ENCLOSURE 2
ATTACHMENT 2

SHINE MEDICAL TECHNOLOGIES, INC.

SHINE MEDICAL TECHNOLOGIES, INC. APPLICATION FOR CONSTRUCTION PERMIT RESPONSE TO REQUEST FOR ADDITIONAL INFORMATION 6B.3-30

ATKINS-NS-DAC-SHN-15-04, REVISION 0
SINGLE PARAMETER SUBCRITICAL LIMITS FOR HOMOGENEOUS 21 WT% ^{235}U URANYL SULFATE, URANIUM OXIDE, AND URANIUM METAL

22 pages follow

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1 INTRODUCTION

1.1 Background/Purpose

The SHINE Medical Technologies project will use uranium sulfate solution as a subcritical neutron fission target to produce ^{99}Mo for medical uses. In addition, the facility will handle uranium metal as a feed material and uranium oxide for recycling uranium during the process. It is important that those who are designing process vessels and material handling equipment know the subcritical limits applicable to the material being processed. This report will provide such information.

1.2 Limits of Applicability

The results of this report are only applicable to the material types that have been studied at the enrichment limit assumed.

2 CONCLUSIONS

Subcritical limits have been determined as follows:

Table 1: Subcritical Limits for 21 wt% ^{235}U

Material type	Parameter studied	Subcritical limit
Uranyl Sulfate	Mass	3.69 kg U (0.7749 kg ^{235}U)
	Volume	9.14 liters (2.41 gallons)
	Infinite concentration	53.16 g U/l
	Infinite cylinder diameter	6.65 in (16.891 cm)
Uranium Oxide (UO_2)	Mass	3.59 kg U (0.7539 kg ^{235}U)
	Volume	7.82 liters (2.07 gallons)
	Infinite cylinder diameter	6.24 in (15.85 cm)
Uranium Metal	Mass	3.57 kg U (0.7497 kg ^{235}U)
	Volume	6.96 liters (1.84 gallons)
	Infinite cylinder diameter	5.96 in (15.138 cm)

3 ANALYSIS/PROCESS METHODOLOGY

This DAC does not model a process. See Section 7.1 for description of the models and calculation methodology.

4 COMPUTER CODES USED IN DAC

MCNP 6.1 is a general-purpose Monte Carlo N–Particle code that can be used for neutron, photon, electron, or coupled neutron/photon/electron transport, including the capability to calculate eigenvalues for critical systems (Reference 1).

MCNP 6.1 was run on the Atkins' Linux computer cluster. All computers have 64-bit hardware and use the 64-bit version of Linux. Distribution of the calculation jobs among the individual CPUs is controlled by the Sun Grid Engine queue software running on the master Linux computer. Additional Linux execution hosts run calculation jobs at the command of the queue master. MCNP 6.1 has been installed in the read only disk area; the installation has been verified with the execution of the sample problems. This disk is shared with the execution hosts. Hardware and software used with the Atkins Linux computer cluster is managed with the Atkins NS System's configuration control.

MCNP models a physical system with a three-dimensional configuration of geometric cells bounded by first and second-degree surfaces and fourth-degree elliptical tori. Each geometric cell contains a material or void as specified by the user to model the physical system. Material characteristics (i.e., cross sections) are represented by point-wise continuous cross-section data. For neutrons, all reactions given in a particular cross-section library (such as ENDF/B-VII) are taken into account. Thermal neutrons are described by the free gas and $S(\alpha, \beta)$ models. The MCNP neutron data library based on Evaluated Neutron Data File B-VII.1 (ENDF/B-VII.1) is the default for continuous energy neutron transport.

The specific elements used in this evaluation are listed here:

^{235}U	92235.80c
^{238}U	92238.80c
S	16032.80c
H	1001.80c
O	8016.80c

The light water $S(\alpha,\beta)$ correction (lwtr.20t) is used for water.

5 ASSUMPTIONS & OPEN ITEMS

5.1 Assumptions

1. Temperature of all cases is assumed to be 20°C. Higher temperatures will result in lower reactivity due to the increase in neutron absorption due to Doppler broadening of the resonance region within ^{238}U.
2. Solute saturation is assumed to be unlimited. Realistic saturation behavior is ignored in favor of showing the peak reactivity for the various materials regardless of concentration.
3. Uranyl sulfate is modeled assuming no excess acid as a conservative simplification, as excess acid reduces reactivity due to increased neutron absorption and decreased moderation within the solution.
4. Uranium is assumed to be enriched to 21 wt% ^{235}U.

5. Uranium dioxide theoretical density is 10.96 g/cc.
6. Uranium metal theoretical density is 19.05 g/cc.
7. Water theoretical density is 0.9982 g/cc.
8. The following atom masses are assumed for the modeled isotopes and molecules.

^{235}U:	235.04392 g/mole
^{238}U:	238.05079 g/mole
U (21 wt%):	237.42 g/mole
S:	32.064388 g/mole
O:	15.999 g/mole
H:	1.0079 g/mole
H_2O:	18.0148 g/mole
H_2SO_4:	98.076188 g/mole
UO_2SO_4:	365.478 g/mole
UO_2:	269.418 g/mole

9. Avogadro's number is assumed to be 0.6022 atom-cm^2/bn.

5.2 Open Items

There are no open items.

