of the Japan Atomic Energy Research Institute.

5.4.3 Bias and Uncertainty

In Table 77, the resulting k_{eff} values are grouped by the nominal U-235 enrichment.

Table 77. Calculated k_{eff} Values.

	Number	Avg. k_{eff}	σ
All Cases	71	0.9985	0.0042
2%	27	0.9971	0.0028
5%	28	1.0006	0.0049
10%	16	0.9973	0.0036

The data is determined to be normal from the Chi-square test. Figure 6 contains the plot of all 71 data points versus the average energy group.

Figure 6. K_{eff} versus H/U Ratio.

No trends are apparent, and the coefficient of regression for the fit is poor ($R^2 = 0.0347$). Since the data is accepted as normal and the correlation coefficient is close to zero, a single-sided lower tolerance limit is established. Equation 1 on page 13 was used to determine the lower tolerance limit.

A single-sided lower tolerance limit of 0.986 is calculated for the 71 experiments.

Table 78 gives the results from the statistical analysis

Table 78. Results from Statistical Analysis.

	All 71 Experiments (WEIGHTED DATA)
One-sided Lower Tolerance Factor (U)	2.065 ^p
Sqrt. of Pooled Variance (Sp)	5.42E-03
Variance About the Mean (S²)	2.12E-05
Average Uncertainty (σ^2)	8.18E-06
Average k_{eff}	0.9985
Lower Tolerance Limit	0.986

5.4.4 Limitations

Since no clear-cut trend in the average k_{eff} values appear with respect to enrichment, no extrapolation to higher enrichments is possible even though the data is normally distributed. The values computed with MCNP (version 4B on the WSMS DEC Alpha workstation) appear to have a downward trend with increasing enrichment. However, extrapolations to higher enrichments would need to be carefully examined and may require the use of an area of applicability margin (AOA)⁴. With this in mind, the lower tolerance band is computed, but its use for extrapolation to higher enrichments can not be conservatively recommended.

^p This is the tolerance factor for 50 data points; therefore, it is conservative for this data set.

6.0 REFERENCES

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9. WSRC-RP-99-00564, "Software Configuration and Control Guidance for MCNP-4B on the WSRC DFS Workstation System (U)." B.T. Baranko, June 30, 1999.
10. WSRC-RP-99-00563, "WSRC MCNP-4B Test Report (U)." B.T. Baranko, June 30, 1999.

APPENDIX A**Table A-1. Parameters Used in Pu Metal Validation Calculations.**

Experimental Descriptor Case Number(Input File)	Exp. k_{eff}	$\sigma_{exp.}$	Calculated Results (all k_{eff} values normalized to Exp. values)		
			K_{eff}	σ_s	AEG (27gr)
PU-MET-FAST-001					
1 (pu-mt001)	1	0.0020	0.9969	0.0006	4.22
PU-MET-FAST-002					
1 (pu-mt002)	1	0.0020	0.9987	0.0006	4.22
PU-MET-FAST-003					
101 (pu-mt003)	1	0.0030	1.0063	0.0006	4.25
102 (pu-mt004)	1	0.0030	0.9990	0.0007	4.82
103 (pu-mt005)	1	0.0030	1.0030	0.0007	4.26
105 (pu-mt007)	1	0.0030	1.0022	0.0006	4.24
PU-MET-FAST-004					
207 (pu-mt008)	1	0.0030	0.9954	0.0013	4.51
208 (pu-mt009)	1	0.0030	0.9933	0.0012	4.55
209 (pu-mt010)	1	0.0030	0.9977	0.0012	4.56
210 (pu-mt011)	1	0.0030	0.9959	0.0012	4.55
211 (pu-mt012)	1	0.0030	0.9949	0.0012	4.56
212 (pu-mt013)	1	0.0030	0.9924	0.0013	4.55
213 (pu-mt014)	1	0.0030	0.9935	0.0012	4.49
214 (pu-mt015)	1	0.0030	0.9935	0.0012	4.49
215 (pu-mt016)	1	0.0030	0.9933	0.0011	4.47
PU-MET-FAST-005					
1 (pu-mt017)	1	0.0013	1.0082	0.0007	4.6
PU-MET-FAST-006					
1 (pu-mt018)	1	0.0030	1.0047	0.0014	4.74
PU-MET-FAST-008					
1 (pu-mt019)	1	0.0006	1.0061	0.0006	4.58
PU-MET-FAST-009					
1 (pu-mt020)	1	0.0027	1.0019	0.0008	4.37
PU-MET-FAST-010					
1 (pu-mt021)	1	0.0018	0.9997	0.0007	4.5
PU-MET-FAST-011					
1 (pu-mt022)	1	0.0010	1.0003	0.0008	6.96
PU-MET-FAST-016					
2 (pu-mt024)	1	0.0038	1.0045	0.0017	5.63
3 (pu-mt025)	1	0.0033	1.0048	0.0018	6.19
4 (pu-mt026)	1	0.0030	1.0024	0.0018	5.48
5 (pu-mt027)	1	0.0034	1.0020	0.0018	7.11
6 (pu-mt028)	1	0.0032	1.0060	0.0018	4.22
PU-MET-FAST-017					
201 (pu-mt029)	1	0.0030	0.9935	0.0012	4.22

Table A-1. Parameters Used in Pu Metal Validation Calculations (Continued).

Experimental Descriptor Case Number(Input File)	Exp. k_{eff}	$\sigma_{exp.}$	Calculated Results (all k_{eff} values normalized to Exp. values)		
			K_{eff}	σ_s	AEG (27gr)
PU-MET-FAST-017 (continued)					
202 (pu-mt030)	1	0.0030	0.9983	0.0012	4.37
203 (pu-mt031)	1	0.0030	0.9994	0.0012	4.37
204 (pu-mt032)	1	0.0030	0.9974	0.0013	9.61
205 (pu-mt033)	1	0.0030	1.0054	0.0013	9.99
PU-MET-FAST-022					
1 (pu-mt035)	1	0.0021	0.9987	0.0006	10.04
PU-MET-FAST-023					
1 (pu-mt036)	1	0.0020	0.9964	0.0010	10.04
PU-MET-FAST-037					
1 (pu-mt037)	1	0.0046	0.9990	0.0024	6.78
2 (pu-mt038)	1	0.0046	1.0016	0.0017	7.38
3 (pu-mt039)	1	0.0046	1.0025	0.0016	7.44
4 (pu-mt040)	1	0.0046	1.0031	0.0017	7.6
5 (pu-mt041)	1	0.0046	1.0010	0.0017	7.89
6 (pu-mt042)	1	0.0038	1.0027	0.0017	8.45
7 (pu-mt043)	1	0.0038	1.0031	0.0017	8.39
8 (pu-mt044)	1	0.0035	1.0008	0.0018	8.99
9 (pu-mt045)	1	0.0038	1.0020	0.0018	9.04
10 (pu-mt046)	1	0.0038	1.0025	0.0018	8.69
11 (pu-mt047)	1	0.0041	0.9978	0.0017	7.45
12 (pu-mt048)	1	0.0039	1.0010	0.0017	8.71
13 (pu-mt049)	1	0.0034	0.9995	0.0018	9.52
14 (pu-mt050)	1	0.0033	1.0047	0.0018	9.26
15 (pu-mt051)	1	0.0033	1.0077	0.0018	9.11
16 (pu-mt052)	1	0.0036	1.0078	0.0017	8.6

Table A-2. Parameters Used in Pu Solutions Validation Calculations.