6 ACCEPTANCE CRITERIA

6.1 Biases and Uncertainties

The methodology and results for the MCNP 6.1 code system validation for its use with the SHINE Medical Technologies applications are documented in Reference 2. Criticality safety experiments were selected from the International Handbook of Evaluated Criticality Safety Benchmark Experiments that adequately match the uranium enrichment, geometry, moderator, reflector, and neutron energy relevant to the processes within the SHINE facility. The bias results demonstrate that the calculated values sufficiently matched the reality of the experiments. The final validation is expressed as an Upper Subcritical Limit (USL) calculated using the statistical accumulation of the experiments' bias and bias uncertainty.

The Upper Subcritical Limit (USL) is calculated using the following equation:

USL = 1.0 + Bias – Bias Uncertainty - MOS

where,

MOS = Margin of Subcriticality = 0.05 Δk, and

Bias = 0.0025 Δk (positive bias is set to zero in the equation.)

Bias Uncertainty = 0.0109 Δk

Therefore the USL = 0.9391.

For an acceptable result, the MCNP $k_{eff} + 2 * \sigma$ must be less than the USL value.

6.2 Area of Applicability (AoA)

The AoA derived in Reference 2 is compared to the calculations performed here in Table 2. All parameters are within the AoA of the MCNP 6.1 validation except for the $H/^{235}U$ ratio. The calculations performed with infinite solutions met the USL at very low uranium concentrations resulting in high ratios. However, the Average Neutron Energy Causing Fission (ANECF) parameter is within the AoA and is a good judge of the validity of the USL to the infinite concentration calculation. Additionally, Reference 2 concludes that the $H/^{235}U$ value characterizes the system neutron moderation only as it is affected by the n-H scatter reaction while the MCNP calculated ANECF is a summation of the effect of all n scatter reactions, and is therefore judged to be a more useful parameter when comparing applications to the validation AoA. Therefore, no additional AoA margin is necessary for the infinite concentration cases.

Table 2: Area of Applicability Summary

Parameter	Area of Applicability from Validation	Area of Applicability for Calculations
Fissile Material	UO_2, UH_3, Metal, $UO_2(NO_3)_2$, UF_4, U-ZrH, UO_2F2, U_xO_y, UO_2SO_4	UO_2, Metal, UO_2SO_4
Fissile Material Form	Solid and Solution	Solid and Solution
$H/^{235}U$ ratio	$0 \le H/^{235}U \le 1400$	$45 \le H/^{235}U \le 2319$[1]
Average Neutron Energy Causing Fission (MeV)	0.0027 < ANECF < 1.46	0.0044 < ANECF < 0.104
Enrichment	10 to 36 wt.% ^{235}U	21 wt.% ^{235}U
Moderating Materials	None, Water, nitric acid, sulfuric acid, Hydrocarbon, CF_2	Water, sulfuric acid
Reflecting Materials	None, Water, Concrete, BeO, Hydrocarbon Material, Iron, Graphite	Water
Absorber Materials	Boron, Cadmium, Aluminium, Steel, Stainless Steel, Hydrocarbon Material	None
Geometry	Homogeneous and Heterogeneous Spheres, Hemispheres, Cylinders, Cuboids Single Units and Arrays	Homogeneous Spheres, Cylinders

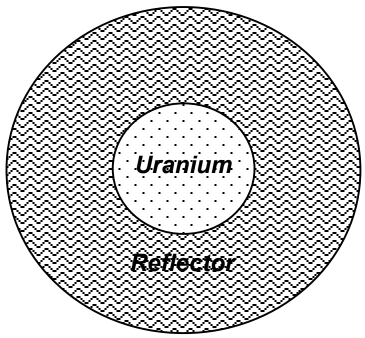
[1] The $H/^{235}U$ value of 2319 corresponds to the infinite concentration calculations. The highest ratio for all other systems is 1233 which is well within the Area of Applicability.

7 CALCULATIONS

7.1 Method Discussion

7.1.1 Geometry Models

For determination of subcritical mass and subcritical volume, a simple sphere model was used. The uranium layer is followed by 12 inches of close-fitting water reflection.



For the infinite fissile solution concentration calculation, a cuboid with a dimension of 200 cm on each side was modeled with a reflective boundary condition on all sides to simulate an infinite amount of material.

For the infinite cylinder, the height of the cylinder was modeled as 200 cm with a reflective boundary condition top and bottom.

7.1.2 Material Specification

Uranyl sulfate, uranium oxide mixed with water, and uranium metal mixed with water were all modeled in this report. The following equations were used to determine the MCNP number density input. MCNP inputs are noted with italics.

Uranyl Sulfate

Uranyl sulfate density is based on an empirical correlation which is specified in Reference 3. No excess acid (molarity = 0, normality = 0) is assumed for conservatism. The temperature is set at 20°C. The following equation was used to determine the uranyl sulfate density:

$$\boldsymbol{\rho_{sol'n}} = \left[\frac{(\boldsymbol{C_U} + \boldsymbol{A})}{\boldsymbol{B} \times \mathbf{10}^{-0.013\boldsymbol{N}}}\right] + \mathbf{0.0003}(\mathbf{25} - \boldsymbol{T})$$

Where:

$\boldsymbol{\rho_{sol'n}} = \ \textbf{\textit{Solution density at T}}℃, \frac{g}{cm^3}$

$\boldsymbol{C_U} = \ \textbf{\textit{Uranium concentration}}, \frac{g}{l}$

$\boldsymbol{T} = \ \textbf{\textit{Temperature}}, ℃$

$\boldsymbol{N} = \ \textbf{\textit{Concentration of free acid in the solution}}\ (\textbf{\textit{moles H}} +/\boldsymbol{L})$

$Constants$	$\leq 150\,\frac{gU}{l}$	$> 150\,\frac{gU}{l}$
A	735.4	743.7
B	737.4	745.4

The uranium concentration is specified which allows the uranyl sulfate solution density to be calculated. Then the number densities for all isotopes can be determined using the following equations:

^{235}U atom density (atoms/bn-cm) = uran_conc/1000 * 235U_wo / 235U_amu * avog
^{238}U atom density (atoms/bn-cm) = uran_conc/1000 * 238U_wo / 238U_amu * avog
U atom density (atoms/bn-cm) = ^{235}U atom density + ^{238}U atom density

UO_2SO_4 density (g/cc) = U atom density/avog * UO2SO4_amu

H_2O density in mix (g/cc) = solution_dens – UO_2SO_4 density

S atom density (atoms/bn-cm) = U atom density
O atom density (atoms/bn-cm) = 6 * (U atom density) + (H_2O density in mix/H2O_amu) * avog
H atom density (atoms/bn-cm) = 2 * (H_2O density in mix/H2O_amu) * avog

where,

uran_conc = uranium concentration in g/liter,
235U_wo = mass fraction of ^{235}U in uranium,
238U_wo = mass fraction of ^{238}U in uranium,
235U_amu = atomic mass of ^{235}U,
238U_amu = atomic mass of ^{238}U,
UO2SO4_amu = atomic mass of UO_2SO_4,
H2O_amu = atomic mass of H_2O.
solution_dens = uranyl sulfate density based on uranium concentration, and
avog = Avogadro's number.

Uranium Oxide and Water

Uranium oxide was modeled as UO_2. This molecule has the least number of oxygen atoms per uranium atoms which will result in the highest reactivity when compared to other oxide compounds (ie. UO_3, U_3O_8, etc.). A simple volume additive relation is used to derive the constituent element atom densities assuming a given uranium density within the mixture. The following equations were used to derive the number densities:

^{235}*U atom density (atoms/bn-cm)* = uran_dens * 235U_wo / 235U_amu * avog
^{238}*U atom density (atoms/bn-cm)* = uran_dens * 238U_wo / 238U_amu * avog
UO_2 density in mixture (g/cc) = uran_dens/U_amu * UO2_amu
H_2O density in mixture (g/cc) = (1 - UO_2 density in mixture/10.96) * 0.9982
O atom density (atoms/bn-cm) = (H_2O density in mixture/H2O_amu) * avog + (2 * UO2 density in mixture/UO2_amu) * avog
H atom density (atoms/bn-cm) = 2 * (H_2O density in mixture/H2O_amu) * avog

where,

uran_dens = uranium density in g/cc,
235U_wo = mass fraction of ^{235}U in uranium,
238U_wo = mass fraction of ^{238}U in uranium,
235U_amu = atomic mass of ^{235}U,
238U_amu = atomic mass of ^{238}U,
U_amu = atomic mass of U,
UO2_amu = atomic mass of UO_2,
H2O_amu = atomic mass of H_2O.
UO_2 density in mixture = uranium dioxide mass density in mixture,
H_2O density in mixture = water mass density in mixture, and
avog = Avogadro's number.

<u>Uranium Metal and Water</u>

A simple volume additive relation is used to derive the constituent element atom densities assuming a uranium metal density within the mixture. The following equations were used to derive the number densities:

^{235}*U atom density (atoms/bn-cm)* = uran_dens * 235U_wo / 235U_amu * avog
^{238}*U atom density (atoms/bn-cm)* = uran_dens * 238U_wo / 238U_amu * avog
H_2O density in mixture (g/cc) = (1 – uran_dens/19.05) * 0.9982
O atom density (atoms/bn-cm) = (H_2O density in mixture/H2O_amu) * avog
H atom density (atoms/bn-cm) = 2 * (H_2O density in mixture/H2O_amu) * avog

where,

uran_dens = uranium density in g/cc,
235U_wo = mass fraction of ^{235}U in uranium,
238U_wo = mass fraction of ^{238}U in uranium,
235U_amu = atomic mass of ^{235}U,
238U_amu = atomic mass of ^{238}U,
H2O_amu = atomic mass of H_2O.
H_2O density in mixture = water mass density in mixture, and
avog = Avogadro's number.

7.1.3 Optimum Value Methodology

For each parameter, a search was performed to find the optimum uranium concentration or density that yields the lowest value. For each uranium concentration, the value at the USL was determined. These values were then compared over the optimum concentration or density range to find the minimum value.

7.2 Evaluations, Analysis, and Detailed Calculations

The results of the single parameter calculations are listed in the following sections.

7.2.1 Uranyl Sulfate Subcritical Mass

Calculations were performed with uranyl sulfate spheres with a uranium concentration ranging from 150 to 300 gU/l. Two data points were calculated at each concentration; one above and one below the USL. Linear interpolation was used to estimate the uranium mass value for the USL of 0.9391. Table 3 presents the MCNP results and Table 4 shows the minimum subcritical uranium mass for each uranium concentration.