Experimental Descriptor Case Number(Input File)	Exp. k _{eff}	σ _{exp.}	Calculated Results (all k _{eff} values normalized to Exp. values)		
			k _{eff}	σ _s	H/Pu
PU-SOL-THERM-009					
1 (pu-sl001)	1.0003	0.0033	1.0192	0.0006	2648.2
2 (pu-sl002)	1.0003	0.0033	1.0241	0.0006	2778.9
3 (pu-sl003)	1.0003	0.0033	1.0238	0.0006	2802.8
PU-SOL-THERM-011					
16-1 (pu-sl004)	1	0.0052	1.0174	0.0010	765
16-2 (pu-sl005)	1	0.0052	1.0235	0.0014	736
16-3 (pu-sl006)	1	0.0052	1.0233	0.0013	691
16-4 (pu-sl007)	1	0.0052	1.0202	0.0013	682
16-5 (pu-sl008)	1	0.0052	1.0155	0.0011	574
18-1 (pu-sl009)	1	0.0052	1.0006	0.0012	1208
18-2 (pu-sl010)	1	0.0052	1.0081	0.0010	1151
18-3 (pu-sl011)	1	0.0052	1.0029	0.0012	1158
18-4 (pu-sl012)	1	0.0052	1.0002	0.0012	1100
18-5 (pu-sl013)	1	0.0052	1.0110	0.0010	1039
18-6 (pu-sl13a)	1	0.0052	1.0062	0.0010	908
18-7 (pu-sl13b)	1	0.0052	1.0063	0.0010	1103
PU-SOL-THERM-012					
1 (pu-sl014)	1	0.0043	1.0117	0.0007	1721.6
2 (pu-sl015)	1	0.0043	1.0124	0.0006	1920.1
3 (pu-sl016)	1	0.0058	1.0131	0.0006	2035.4
4 (pu-sl017)	1	0.0058	1.0133	0.0005	2311.6
5 (pu-sl018)	1	0.0058	1.0145	0.0005	2573.3
6 (pu-sl019)	1	0.0007	1.0095	0.0010	309.1
7 (pu-sl020)	1	0.0013	1.0087	0.0009	398.8
8 (pu-sl021)	1	0.0013	1.0109	0.0007	632.5
9 (pu-sl022)	1	0.0043	1.0157	0.0008	1054.1
10 (pu-sl023)	1	0.0043	1.0122	0.0006	1251.8
11 (pu-sl024)	1	0.0043	1.0140	0.0007	1566.7
12 (pu-sl025)	1	0.0043	1.0158	0.0006	1721.6
13 (pu-sl026)	1	0.0058	1.0151	0.0004	2573.3
PU-SOL-THERM-001					
1 (pu-sl037)	1	0.005	1.0086	0.0014	371.3
2 (pu-sl038)	1	0.005	1.0136	0.0015	271.5
3 (pu-sl039)	1	0.005	1.0133	0.0014	215.9
4 (pu-sl040)	1	0.005	1.0090	0.0015	190.4
5 (pu-sl041)	1	0.005	1.0103	0.0014	180.2
6 (pu-sl042)	1	0.005	1.0092	0.0015	91.2
PU-SOL-THERM-002					
1 (pu-sl043)	1	0.0047	1.0108	0.0012	524
2 (pu-sl044)	1	0.0047	1.0122	0.0013	505
3 (pu-sl045)	1	0.0047	1.0096	0.0013	451
4 (pu-sl046)	1	0.0047	1.0098	0.0012	421
5 (pu-sl047)	1	0.0047	1.0133	0.0012	393

Table A-2. Parameters Used in Pu Solutions Validation Calculations (Continued).

Experimental Descriptor Case Number(Input File)	Exp. k_{eff}	$\sigma_{exp.}$	Calculated Results (all k_{eff} values normalized to Exp. values)		
			k_{eff}	σ_s	H/Pu
PU-SOL-THERM-002 (continued)					
6 (pu-sl048)	1	0.0047	1.0109	0.0013	344
7 (pu-sl049)	1	0.0047	1.0123	0.0013	309
PU-SOL-THERM-003					
1 (pu-sl050)	1	0.0047	1.0104	0.0012	788
2 (pu-sl051)	1	0.0047	1.0089	0.0011	756
3 (pu-sl052)	1	0.0047	1.0093	0.0012	698.9
4 (pu-sl053)	1	0.0047	1.0107	0.0012	681.7
5 (pu-sl054)	1	0.0047	1.0120	0.0012	626.7
6 (pu-sl055)	1	0.0047	1.0135	0.0012	562.8
7 (pu-sl056)	1	0.0047	1.0148	0.0012	737.8
8 (pu-sl057)	1	0.0047	1.0144	0.0012	714.3
PU-SOL-THERM-004					
1 (pu-sl058)	1	0.0047	1.0096	0.0013	987
2 (pu-sl059)	1	0.0047	1.0072	0.0012	977
3 (pu-sl060)	1	0.0047	1.0093	0.0013	935
4 (pu-sl061)	1	0.0047	1.0077	0.0013	889
5 (pu-sl062)	1	0.0047	1.0105	0.0013	942
6 (pu-sl063)	1	0.0047	1.0095	0.0012	927
7 (pu-sl064)	1	0.0047	1.0126	0.0012	892
8 (pu-sl065)	1	0.0047	1.0077	0.0012	869
9 (pu-sl066)	1	0.0047	1.0082	0.0013	805
10 (pu-sl067)	1	0.0047	1.0105	0.0013	689
11 (pu-sl068)	1	0.0047	1.0086	0.0014	592
12 (pu-sl069)	1	0.0047	1.0131	0.0012	893
13 (pu-sl070)	1	0.0047	1.0080	0.0013	903
PU-SOL-THERM-005					
1 (pu-sl071)	1	0.0047	1.0092	0.0012	902.8
2 (pu-sl072)	1	0.0047	1.0107	0.0012	867.7
3 (pu-sl073)	1	0.0047	1.0110	0.0011	834.4
4 (pu-sl074)	1	0.0047	1.0116	0.0012	765.2
5 (pu-sl075)	1	0.0047	1.0126	0.0011	694.1
6 (pu-sl076)	1	0.0047	1.0119	0.0011	633.4
7 (pu-sl077)	1	0.0047	1.0128	0.0012	580.6
8 (pu-sl078)	1	0.0047	1.0039	0.0012	868.7
9 (pu-sl079)	1	0.0047	1.0105	0.0011	825.1
PU-SOL-THERM-006					
1 (pu-sl080)	1	0.0035	1.0092	0.0011	1061
2 (pu-sl081)	1	0.0035	1.0081	0.0011	1018
3 (pu-sl082)	1	0.0035	1.0105	0.0010	940
PU-SOL-THERM-007					
1 (pu-sl083)	1	0.0048	1.0116	0.0012	109.6
2 (pu-sl084)	1	0.0048	1.0044	0.0012	114
3 (pu-sl085)	1	0.0048	1.0119	0.0012	267.5
4 (pu-sl086)	1	0.0048	1.0080	0.0012	262