Table 3: Uranyl Sulfate Sphere MCNP Results for Minimum Subcritical Mass

Case	Uranium Concentration (gU/l)	Sphere Diameter (cm)	k_{eff}	σ	$k_{eff}+2\sigma$	Sphere Volume (l)	Uranium Mass (kg)
sphere_sulfate_150_37.2	150	37.2	0.93437	0.00076	0.93589	26.95	4.04
sphere_sulfate_150_37.4	150	37.4	0.93779	0.00070	0.93919	27.39	4.11
sphere_sulfate_200_32.8	200	32.8	0.93691	0.00079	0.93849	18.48	3.70
sphere_sulfate_200_33	200	33	0.93881	0.00072	0.94025	18.82	3.76
sphere_sulfate_225_31.4	225	31.4	0.93494	0.00075	0.93644	16.21	3.65
sphere_sulfate_225_31.6	225	31.6	0.93855	0.00094	0.94043	16.52	3.72
sphere_sulfate_250_30.4	250	30.4	0.93541	0.00077	0.93695	14.71	3.68
sphere_sulfate_250_30.6	250	30.6	0.94087	0.00082	0.94251	15.00	3.75
sphere_sulfate_300_29	300	29	0.93687	0.00078	0.93843	12.77	3.83
sphere_sulfate_300_29.2	300	29.2	0.93912	0.00080	0.94072	13.04	3.91

Table 4: Minimum Subcritical Mass for each Uranyl Sulfate Uranium Concentration

Uranium Concentration (gU/l)	Subcritical Uranium Mass (kg)
150	4.11
200	3.72
225	3.69
250	3.71
300	3.85

Examination of the Table 4 results shows a subcritical uranium mass limit of 3.69 kg U for uranyl sulfate.

7.2.2 Uranyl Sulfate Subcritical Volume

Calculations were performed with uranyl sulfate spheres with a uranium concentration ranging from 600 to 1200 gU/l. Two data points were calculated at each concentration; one above and one below the USL. Linear interpolation was used to estimate the uranium volume value for the

USL of 0.9391. Table 5 presents the MCNP results and Table 6 shows the minimum subcritical uranium volume for each uranium concentration.

Table 5: Uranyl Sulfate Sphere MCNP Results for Minimum Subcritical Volume

Case	Uranium Concentration (gU/l)	Sphere Diameter (cm)	k_{eff}	σ	k_{eff}+2σ	Sphere Volume (l)
sphere_sulfate_600_26.2	600	26.2	0.93691	0.00095	0.93881	9.42
sphere_sulfate_600_26.3	600	26.3	0.93931	0.00097	0.94125	9.53
sphere_sulfate_700_25.9	700	25.9	0.93471	0.00089	0.93649	9.10
sphere_sulfate_700_26	700	26	0.93730	0.00092	0.93914	9.20
sphere_sulfate_800_25.9	800	25.9	0.93549	0.00088	0.93725	9.10
sphere_sulfate_800_26	800	26	0.94017	0.00091	0.94199	9.20
sphere_sulfate_900_25.9	900	25.9	0.93343	0.00096	0.93535	9.10
sphere_sulfate_900_26	900	26	0.93831	0.00085	0.94001	9.20
sphere_sulfate_1000_26.1	1000	26.1	0.93720	0.00089	0.93898	9.31
sphere_sulfate_1000_26.2	1000	26.2	0.94093	0.00093	0.94279	9.42
sphere_sulfate_1100_26.4	1100	26.4	0.93711	0.00095	0.93901	9.63
sphere_sulfate_1100_26.5	1100	26.5	0.94104	0.00097	0.94298	9.74
sphere_sulfate_1200_26.5	1200	26.5	0.93548	0.00097	0.93742	9.74
sphere_sulfate_1200_26.6	1200	26.6	0.93740	0.00092	0.93924	9.85

Table 6: Minimum Subcritical Volume for each Uranyl Sulfate Uranium Concentration

Uranium Concentration (gU/l)	Subcritical Volume (l)
600	9.43
700	9.20
800	9.14
900	9.18
1000	9.31
1100	9.64
1200	9.85

Examination of the Table 6 results shows a subcritical uranium volume limit of 9.14 liters for uranyl sulfate.

7.2.3 Uranyl Sulfate Infinite Subcritical Concentration

Calculations were performed with an infinite amount of uranyl sulfate with a uranium concentration of 53.0 and 53.2 gU/l. Table 7 presents the MCNP results.

Table 7: Infinite Subcritical Concentration MCNP Results for Uranyl Sulfate

Case	Uranium Concentration (gU/l)	k_{eff}	σ	k_{eff}+2σ
inf_sulfate_53	53.0	0.93730	0.00020	0.93770
inf_sulfate_53.2	53.2	0.93906	0.00019	0.93944

Linear interpolation of the Table 7 results shows an infinite subcritical uranium concentration limit of 53.16 gU/l for uranyl sulfate.

7.2.4 Uranyl Sulfate Subcritical Cylinder Diameter

Calculations were performed with uranyl sulfate cylinders of infinite height with a uranium concentration ranging from 600 to 1100 gU/l. Two data points were calculated at each concentration; one above and one below the USL. Linear interpolation was used to estimate the cylinder diameter value for the USL of 0.9391. Table 8 presents the MCNP results and Table 9 shows the minimum subcritical cylinder diameter for each uranium concentration.

Table 8: Uranyl Sulfate Cylinder MCNP Results for Minimum Cylinder Diameter

Case	Uranium Concentration (gU/l)	Cylinder Diameter (in)	k_{eff}	σ	k_{eff}+2σ
cyl_sulfate_600_6.75	600	6.75	0.93662	0.00085	0.93832
cyl_sulfate_600_6.8	600	6.8	0.94178	0.00087	0.94352
cyl_sulfate_700_6.65	700	6.65	0.93542	0.00086	0.93714
cyl_sulfate_700_6.7	700	6.7	0.93828	0.00079	0.93986
cyl_sulfate_800_6.64	800	6.64	0.93523	0.00080	0.93683
cyl_sulfate_800_6.65	800	6.65	0.93784	0.00097	0.93978
cyl_sulfate_850_6.65	850	6.65	0.93584	0.00090	0.93764
cyl_sulfate_850_6.66	850	6.66	0.93837	0.00088	0.94013
cyl_sulfate_900_6.64	900	6.64	0.93706	0.00084	0.93874
cyl_sulfate_900_6.66	900	6.66	0.93781	0.00081	0.93943
cyl_sulfate_1000_6.65	1000	6.65	0.93466	0.00072	0.93610
cyl_sulfate_1000_6.7	1000	6.7	0.93978	0.00101	0.94180
cyl_sulfate_1100_6.7	1100	6.7	0.93492	0.00083	0.93658
cyl_sulfate_1100_6.75	1100	6.75	0.94029	0.00081	0.94191

Table 9: Minimum Subcritical Cylinder Diameter for each Uranyl Sulfate Uranium Concentration

Uranium Concentration (gU/l)	Cylinder Diameter (in)
600	6.76
700	6.69
800	6.65
850	6.66
900	6.65
1000	6.68
1100	6.72

Examination of the Table 9 results shows a subcritical cylinder diameter limit of 6.65 inches for uranyl sulfate.

7.2.5 Uranium Oxide Subcritical Mass

Calculations were performed with uranium dioxide spheres with a uranium density ranging from 0.15 to 0.35 gU/cc. Two data points were calculated at each density; one below and one above the USL. Linear interpolation was used to estimate the uranium mass value for the USL of 0.9391. Table 10 presents the MCNP results and Table 11 shows the minimum subcritical uranium mass for each uranium density.

Table 10: Uranium Dioxide Sphere MCNP Results for Minimum Subcritical Mass

Case	Uranium Density (gU/cc)	Sphere Diameter (cm)	k_{eff}	σ	k_{eff}+2σ	Uranium Mass (kg)
sphere_oxide_0.15_37	0.15	37	0.93333	0.00062	0.93457	3.98
sphere_oxide_0.15_37.5	0.15	37.5	0.94027	0.00073	0.94173	4.14
sphere_oxide_0.2_32.6	0.2	32.6	0.93531	0.00084	0.93699	3.63
sphere_oxide_0.2_32.7	0.2	32.7	0.93828	0.00080	0.93988	3.66
sphere_oxide_0.225_31.2	0.225	31.2	0.93680	0.00077	0.93834	3.58
sphere_oxide_0.225_31.3	0.225	31.3	0.93800	0.00076	0.93952	3.61
sphere_oxide_0.25_30.1	0.25	30.1	0.93458	0.00084	0.93626	3.57
sphere_oxide_0.25_30.2	0.25	30.2	0.93872	0.00089	0.94050	3.61
sphere_oxide_0.3_28.6	0.3	28.6	0.93457	0.00080	0.93617	3.67
sphere_oxide_0.3_28.7	0.3	28.7	0.93759	0.00086	0.93931	3.71
sphere_oxide_0.35_27.6	0.35	27.6	0.93652	0.00077	0.93806	3.85
sphere_oxide_0.35_27.7	0.35	27.7	0.93830	0.00069	0.93968	3.89

Table 11: Minimum Subcritical Mass for each Uranium Dioxide Uranium Density

Uranium Density (gU/cc)	Subcritical Uranium Mass (kg)
0.15	4.08
0.2	3.65
0.225	3.60
0.25	3.59
0.3	3.71
0.35	3.88

Examination of the Table 11 results shows a subcritical uranium mass limit of 3.59 kg U for uranium dioxide.

7.2.6 Uranium Oxide Subcritical Volume

Calculations were performed with uranium dioxide spheres with a uranium density ranging from 0.8 to 1.4 gU/cc. Seven data points were calculated at each density. Linear interpolation was used to estimate the uranium volume value for the USL of 0.9391. Table 12 presents the MCNP results and Table 13 shows the minimum subcritical volume for each uranium density.

Table 12: Uranium Dioxide Sphere MCNP Results for Minimum Subcritical Volume

Case	Uranium Density (gU/cc)	Sphere Diameter (cm)	k_{eff}	σ	$k_{eff}+2\sigma$	Sphere Volume (l)
sphere_oxide_0.8_24.8	0.8	24.8	0.93579	0.00088	0.93755	7.99
sphere_oxide_0.8_24.85	0.8	24.85	0.93798	0.00083	0.93964	8.03
sphere_oxide_0.85_24.75	0.85	24.75	0.93594	0.00075	0.93744	7.94
sphere_oxide_0.85_24.8	0.85	24.8	0.93742	0.00093	0.93928	7.99
sphere_oxide_0.9_24.65	0.9	24.65	0.93366	0.00095	0.93556	7.84
sphere_oxide_0.9_24.7	0.9	24.7	0.93783	0.00099	0.93981	7.89
sphere_oxide_1_24.65	1	24.65	0.93696	0.00094	0.93884	7.84
sphere_oxide_1_24.7	1	24.7	0.93802	0.00094	0.93990	7.89
sphere_oxide_1.05_24.6	1.05	24.6	0.93467	0.00096	0.93659	7.79
sphere_oxide_1.05_24.65	1.05	24.65	0.93796	0.00080	0.93956	7.84
sphere_oxide_1.1_24.6	1.1	24.6	0.93646	0.00091	0.93828	7.79
sphere_oxide_1.1_24.65	1.1	24.65	0.93812	0.00090	0.93992	7.84
sphere_oxide_1.2_24.6	1.2	24.6	0.93676	0.00081	0.93838	7.79
sphere_oxide_1.2_24.65	1.2	24.65	0.93778	0.00097	0.93972	7.84
sphere_oxide_1.3_24.7	1.3	24.7	0.93564	0.00088	0.93740	7.89
sphere_oxide_1.3_24.75	1.3	24.75	0.93735	0.00097	0.93929	7.94
sphere_oxide_1.4_24.75	1.4	24.75	0.93342	0.00092	0.93526	7.94
sphere_oxide_1.4_24.8	1.4	24.8	0.93749	0.00095	0.93939	7.99