Table A-2. Parameters Used in Pu Solutions Validation Calculations (Continued).

Experimental Descriptor Case Number(Input File)	Exp. k_{eff}	$\sigma_{exp.}$	Calculated Results (all k_{eff} values normalized to Exp. values)		
			k_{eff}	σ_s	H/Pu
PU-SOL-THERM-007 (continued)					
5 (pu-sl087)	1	0.0048	1.0086	0.0012	265.8
6 (pu-sl088)	1	0.0048	1.0033	0.0012	258.5
7 (pu-sl089)	1	0.0048	1.0024	0.0012	259.7
8 (pu-sl090)	1	0.0048	1.0054	0.0012	285
PU-SOL-THERM-010					
1 (pu-sl091)	1	0.0048	1.0215	0.0011	266.9
2 (pu-sl092)	1	0.0048	1.0195	0.0011	356.9
3 (pu-sl093)	1	0.0048	1.0140	0.0010	484.2
4 (pu-sl094)	1	0.0048	1.0181	0.0010	485
5 (pu-sl095)	1	0.0048	1.0158	0.0010	558.1
6 (pu-sl096)	1	0.0048	1.0157	0.0010	558.1
7 (pu-sl097)	1	0.0048	1.0096	0.0010	605.9
8 (pu-sl098)	1	0.0048	1.0104	0.0009	665.4
9 (pu-sl099)	1	0.0048	1.0197	0.0011	414.3
10 (pu-sl100)	1	0.0048	1.0079	0.0010	535.2
11 (pu-sl101)	1	0.0048	1.0161	0.0010	543.4
12 (pu-sl102)	1	0.0048	1.0156	0.0010	618.4
13 (pu-sl103)	1	0.0048	1.0231	0.0010	728.1
14 (pu-sl104)	1	0.0048	1.0155	0.0010	849.7

Table A-3. Parameters Used in Uranium Metal (Fast) Validation Calculations.

Experimental Descriptor Case Number(Input File)	Exp. k _{eff}	σ _{exp}	Calculated Results (all k _{eff} values normalized to Exp. values)		
			k _{eff}	σ _s	AEG (27gr)
HEU-MET-FAST-001					
1 (heumt002)	1	0.0010	0.9993	0.0010	4.85
2 (heumt001)	1	0.0010	0.9985	0.0008	4.86
HEU-MET-FAST-002					
1 (heumt003)	1	0.0030	1.0028	0.0011	4.87
2 (heumt004)	1	0.0030	1.0060	0.0011	4.89
3 (heumt005)	1	0.0030	1.0014	0.0011	4.89
4 (heumt006)	1	0.0030	1.0009	0.0010	4.91
5 (heumt007)	1	0.0030	1.0007	0.0011	4.91
6 (heumt008)	1	0.0030	1.0040	0.0010	4.90
HEU-MET-FAST-003					
1 (heumt009)	1	0.0050	0.9938	0.0010	4.88
2 (heumt010)	1	0.0050	0.9931	0.0010	4.87
3 (heumt011)	1	0.0050	1.0001	0.0011	4.87
4 (heumt012)	1	0.0050	1.0002	0.0010	4.86
5 (heumt013)	1	0.0050	1.0045	0.0010	4.87
6 (heumt014)	1	0.0050	1.0018	0.0010	4.87
7.(heumt015)	1	0.0050	1.0009	0.0012	4.89
8 (heumt016)	1	0.0050	0.9983	0.0010	5.20
9 (heumt017)	1	0.0050	0.9986	0.0009	5.03
10 (heumt018)	1	0.0050	1.0021	0.0009	5.37
11 (heumt019)	1	0.0050	1.0036	0.0010	5.39
HEU-MET-FAST-004					
2 (heumt 022)	1.002	0.0020	0.9985	0.0011	8.50
HEU-MET-FAST-007					
1 (heumt023)	0.9971	0.0001	0.9965	0.0009	4.84
2 (heumt024)	0.9986	0.0001	0.9954	0.0010	5.39
3 (heumt025)	1.0012	0.0001	0.9918	0.0011	5.63
4 (heumt026)	0.997	0.0001	0.9963	0.0011	5.73
5 (heumt027)	1	0.0001	0.9930	0.0011	5.96
6 (heumt028)	1.0028	0.0001	0.9986	0.0012	6.40
7 (heumt029)	0.9996	0.0001	0.9950	0.0012	6.17
8 (heumt030)	0.9992	0.0001	0.9957	0.0011	6.14
9 (heumt031)	1.0017	0.0008	0.9932	0.0011	6.27
10 (heumt032)	1	0.0001	0.9907	0.0014	8.08
11 (heumt033)	0.9982	0.0001	0.9918	0.0013	9.65
12 (heumt034)	0.9951	0.0001	0.9909	0.0013	9.99
13 (heumt035)	1.0009	0.0001	0.9929	0.0014	10.65
14 (heumt036)	0.9983	0.0001	0.9921	0.0015	10.07
15 (heumt037)	0.9978	0.0001	0.9910	0.0013	10.54
16 (heumt038)	0.9988	0.0001	0.9919	0.0013	10.57
17 (heumt039)	0.9972	0.0001	0.9913	0.0014	12.83
18 (heumt040)	0.9991	0.0001	0.9945	0.0014	12.88

Table A-3. Parameters Used in Uranium Metal (Fast) Validation Calculations (Continued).