Table 13: Minimum Subcritical Volume for each Uranium Dioxide Uranium Density

Uranium Density (gU/cc)	Subcritical Volume (l)
0.8	8.02
0.9	7.98
1	7.88
1.05	7.84
1.1	7.82
1.2	7.82
1.3	7.93
1.4	7.98

Examination of the Table 13 results shows a subcritical uranium volume limit of 7.82 liters for uranium oxide.

7.2.7 Uranium Oxide Subcritical Cylinder Diameter

Calculations were performed with uranium dioxide cylinders of infinite height with a uranium density ranging from 0.8 to 1.5 gU/cc. Two data points were calculated at each density; one below and one above the USL. Linear interpolation was used to estimate the cylinder diameter

value for the USL of 0.9391. Table 14 presents the MCNP results and Table 15 shows the minimum subcritical cylinder diameter for each uranium density.

Table 14: Uranium Dioxide Cylinder MCNP Results for Minimum Cylinder Diameter

Case	Uranium Density (gU/cc)	Cylinder Diameter (in)	k_{eff}	σ	$k_{eff}+2\sigma$
cyl_oxide_0.8_6.3	0.8	6.3	0.93422	0.00094	0.93610
cyl_oxide_0.8_6.35	0.8	6.35	0.93815	0.00092	0.93999
cyl_oxide_0.9_6.25	0.9	6.25	0.93414	0.00086	0.93586
cyl_oxide_0.9_6.3	0.9	6.3	0.93946	0.00080	0.94106
cyl_oxide_1_6.25	1	6.25	0.93583	0.00078	0.93739
cyl_oxide_1_6.3	1	6.3	0.94183	0.00077	0.94337
cyl_oxide_1.1_6.2	1.1	6.2	0.93412	0.00088	0.93588
cyl_oxide_1.1_6.25	1.1	6.25	0.93790	0.00085	0.93960
cyl_oxide_1.2_6.2	1.2	6.2	0.93341	0.00077	0.93495
cyl_oxide_1.2_6.25	1.2	6.25	0.93847	0.00091	0.94029
cyl_oxide_1.3_6.2	1.3	6.2	0.93296	0.00096	0.93488
cyl_oxide_1.3_6.25	1.3	6.25	0.93837	0.00087	0.94011
cyl_oxide_1.4_6.25	1.4	6.25	0.93624	0.00091	0.93806
cyl_oxide_1.4_6.3	1.4	6.3	0.94098	0.00086	0.94270
cyl_oxide_1.5_6.25	1.5	6.25	0.93575	0.00094	0.93763
cyl_oxide_1.5_6.3	1.5	6.3	0.93930	0.00080	0.94090

Table 15: Minimum Subcritical Cylinder Diameter for each Uranium Dioxide Density

Uranium Density (gU/cc)	Cylinder Diameter (in)
0.8	6.34
0.9	6.28
1.0	6.26
1.1	6.24
1.2	6.24
1.3	6.24
1.4	6.26
1.5	6.27

Examination of the Table 15 results shows a subcritical cylinder diameter limit of 6.24 inches for uranium oxide.

7.2.8 Uranium Metal Subcritical Mass

Calculations were performed with uranium metal spheres with a uranium density ranging from 0.10 to 0.30 gU/cc. Two data points were calculated at each density; one below and one above the USL. Linear interpolation was used to estimate the uranium mass value for the USL of

0.9391. Table 16 presents the MCNP results and Table 17 shows the minimum subcritical uranium mass for each uranium density.

Table 16: Uranium Metal Sphere MCNP Results for Minimum Subcritical Mass

Case	Uranium Density (gU/cc)	Sphere Diameter (cm)	k_{eff}	σ	k_{eff}+2σ	Uranium Mass (kg)
sphere_metal_0.1_49	0.1	49	0.93316	0.00064	0.93444	6.16
sphere_metal_0.1_50	0.1	50	0.94189	0.00061	0.94311	6.54
sphere_metal_0.15_37.3	0.15	37.3	0.93700	0.00064	0.93828	4.08
sphere_metal_0.15_37.4	0.15	37.4	0.93850	0.00067	0.93984	4.11
sphere_metal_0.2_32.6	0.2	32.6	0.93682	0.00070	0.93822	3.63
sphere_metal_0.2_32.7	0.2	32.7	0.93876	0.00074	0.94024	3.66
sphere_metal_0.225_31.2	0.225	31.2	0.93557	0.00080	0.93717	3.58
sphere_metal_0.225_31.3	0.225	31.3	0.94079	0.00079	0.94237	3.61
sphere_metal_0.25_30	0.25	30	0.93379	0.00080	0.93539	3.53
sphere_metal_0.25_30.1	0.25	30.1	0.93775	0.00082	0.93939	3.57
sphere_metal_0.3_28.5	0.3	28.5	0.93648	0.00086	0.93820	3.64
sphere_metal_0.3_28.6	0.3	28.6	0.93835	0.00086	0.94007	3.67

Table 17: Minimum Subcritical Mass for each Uranium Metal Density

Uranium Density (gU/cc)	Subcritical Uranium Mass (kg)
0.10	6.37
0.15	4.09
0.20	3.64
0.225	3.59
0.25	3.57
0.30	3.65

Examination of the Table 17 results shows a subcritical uranium mass limit of 3.57 kg U for uranium metal.