Experimental Descriptor Case Number(Input File)	Exp. k _{eff}	σ _{exp.}	Calculated Results (all k _{eff} values normalized to Exp. values)		
			k _{eff}	σ _s	AEG (27gr)
HEU-MET-FAST-007 (continued)					
19 (heumt041)	0.9983	0.0001	0.9960	0.0009	4.84
20 (heumt042)	0.9981	0.0001	0.9931	0.0011	6.13
21 (heumt043)	0.9987	0.0001	0.9916	0.0012	6.20
22 (heumt044)	0.9994	0.0001	0.9922	0.0011	6.29
23 (heumt045)	0.9993	0.0001	0.9916	0.0012	7.37
24 (heumt046)	1.0001	0.0001	0.9907	0.0012	7.45
25 (heumt047)	0.999	0.0001	0.9928	0.0012	8.23
26 (heumt048)	0.9997	0.0001	0.9919	0.0012	8.31
27 (heumt049)	0.9965	0.0002	0.9959	0.0012	5.44
28 (heumt050)	0.9987	0.0002	0.9911	0.0010	5.89
29 (heumt051)	0.9978	0.0002	0.9940	0.0012	6.36
30 (heumt052)	0.9981	0.0002	0.9936	0.0011	8.54
31 (heumt053)	1.0013	0.0002	0.9969	0.0013	11.06
32 (heumt054)	0.9959	0.0001	1.0045	0.0010	5.02
33 (heumt055)	0.9995	0.0001	1.0062	0.0011	5.12
34 (heumt056)	0.9977	0.0001	1.0085	0.0010	5.23
35 (heumt057)	1.0011	0.0001	0.9863	0.0012	10.01
36 (heumt058)	0.9999	0.0001	0.9960	0.0012	10.62
37 (heumt059)	0.9988	0.0001	0.9986	0.0014	11.19
38 (heumt060)	1	0.0001	0.9929	0.0012	11.36
39 (heumt061)	1.0018	0.0001	0.9954	0.0014	11.37
40 (heumt062)	1.0013	0.0001	0.9989	0.0013	11.35
41 (heumt063)	0.9994	0.0001	0.9970	0.0014	13.15
42 (heumt064)	1.0016	0.0001	0.9963	0.0012	13.19
43 (heumt065)	0.9998	0.0001	0.9970	0.0015	15.81
HEU-MET-FAST-012					
1 (heumt088)	0.9992	0.0018	0.9945	0.0005	4.92
HEU-MET-FAST-013					
1 (heumt089)	0.9990	0.0015	1.0027	0.0006	4.99
HEU-MET-FAST-021					
1 (heumt090)	1	0.0024	1.0070	0.0006	5.09
HEU-MET-FAST-022					
1 (heumt091)	1	0.0019	0.9929	0.0006	4.94
HEU-MET-FAST-023					
2 (heumt066)	1	0.0052	0.9943	0.0006	5.43
3 (heumt067)	1	0.0052	1.0001	0.0007	8.33
4 (heumt068)	1	0.0052	1.0023	0.0007	10.06
5 (heumt069)	1	0.0052	0.9989	0.0007	10.28
6 (heumt070)	1	0.0052	0.9942	0.0006	4.87
7 (heumt071)	1	0.0052	0.9916	0.0007	5.48
8 (heumt072)	1	0.0052	0.9987	0.0007	8.66
9 (heumt073)	1	0.0052	0.9975	0.0007	10.50

10 (heumt074)	1	0.0052	0.9949	0.0005	10.74
12(heumt075)	1	0.0052	0.9932	0.0007	5.42

Table A-3. Parameters Used in Uranium Metal (Fast) Validation Calculations (Continued).

Experimental Descriptor Case Number(Input File)	Exp. k_{eff}	$\sigma_{exp.}$	Calculated Results (all k_{eff} values normalized to Exp. values)		
			k_{eff}	σ_s	AEG (27gr)
HEU-MET-FAST-023 (continued)					
13 (heumt076)	1	0.0052	1.0071	0.0007	8.30
14 (heumt077)	1	0.0052	1.0037	0.0007	9.97
15 (heumt078)	1	0.0052	0.9987	0.0006	10.21
16 (heumt079)	1	0.0052	0.9980	0.0005	4.87
17 (heumt080)	1	0.0052	0.9962	0.0005	5.46
18 (heumt081)	1	0.0052	0.9977	0.0006	8.67
19 (heumt082)	1	0.0052	0.9986	0.0005	10.37
20 (heumt083)	1	0.0052	0.9959	0.0005	10.59
21 (heumt084)	1	0.0057	0.9942	0.0005	4.91
22 (heumt085)	1	0.0052	0.9949	0.0006	10.88
28 (heumt086)	1	0.0052	0.9940	0.0005	4.86
29 (heumt087)	1	0.0052	0.9955	0.0006	4.89
HEU-MET-FAST-024					
1 (heumt092)	0.9990	0.0015	0.9977	0.0011	7.55
HEU-MET-FAST-026					
b-1 (heumt099)	0.9982	0.0042	1.0042	0.0014	4.86
b-2 (heumt100)	0.9982	0.0042	0.9984	0.0014	5.42
b-3 (heumt101)	1	0.0038	0.9988	0.0016	8.39
b-4 (heumt102)	1	0.0038	0.9977	0.0019	9.94
b-5 (heumt103)	1	0.0038	0.9938	0.0016	10.18
b-6 (heumt104)	0.9982	0.0042	0.9977	0.0014	4.89
b-7 (heumt105)	0.9982	0.0042	0.9968	0.0016	5.44
b-8 (heumt106)	1	0.0038	0.9990	0.0018	8.56
b-9 (heumt107)	1	0.0038	0.9968	0.0017	10.12
b-10 (heumt108)	1	0.0038	0.9927	0.0018	10.29
c-1 (heumt109)	0.9982	0.0042	0.9981	0.0013	4.86
c-2 (heumt110)	0.9982	0.0042	0.9959	0.0013	4.86
c-3 (heumt111)	0.9982	0.0042	0.9977	0.0015	5.39
c-4 (heumt112)	1	0.0038	1.0004	0.0017	6.88
c-5 (heumt113)	1	0.0038	0.9973	0.0018	8.30
c-6 (heumt114)	1	0.0038	0.9966	0.0016	9.69
c-7 (heumt115)	1	0.0038	0.9993	0.0017	9.83
c-8 (heumt116)	0.9982	0.0042	0.9997	0.0014	4.90
c-9 (heumt117)	0.9982	0.0042	0.9880	0.0015	5.45
c-10 (heumt118)	1	0.0038	0.9962	0.0017	8.39
c-11 (heumt119)	1	0.0038	1.0011	0.0018	9.72
c-12 (heumt120)	1	0.0038	1.0027	0.0017	9.84
d-1 (heumt121)	0.9982	0.0042	0.9989	0.0013	4.87
d-2 (heumt122)	0.9982	0.0042	0.9935	0.0015	5.40
d-3 (heumt123)	1	0.0038	0.9959	0.0019	8.14