7.2.9 Uranium Metal Subcritical Volume

Calculations were performed with uranium metal spheres with a uranium density ranging from 0.8 to 2.0 gU/cc. Two data points were calculated at each density; one below and one above the USL. Linear interpolation was used to estimate the volume for the USL of 0.9391. Table 18 presents the MCNP results and Table 19 shows the minimum subcritical volume for each uranium density.

Table 18: Uranium Metal Sphere MCNP Results for Minimum Subcritical Volume

Case	Uranium Density (gU/cc)	Sphere Diameter (cm)	k_{eff}	σ	$k_{eff}+2\sigma$	Sphere Volume (l)
sphere_metal_0.8_24.2	0.8	24.2	0.93353	0.00087	0.93527	7.42
sphere_metal_0.8_24.3	0.8	24.3	0.93849	0.00094	0.94037	7.51
sphere_metal_0.9_24.1	0.9	24.1	0.93718	0.00085	0.93888	7.33
sphere_metal_0.9_24.2	0.9	24.2	0.93958	0.00097	0.94152	7.42
sphere_metal_1_23.9	1	23.9	0.93542	0.00091	0.93724	7.15
sphere_metal_1_24	1	24	0.93791	0.00090	0.93971	7.24
sphere_metal_1.1_23.9	1.1	23.9	0.93673	0.00097	0.93867	7.15
sphere_metal_1.1_24	1.1	24	0.94201	0.00082	0.94365	7.24
sphere_metal_1.2_23.7	1.2	23.7	0.93450	0.00097	0.93644	6.97
sphere_metal_1.2_23.8	1.2	23.8	0.93861	0.00081	0.94023	7.06
sphere_metal_1.3_23.7	1.3	23.7	0.93462	0.00090	0.93642	6.97
sphere_metal_1.3_23.8	1.3	23.8	0.94058	0.00093	0.94244	7.06
sphere_metal_1.4_23.7	1.4	23.7	0.93557	0.00090	0.93737	6.97
sphere_metal_1.4_23.8	1.4	23.8	0.93978	0.00102	0.94182	7.06
sphere_metal_1.5_23.7	1.5	23.7	0.93603	0.00084	0.93771	6.97
sphere_metal_1.5_23.72	1.5	23.72	0.93744	0.00093	0.93930	6.99
sphere_metal_1.6_23.6	1.6	23.6	0.93419	0.00090	0.93599	6.88
sphere_metal_1.6_23.7	1.6	23.7	0.93749	0.00094	0.93937	6.97
sphere_metal_1.7_23.7	1.7	23.7	0.93651	0.00090	0.93831	6.97
sphere_metal_1.7_23.8	1.7	23.8	0.94007	0.00100	0.94207	7.06
sphere_metal_1.8_23.7	1.8	23.7	0.93597	0.00097	0.93791	6.97
sphere_metal_1.8_23.8	1.8	23.8	0.93924	0.00097	0.94118	7.06
sphere_metal_1.9_23.8	1.9	23.8	0.93706	0.00087	0.93880	7.06
sphere_metal_1.9_23.9	1.9	23.9	0.94004	0.00101	0.94206	7.15
sphere_metal_2_23.7	2	23.7	0.93426	0.00093	0.93612	6.97
sphere_metal_2_23.8	2	23.8	0.93827	0.00091	0.94009	7.06

Table 19: Minimum Subcritical Volume for each Uranium Metal Uranium Density

Uranium Density (gU/cc)	Subcritical Volume (l)
0.8	7.49
0.9	7.34
1	7.22
1.1	7.16

Uranium Density (gU/cc)	Subcritical Volume (l)
1.2	7.03
1.3	7.01
1.4	7.00
1.5	6.99
1.6	6.96
1.7	6.99
1.8	7.00
1.9	7.07
2	7.04

Examination of the Table 19 results shows a subcritical uranium volume limit of 6.96 liters for uranium metal.

7.2.10 Uranium Metal Subcritical Cylinder Diameter

Calculations were performed with uranium metal cylinders of infinite height with a uranium density ranging from 1.2 to 2.4 gU/cc. Two data points were calculated at each density; one below and one above the USL. Linear interpolation was used to estimate the cylinder diameter value for the USL of 0.9391. Table 20 presents the MCNP results and Table 21 shows the minimum subcritical cylinder diameter for each uranium density.