d-4 (heumt124)	1	0.0038	0.9966	0.0018	9.28
d-5 (heumt125)	1	0.0038	0.9956	0.0018	9.44
d-6 (heumt126)	0.9982	0.0042	0.9990	0.0015	4.92
d-7 (heumt127)	0.9982	0.0042	0.9911	0.0014	5.44

Table A-3. Parameters Used in Uranium Metal (Fast) Validation Calculations (Continued).

Experimental Descriptor Case Number(Input File)	Exp. k_{eff}	$\sigma_{exp.}$	Calculated Results (all k_{eff} values normalized to Exp. values)		
			k_{eff}	σ_s	AEG (27gr)
HEU-MET-FAST-026 (continued)					
d-8 (heumt128)	1	0.0038	0.9970	0.0017	8.02
d-9 (heumt129)	1	0.0038	0.9981	0.0017	9.23
d-10 (heumt130)	1	0.0038	0.9990	0.0017	9.38
HEU-MET-FAST-033					
1 (heumt93)	0.9991	0.0014	0.9953	0.0004	8.63
2 (heumt94)	0.9991	0.0014	0.9948	0.0004	10.93
HEU-MET-FAST-034					
1 (heumt95)	0.9990	0.0012	0.9923	0.0004	8.65
2 (heumt96)	0.9990	0.0012	0.9922	0.0004	8.75
3 (heumt97)	0.9990	0.0012	0.9954	0.0004	8.87
HEU-MET-FAST-036					
1 (heumt98)	0.9995	0.0013	0.9993	0.0004	10.97
IEU-MET-FAST-005					
1 (ieumt001)	1	0.0021	1.0138	0.0006	5.38
IEU-MET-FAST-006					
1 (ieumt002)	1	0.0023	0.9969	0.0006	5.32

Table A-4. Parameters Used in Uranium Metal (Thermal) Validation Calculations.

Experimental Descriptor Case Number(Input File)	Exp. k_{eff}	$\sigma_{\text{exp.}}$	Calculated Results (all k_{eff} values normalized to Exp. values)			
			k_{eff}	σ_s	AEG (18gr)	E (eV)
Research Reactor Fuel HEU-MET-THERM-006						
1(1)	1	0.0040	0.9979	0.0017	12.89	0.146
2(2)	1	0.0040	1.0007	0.0014	13.05	0.098
3(3)	1	0.0040	1.0074	0.0013	13.14	0.093
4(4)	1	0.0040	0.9969	0.0014	13.16	0.092
5(5)	1	0.0040	1.0047	0.0014	13.21	0.090
6(6)	1	0.0040	1.0002	0.0014	13.25	0.088
7(7)	1	0.0040	1.0003	0.0014	13.28	0.086
8(8)	1	0.0040	0.9945	0.0013	13.31	0.085
9(9)	1	0.0040	0.9955	0.0014	13.31	0.084
10(10)	1	0.0040	1.0059	0.0016	12.90	0.135
11(11)	1	0.0040	0.9987	0.0015	13.16	0.092
12(12)	1	0.0040	1.0066	0.0014	13.28	0.086
13(13)	1	0.0040	1.0302	0.0015	12.91	0.138
16(16)	1	0.0040	0.9974	0.0018	13.14	0.069

Table A-5. Parameters Used in Uranium Solutions (HEU) Validation Calculations.

Experimental Descriptor Case Number(Input File)	Exp. k _{eff}	σ _{exp.}	Calculated Results (all k _{eff} values normalized to Exp. values)		
			k _{eff}	σ _s	AEG (27gr)
HEU-SOL-THERM-001					
1 (heusl001)	1	0.0025	1.0008	0.0020	23.58
2 (heusl002)	1	0.0025	1.0007	0.0020	21.69
3 (heusl003)	1	0.0025	1.0089	0.0020	23.61
4 (heusl004)	1	0.0025	1.0046	0.0022	21.58
5 (heusl005)	1	0.0025	1.0036	0.0017	24.57
6 (heusl006)	1	0.0025	1.0104	0.0019	24.52
7 (heusl007)	1	0.0025	1.0023	0.0020	23.66
8 (heusl008)	1	0.0025	1.0051	0.0021	23.58
9 (heusl009)	1	0.0025	0.9976	0.0022	21.59
10 (heusl010)	1	0.0025	0.9995	0.0018	24.46
HEU-SOL-THERM-002					
1 (heusl011)	1	0.0020	1.0093	0.0022	23.61
2 (heusl012)	1	0.0020	1.0113	0.0020	23.62
3 (heusl013)	1	0.0020	1.0008	0.0019	21.84
4 (heusl014)	1	0.0020	1.0083	0.0020	21.90
5 (heusl015)	1	0.0020	1.0058	0.0021	23.62
6 (heusl016)	1	0.0020	1.0125	0.0019	23.65
7 (heusl017)	1	0.0020	1.0040	0.0021	21.86
8 (heusl018)	1	0.0020	1.0073	0.0020	21.94
9 (heusl019)	1	0.0020	1.0053	0.0019	24.52
10 (heusl020)	1	0.0020	1.0072	0.0016	24.53
11 (heusl021)	1	0.0020	1.0044	0.0020	23.62
12 (heusl022)	1	0.0020	1.0131	0.0021	23.65
13 (heusl023)	1	0.0020	1.0010	0.0021	21.86
14 (heusl024)	1	0.0020	1.0051	0.0022	21.97
HEU-SOL-THERM-003					
1 (heusl025)	1	0.0050	1.0039	0.0017	24.53
2 (heusl026)	1	0.0050	1.0047	0.0018	24.52
3 (heusl027)	1	0.0050	1.0041	0.0019	23.59
4 (heusl028)	1	0.0050	1.0084	0.0020	23.63
5 (heusl029)	1	0.0050	1.0041	0.0021	21.78
6 (heusl030)	1	0.0050	1.0036	0.0021	21.89
7 (heusl031)	1	0.0050	1.0044	0.0016	24.54
8 (heusl032)	1	0.0050	1.0066	0.0021	23.60
9 (heusl033)	1	0.0050	1.0071	0.0020	23.66
10 (heusl034)	1	0.0050	0.9989	0.0022	21.80
11 (heusl035)	1	0.0050	1.0055	0.0021	21.97
12 (heusl036)	1	0.0050	1.0077	0.0018	24.52
13 (heusl037)	1	0.0050	1.0033	0.0017	24.55
14 (heusl038)	1	0.0050	1.0058	0.0018	24.53
15 (heusl039)	1	0.0050	0.9921	0.0017	24.48
16 (heusl040)	1	0.0050	1.0044	0.0021	23.60
17 (heusl041)	1	0.0050	1.0096	0.0019	23.69
18 (heusl042)	1	0.0050	0.9985	0.0021	21.80
19 (heusl043)	1	0.0050	1.0087	0.0020	22.01

Table A-5. Parameters Used in Uranium Solutions (HEU) Validation Calculations (Continued).

Experimental Descriptor Case Number(Input File)	Exp. k_{eff}	$\sigma_{exp.}$	Calculated Results (all k_{eff} values normalized to Exp. values)		
			k_{eff}	σ_c	AEG (27gr)
HEU-SOL-THERM-007					
1 (heusl044)	1	0.0030	1.0134	0.0015	24.42
2 (heusl045)	1	0.0030	1.0168	0.0017	21.74
3 (heusl046)	1	0.0030	1.0082	0.0015	24.46
4 (heusl047)	1	0.0030	1.0108	0.0018	21.92
5 (heusl048)	1	0.0030	1.0092	0.0017	24.33
6 (heusl049)	1	0.0030	1.0096	0.0019	21.71
7 (heusl050)	1	0.0030	1.0075	0.0017	24.35
8 (heusl051)	1	0.0030	1.0008	0.0020	21.73
9 (heusl052)	1	0.0030	1.0084	0.0018	24.30
10 (heusl053)	1	0.0030	1.0141	0.0016	24.25
11 (heusl054)	1	0.0030	1.0115	0.0018	21.81
12 (heusl055)	1	0.0030	1.0080	0.0015	24.30
13 (heusl056)	1	0.0030	1.0096	0.0019	21.97
14 (heusl057)	1	0.0030	1.0067	0.0019	21.92
15 (heusl058)	1	0.0035	1.0080	0.0018	21.90
16 (heusl059)	1	0.0035	1.0075	0.0019	21.82
17 (heusl060)	1	0.0035	1.0083	0.0018	21.91
HEU-SOL-THERM-008					
1 (heusl061)	1	0.0035	1.0026	0.0016	24.52
2 (heusl062)	1	0.0035	1.0122	0.0019	21.95
3 (heusl063)	1	0.0035	0.9958	0.0016	24.56
4 (heusl064)	1	0.0035	1.0072	0.0017	22.13
5 (heusl065)	1	0.0035	1.0002	0.0016	24.52
6 (heusl066)	1	0.0035	1.0084	0.0018	21.82
7 (heusl067)	1	0.0035	0.9975	0.0017	24.55
8 (heusl068)	1	0.0035	1.0026	0.0018	21.89
9 (heusl069)	1	0.0035	1.0006	0.0015	24.52
10 (heusl070)	1	0.0035	1.0088	0.0019	21.96
11 (heusl071)	1	0.0035	0.9961	0.0015	24.58
12 (heusl072)	1	0.0035	1.0048	0.0018	22.17
13 (heusl073)	1	0.0035	1.0073	0.0018	21.98
14 (heusl074)	1	0.0035	1.0057	0.0017	22.13
HEU-SOL-THERM-009					
1 (heusl075)	1	0.0057	1.0037	0.0017	20.73
2 (heusl076)	1	0.0057	1.0061	0.0016	21.47
3 (heusl078)	1	0.0057	1.0072	0.0016	22.55
4 (heusl079)	1	0.0057	1.0021	0.0016	23.42
HEU-SOL-THERM-011					
1 (heusl080)	1	0.0019	1.0119	0.0013	24.69
2 (heusl081)	1	0.0019	1.0042	0.0014	24.70

Table A-5. Parameters Used in Uranium Solutions (HEU) Validation Calculations (Continued).

Experimental Descriptor Case Number(Input File)	Exp. k_{eff}	$\sigma_{exp.}$	Calculated Results (all k_{eff} values normalized to Exp. values)		
			k_{eff}	σ_s	AEG (27gr)
HEU-SOL-THERM-012					
1 (heusl082)	0.9999	0.0058	1.0042	0.0009	24.99
HEU-SOL-THERM-010					
1 (heusl083)	1	0.0018	1.0066	0.0015	24.26
2 (heusl084)	1	0.0018	1.0074	0.0014	24.24
3 (heusl085)	1	0.0018	1.0041	0.0015	24.18
4 (heusl086)	1	0.0018	1.0022	0.0015	24.16

Table A-6. Parameters Used in Uranium Compounds Validation Calculations.