Table 20: Uranium Metal Cylinder MCNP Results for Minimum Cylinder Diameter

Case	Uranium Density (gU/cc)	Cylinder Diameter (in)	k_{eff}	σ	$k_{eff}+2\sigma$
cyl_metal_1.2_6	1.2	6	0.93724	0.00090	0.93904
cyl_metal_1.2_6.02	1.2	6.02	0.93918	0.00082	0.94082
cyl_metal_1.4_5.96	1.4	5.96	0.93624	0.00090	0.93804
cyl_metal_1.4_5.98	1.4	5.98	0.93865	0.00094	0.94053
cyl_metal_1.6_5.94	1.6	5.94	0.93684	0.00093	0.93870
cyl_metal_1.6_5.96	1.6	5.96	0.93821	0.00090	0.94001
cyl_metal_1.8_5.96	1.8	5.96	0.93747	0.00071	0.93889
cyl_metal_1.8_5.98	1.8	5.98	0.94005	0.00089	0.94183
cyl_metal_2_5.94	2	5.94	0.93390	0.00090	0.93570
cyl_metal_2_5.96	2	5.96	0.93813	0.00090	0.93993
cyl_metal_2.2_5.96	2.2	5.96	0.93610	0.00070	0.93750
cyl_metal_2.2_5.98	2.2	5.98	0.93820	0.00090	0.94000
cyl_metal_2.4_5.98	2.4	5.98	0.93643	0.00072	0.93787
cyl_metal_2.4_6	2.4	6	0.93821	0.00084	0.93989

Table 21: Minimum Subcritical Cylinder Diameter for each Uranium Metal Density

Uranium Density (gU/cc)	Cylinder Diameter (in)
1.2	6.00
1.4	5.97
1.6	5.95
1.8	5.96
2.0	5.96
2.2	5.97
2.4	5.99

Examination of the Table 21 results shows a subcritical cylinder diameter limit of 5.96 in. for uranium metal.

8 REFERENCES

1. *MCNP6 USER MANUAL,* LA-CP-13-00634, Rev. 0, Los Alamos National Laboratory, May 2013.
2. Revolinski, S., *MCNP 6.1 Validation with Continuous Energy ENDF/B-VII.1 Cross Sections for SHINE Medical Technologies*, Atkins-NS-DAC-SHN-15-03, Rev. 1, June 2015.
3. Glunz, H., *V and V Report: Uranyl Sulfate Solution Densities*, NSA-TR-SHN-12-03, Rev. 1, February 2012.

APPENDIX 1: REPRESENTATIVE INPUT FILES

Sphere Model

All sphere model inputs are a variation of the model described in this input file, with case descriptive information, sphere radii and material #1 changed as appropriate.

```
Uranyl Sulfate Sphere at          150 g/l,         37.2 cm dia
c
c Uranium Concentration =          150
c Acid molarity =            0
c Soln temperautre =           20
c Sphere diameter =          37.2
c Sphere volume =        26954
c Sphere mass =       4043.1
c
c cells
1 1       -1.2022 -10   imp:n=1
2 15 -0.9982 -20 10       imp:n=1
3 0 20                   imp:n=0

c surfaces
10 so         18.6
20 so        49.08

c Data
kcode 5000 1.0 100 300
ksrc 0 0 0
c materials
c           150 g/L U
c Density (g/cm3):        1.2022
m1      92235.80c  8.0705e-05
        92238.80c  2.9977e-04
        16032.80c  3.6153e-04
        16033.80c  2.8536e-06
        16034.80c  1.6018e-05
        16036.80c  7.6095e-08
         8016.80c  3.4751e-02
         1001.80c  6.4937e-02
mt1     lwtr.20t
c Water (0.9982 g/cc)
m15 1001.80c 2  8016.80c 1
mt15 lwtr.20t
```

Infinite Concentration Model

All infinite concentration inputs are a variation of the model described in this input file, with case descriptive information and material #1 changed as appropriate.

```
Uranyl Sulfate Sphere at          53 g/l,           0 cm dia
c
c Uranium Concentration =          53
c Acid molarity =            0
c Soln temperature =           20
c
c cells
1 1      -1.0707 -10 11 -12 13 -14 15 imp:n=1
3 0 #1                                 imp:n=0

c surfaces
*10 px  100
*11 px -100
*12 py  100
*13 py -100
*14 pz  100
*15 pz -100

c Data
kcode 5000 1.0 100 300
ksrc 0 0 0
c materials
c           53 g/L U
c Density (g/cm3):        1.0707
m1      92235.80c  2.8516e-05
        92238.80c  1.0592e-04
        16032.80c  1.2774e-04
        16033.80c  1.0083e-06
        16034.80c  5.6597e-06
        16036.80c  2.6887e-08
         8016.80c  3.3869e-02
         1001.80c  6.6126e-02
mt1     lwtr.20t
```

Infinite Cylinder Model

All infinite cylinder inputs are a variation of the model described in this input file, with case descriptive information, cylinder radii and material #1 changed as appropriate.

```
Uranyl Sulfate Cylinder at        1000 g/l,          6.7 in dia
c
c Uranium Concentration =        1000
c Soltn Dens =       2.3408
c Excess acid (M) =           0
c Temperature (C) =          20
c Cylinder diameter (in) =        6.7
c
c cells
1 1      -2.3408 -10 -12 14  imp:n=1
2 15 -0.9982 -20 10 -12 14     imp:n=1
3 0 (20:12:-14)               imp:n=0

c surfaces
10 cz        8.509
*12 pz  100
*14 pz -100
20 cz       38.989

c Data
kcode 5000 1.0 100 300
ksrc 0 0 0
c materials
c         1000 g/L U
c Density (g/cm3):        2.3408
m1      92235.80c  5.3804e-04
        92238.80c  1.9985e-03
        16032.80c  2.4102e-03
        16033.80c  1.9024e-05
        16034.80c  1.0679e-04
        16036.80c  5.0730e-07
         8016.80c  4.2008e-02
         1001.80c  5.3578e-02
mt1     lwtr.20t
c Water (0.9982 g/cc)
m15 1001.80c 2  8016.80c 1
mt15 lwtr.20t
```