Experimental Descriptor Case Number(Input File)	Exp. k_{eff}	σ_{exp}	Calculated Results (all k_{eff} values normalized to Exp. values)			
			k_{eff}	σ_s	AEG (27 gr)	H/U
LEU-COMP-THERM-001						
1 (Leum0101)	0.9998	0.0030	0.9975	0.0017	23.56	399
2 (Leum0102)	0.9998	0.0030	0.9984	0.0016	23.57	399
3 (Leum0103)	0.9998	0.0030	0.9963	0.0016	23.57	399
4 (Leum0104)	0.9998	0.0030	0.9967	0.0017	23.57	399
5 (Leum0105)	0.9998	0.0030	0.9928	0.0015	23.58	399
6 (Leum0106)	0.9998	0.0030	0.9985	0.0017	23.57	399
7 (Leum0107)	0.9998	0.0031	0.9955	0.0015	23.61	399
8 (Leum0108)	0.9998	0.0030	0.9951	0.0015	23.59	399
LEU-COMP-THERM-002						
1 (Leum0201)	0.9997	0.0020	0.9954	0.0018	23.3	256
2 (Leum0202)	0.9997	0.0020	1.0010	0.0016	23.31	256
3 (Leum0203)	0.9997	0.0020	0.9953	0.0019	23.31	256
4 (Leum0204)	0.9997	0.0018	0.9946	0.0017	23.33	256
5 (Leum0205)	0.9997	0.0019	0.9955	0.0020	23.34	256
LEU-COMP-THERM-010						
1 (Leum1001)	1.0000	0.0021	1.0061	0.0020	23.23	256
2 (Leum1002)	1.0000	0.0021	1.0082	0.0017	23.27	256
3 (Leum1003)	1.0000	0.0021	1.0037	0.0017	23.30	256
4 (Leum1004)	1.0000	0.0021	0.9954	0.0016	23.35	256
9 (Leum1009)	1.0000	0.0021	1.0006	0.0018	23.19	256
10 (Leum1010)	1.0000	0.0021	0.9999	0.0018	23.24	256
11 (Leum1011)	1.0000	0.0021	1.0027	0.0019	23.27	256
12 (Leum1012)	1.0000	0.0021	1.0037	0.0019	23.31	256
13 (Leum1013)	1.0000	0.0021	0.9976	0.0020	23.35	256
14 (Leum1014)	1.0000	0.0028	0.9980	0.0018	21.84	106
15 (Leum1015)	1.0000	0.0028	1.0005	0.0020	21.91	106
16 (Leum1016)	1.0000	0.0028	1.0054	0.0019	21.95	106
17 (Leum1017)	1.0000	0.0028	1.0054	0.0019	21.98	106
18 (Leum1018)	1.0000	0.0028	1.0033	0.0021	22.00	106
19 (Leum1019)	1.0000	0.0028	0.9952	0.0021	22.05	106
20 (Leum1020)	1.0000	0.0028	1.0024	0.0019	21.89	106
21 (Leum1021)	1.0000	0.0028	1.0028	0.0021	21.96	106
22 (Leum1022)	1.0000	0.0028	1.0039	0.0021	22.03	106
23 (Leum1023)	1.0000	0.0028	0.9961	0.0020	22.05	106
LEU-COMP-THERM-017						
1 (Leum1701)	1.0000	0.0031	1.0025	0.0017	23.53	399
2 (Leum1702)	1.0000	0.0031	1.0021	0.0018	23.56	399
3 (Leum1703)	1.0000	0.0031	1.0007	0.0016	23.56	399
10 (Leum1710)	1.0000	0.0031	0.9957	0.0016	23.50	399
11 (Leum1711)	1.0000	0.0031	0.9986	0.0016	23.54	399
12 (Leum1712)	1.0000	0.0031	0.9958	0.0013	23.56	399
13 (Leum1713)	1.0000	0.0031	0.9969	0.0015	23.57	399
14 (Leum1714)	1.0000	0.0031	0.9978	0.0016	23.58	399
15 (Leum1715)	1.0000	0.0028	0.9923	0.0017	22.69	219
16 (Leum1716)	1.0000	0.0028	0.9929	0.0017	22.74	219
17 (Leum1717)	1.0000	0.0028	0.9984	0.0015	22.79	219

Table A-6. Parameters Used in Uranium Compounds Validation Calculations (Continued).

Experimental Descriptor Case Number(Input File)	Exp. k_{eff}	$\sigma_{exp.}$	Calculated Results (all k_{eff} values normalized to Exp. values)			
			k_{eff}	σ_s	AEG (27 gr)	H/U
LEU-COMP-THERM-017 (continued)						
18 (Leum1718)	1.0000	0.0028	0.9987	0.0016	22.79	219
19 (Leum1719)	1.0000	0.0028	1.0001	0.0018	22.82	219
20 (Leum1720)	1.0000	0.0028	0.9948	0.0017	22.83	219
21 (Leum1721)	1.0000	0.0028	0.9958	0.0017	22.85	219
22 (Leum1722)	1.0000	0.0028	0.9933	0.0016	22.85	219
23 (Leum1723)	1.0000	0.0028	0.9981	0.0016	22.75	219
24 (Leum1724)	1.0000	0.0028	1.0017	0.0016	22.80	219
25 (Leum1725)	1.0000	0.0028	0.9948	0.0017	22.87	219

Table A-7. Parameters Used in Uranium Solutions (LEU) Validation Calculations.

Experimental Descriptor case Number(Input File)	Exp. k_{eff}	$\sigma_{exp.}$	Calculated Results (all k_{eff} values normalized to Exp. values)			
			k_{eff}	σ_s	AEG (27 gr)	H/U
LEU-SOL-THERM-001						
1 (Solm101)	0.9991	0.0029	1.0141	0.0010	24.15	454
LEU-SOL-THERM-002						
1 (Solm201)	1.0038	0.0040	0.9969	0.0011	24.78	1098
2 (Solm202)	1.0024	0.0037	0.9945	0.0013	24.72	1002
3 (Solm203)	1.0024	0.0044	0.9974	0.0012	24.75	1002
LEU-SOL-THERM-003						
1 (Solm301)	0.9997	0.0039	0.9998	0.0014	24.67	771
2 (Solm302)	0.9993	0.0042	0.9986	0.0013	24.74	878
3 (Solm303)	0.9995	0.0042	1.0008	0.0013	24.75	898
4 (Solm304)	0.9995	0.0042	0.9959	0.0013	24.76	914
5 (Solm305)	0.9997	0.0048	0.9973	0.0011	24.86	1173
6 (Solm306)	0.9999	0.0049	0.9988	0.0010	24.87	1214
7 (Solm307)	0.9994	0.0049	0.9978	0.0010	24.88	1241
8 (Solm308)	0.9993	0.0052	1.0020	0.0009	24.93	1400
9 (Solm309)	0.9996	0.0052	0.9987	0.0009	24.93	1438
LEU-SOL-THERM-004						
1 (Leu401)	0.9994	0.0008	1.0039	0.0013	24.64	719
29 (Leu402)	0.9999	0.0009	0.9945	0.0013	24.68	772
33 (Leu403)	0.9999	0.0009	0.9893	0.0012	24.72	843
34 (Leu404)	0.9999	0.0010	0.9958	0.0012	24.75	896
46 (Leu405)	0.9999	0.0010	0.9952	0.0013	24.77	942
51 (Leu406)	0.9993	0.0010	0.9957	0.0012	24.79	983
54 (Leu407)	0.9996	0.0011	0.9932	0.0011	24.81	1018

APPENDIX B: Comparison of WSRC and WSMS MCNP-4B Validation Results

MCNP-4B has been validated on the WSMS DEC Alpha machines in the Centennial Complex. Since this same version of the code will be run at WSRC on their RS/6000 workstations, it was desirable to determine if the validation that was performed for MCNP-4B on the WSMS platform could be used for the WSRC platform as well. In order to determine if this comparison could be used in support of the SRS MCNP-4B validation, a representative sample of input files from each of the major fissile types and forms were run under the SRS certified MCNP-4B code and subsequently compared to the validated WSMS certified MCNP-4B code. The results of these comparisons are shown in Table B.1, and demonstrate that the two platforms provide statistically similar k_{eff} values; therefore, this appendix gives sufficient certification that the validation for MCNP-4B under the WSMS system is directly compatible as the MCNP-4B validation for the WSRC system. The results are listed in the following table (DFS signifies the WSRC platform).

Table B-1. Results From SRS and WSMS MCNP-4B Comparison.

	file	DFS	DFS	WSMS	WSMS	
		k_{eff}	σ	k_{eff}	σ	Δk
1	heumt034.out	0.9860	0.0013	0.9860	0.0013	0.0000
2	heumt037.out	0.9877	0.0013	0.9888	0.0013	-0.0011
3	heumt039.out	0.9885	0.0014	0.9885	0.0014	0.0000
4	heumt043.out	0.9903	0.0012	0.9903	0.0012	0.0000
5	heumt045.out	0.9909	0.0012	0.9909	0.0012	0.0000
6	heumt046.out	0.9908	0.0012	0.9908	0.0012	0.0000
7	heumt050.out	0.9898	0.0010	0.9898	0.0010	0.0000
8	heumt057.out	0.9878	0.0013	0.9874	0.0012	0.0004
9	heumt071.out	0.9921	0.0006	0.9916	0.0006	0.0004
10	heumt117.out	0.9854	0.0015	0.9862	0.0015	-0.0008
11	heumt127.out	0.9888	0.0015	0.9893	0.0014	-0.0005
12	heusl004.out	1.0046	0.0022	1.0046	0.0022	0.0000
13	heusl014.out	1.0063	0.0020	1.0083	0.002	-0.0020
14	heusl039.out	0.9946	0.0017	0.9921	0.0017	0.0025
15	heusl050.out	1.0057	0.0016	1.0075	0.0017	-0.0019
16	heusl063.out	0.9982	0.0016	0.9958	0.0016	0.0024
17	heusl071.out	0.9957	0.0015	0.9961	0.0015	-0.0004
18	heusl078.out	1.0060	0.0016	1.0072	0.0016	-0.0012
19	heusl084.out	1.0074	0.0014	1.0074	0.0014	0.0000
20	heusl087.out	0.9990	0.0013	0.9990	0.0013	0.0000
21	heusl088.out	0.9914	0.0013	0.9911	0.0014	0.0003
22	heusl089.out	0.9934	0.0010	0.9951	0.0010	-0.0017
23	heusl090.out	0.9841	0.0010	0.9840	0.0010	0.0001
24	heusl091.out	0.9983	0.0010	0.9972	0.0010	0.0011
25	heusl094.out	0.9997	0.0009	0.9975	0.0009	0.0022
26	pu-mt006.out	0.9802	0.0007	0.9817	0.0007	-0.0015

Table B-1. Results From SRS and WSMS MCNP-4B Comparison (Continued).

	file	DFS k_{eff}	DFS σ	WSMS k_{eff}	WSMS σ	Δk
27	pu-mt008.out	0.9951	0.0013	0.9954	0.0013	-0.0003
28	pu-mt009.out	0.9951	0.0013	0.9933	0.0012	0.0018
29	pu-mt011.out	1.0003	0.0008	1.0003	0.0008	0.0000
30	pu-mt012.out	0.9949	0.0012	0.9949	0.0012	0.0000
31	pu-mt013.out	0.9932	0.0012	0.9924	0.0013	0.0008
32	pu-mt014.out	0.9935	0.0012	0.9935	0.0012	0.0000
33	pu-mt015.out	0.9929	0.0012	0.9935	0.0012	-0.0006
34	pu-mt016.out	0.9933	0.0011	0.9933	0.0011	0.0000
35	pu-mt029.out	0.9939	0.0013	0.9935	0.0012	0.0004
36	pu-sl078.out	1.0039	0.0012	1.0039	0.0012	-0.0001
37	pu-sl084.out	1.0046	0.0012	1.0044	0.0012	0.0002
38	pu-sl088.out	1.0020	0.0012	1.0033	0.0012	-0.0014
39	pu-sl089.out	1.0024	0.0012	1.0024	0.0012	0.0000
40	pu-sl090.out	1.0060	0.0012	1.0054	0.0012	0.0005
41	pu_sl009.out	1.0015	0.0011	1.0006	0.0012	0.0009
42	pu_sl011.out	1.0029	0.0012	1.0029	0.0012	0.0000
43	pu_sl012.out	1.0002	0.0012	1.0002	0.0012	0.0000
44	pu_sl013.out	1.0110	0.0010	1.0110	0.0010	0.0000
45	pu_sl059.out	1.0057	0.0019	1.0072	0.0012	-0.0015
46	1.out (MTR)	0.9982	0.0015	0.9979	0.0017	0.0003
47	2.out (MTR)	1.0044	0.0016	1.0007	0.0014	0.0037
48	4.out (MTR)	0.9964	0.0016	0.9969	0.0014	-0.0005
49	5.out (MTR)	1.0055	0.0015	1.0047	0.0014	0.0008
50	6.out (MTR)	1.0007	0.0014	1.0002	0.0014	0.0006
51	7.out (MTR)	0.9987	0.0014	1.0003	0.0014	-0.0016
52	8.out (MTR)	0.9959	0.0015	0.9945	0.0013	0.0014
	Mean	0.9968	0.0013	0.9967	0.0013	
	Std. Deviation About Mean	0.0070	0.0003	0.0070	0.0003	

Given that the means and the standard deviations are so close (small differences in the 4th decimal place), and that the bias/bias uncertainties determined in the WSMS validation documents are only reported to three decimal places, the WSMS validation results and the WSRC validation results would be the same. This is due to the fact that a lower tolerance limit is calculated by the equation :

$$K_L = (\text{Mean } K_{eff}) - US_p$$

where U is a constant (one-sided lower tolerance factor) and S_p is the square root of the pooled variance. S_p is given by:

$$S_p = \sqrt{(s)^2 + (\sigma)^2}$$

where s^2 is the variance (standard deviation) about the mean squared, and σ^2 is the average uncertainty squared. As seen in Table B-1, all of these values are the same between the WSRC and WSMS data, except for the mean K_{eff} , which is within one unit of the fourth decimal place. This insignificant difference would vanish due to the truncation of the fourth decimal place when LTL values are reported, yielding the same result.

In conclusion, the above results of the subset comparisons prove that the WSMS MCNP-4B validation serves as an effective validation of the WSRC certified MCNP-4B code, in addition to providing correct and accurate bias and bias uncertainty.