ENCLOSURE 2
ATTACHMENT 11

SHINE MEDICAL TECHNOLOGIES, INC.

SHINE MEDICAL TECHNOLOGIES, INC. APPLICATION FOR CONSTRUCTION PERMIT RESPONSE TO REQUEST FOR ADDITIONAL INFORMATION

NSA-TR-SHN-13-05, REVISION 1
SHINE PHYSICS VALIDATION

53 pages follow

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1.0 INTRODUCTION

SHINE Medical Technologies is designing a system to generate molybdenum-99 for use as a medical isotope. The SHINE system is described in detail in Reference 7. In summary the system consists of (1) a neutron driver defined by an accelerator deuteron source directed into tritium target generating high energy fusion neutrons that pass through (2) a [Proprietary Information] neutron multiplier resulting in a spectrum of [Proprietary Information] neutrons which then enter (3) a Target Solution Vessel (TSV) containing uranyl sulfate (UO_2SO_4) in solution.

The purpose of this technical report is to document a validation of the calculational methods, specifically the MCNP5-1.60 code (with [Proprietary Information] cross-sections), used to analyze the SHINE system. ANSI/ANS-19.3 (Reference 8) requires that calculational methods used for steady-state neutronics calculations of reactor systems (e.g., neutron reaction-rate spatial distributions, power distributions, and effective neutron multiplication constants of nuclear power reactors) be validated to determine any appropriate biases and uncertainties for the areas of applicability (AoAs). Bias represents any numerical difference between the results of modeling benchmark experiments with a computer code and the experimental results.

2.0 ASSUMPTIONS

The modeling assumptions made for the benchmark experiments are consistent with those described in Reference 1.

3.0 COMPUTER CODES

a. MCNP5-1.60 (Reference 2), the Los Alamos National Laboratory (LANL) Monte Carlo N-Particle (MCNP) radiation transport code was used to calculate eigenvalues of the benchmark systems, as well as effective delayed neutron fractions for the calculation of mean neutron lifetime. MCNP5-1.60 is developed and maintained under a configuration management plan by LANL. The code is distributed by the Radiation Safety Information Computational Center (RSICC).

   The installation of MCNP5 version 1.60 has been verified on the NSA system. The NSA system is a computer cluster composed of several servers that use Intel processors running the Fedora Linux operating system. MCNP5 has been installed in the read only disk area; the installation has been verified with the execution of the sample problems (Reference 3).

b. ORIGEN-S (Reference 4), a module of the larger SCALE-6.1 (Standardized Computer Analyses for Licensing Evaluations) computational system from Oak Ridge National Laboratory (ORNL), was used to generate fission product inventories for the calculation of mean neutron lifetime. As part of the larger SCALE computational system the ORIGEN-S code is developed and maintained under a configuration management plan by

ORNL. The code is distributed by the Radiation Safety Information Computational Center (RSICC).

The installation of ORIGEN-S/SCALE6.1 has been verified on the NSA system. The NSA system is a computer cluster composed of several servers that use Intel processors running the Fedora Linux operating system. SCALE6.1 has been installed in the read only disk area; the installation has been verified with the execution of the sample problems (Reference 5).

c. Microsoft Office Excel, 2010. The Excel spreadsheet software was used to process ORIGEN-S and MCNP5 calculation results. The calculations consist of mathematical equations which can be verified by hand calculations.

Computer type: Dell Latitude E6520
Operating System: Microsoft Windows 7
Serial Numbers: NSA-211

4.0 BENCHMARKS

The following subsections describe two benchmarks involving uranyl sulfate solutions taken from the International Handbook of Evaluated Criticality Safety Benchmark Experiments (Reference 1). Each of the benchmarks involves multiple individual cases that are modeled herein using MCNP5-1.60. The MCNP5 results are then compared to the sample results presented in Reference 1. Appendix A of this report contains an MCNP5 input listing for each of the benchmark cases.

Note that the methodology employed herein compares the MCNP5 results to the sample calculations provided in both benchmarks using the MCU code (IEU-SOL-THERM-001) and the APOLLO-MORET code suite (HEU-SOL-THERM-046), both of which employ Monte Carlo techniques. The benchmark experimental results for these two benchmarks were deemed to be unacceptable for direct validation because of the unresolved historical differences between them and results calculated by other physics codes (average $\Delta k = -0.021$ for IST-001 and average $\Delta k = 0.014$ for HST-046). Given the lack of other suitable uranyl sulfate benchmarks, it was judged that a favorable comparison of MCNP5 results to the results of these other codes provides the best available measure of MCNP5's ability to suitably model the benchmark systems.

One other potential benchmark was identified: the LOPO low power reactor built in 1944 at the Los Alamos National Laboratory. This reactor consisted of a one foot diameter stainless steel spherical shell, reflected by beryllium oxide on a graphite base. The vessel was filled with a homogeneous uranyl sulfate solution enriched to 14 wt.% ^{235}U. However, sufficient data could not be located to accurately model the reactor, and it was dismissed as a benchmark.

4.1 IEU-SOL-THERM-001

The purpose of these experiments, performed at the Russian Research Center "Kurchatov Institute" in 1980-1981, was to investigate nuclear safety issues for a special-purpose compact reactor with an aqueous solution of uranyl sulfate (~20.71 wt.% ^{235}U) and graphite reflector. Four configurations of critical assemblies with different concentrations of uranium in the solution were included, with the solution volume controlled to achieve criticality.

An aqueous solution of uranyl sulfate was placed in the core vessel, a welded steel cylinder with a hemispherical bottom and a lid, the latter penetrated by vertically arranged steel pipes which form leak-tight channels. Core vessels of two wall thicknesses were used (0.5 cm and 0.3 cm), both with an inner diameter of 30.5 mm. The thicker vessel was 71.5 cm high from its end to the inner surface of the bottom (along the axis), and its cylindrical part is 56.25 cm long. A coiled cooling pipe was placed inside the vessel.

The core vessel was surrounded with a graphite reflector which contains five vertical channels and one horizontal channel machined into the graphite blocks. The vessel was recessed into the graphite reflector to a depth of 65.6 cm from the reflector top. The side surfaces of the graphite reflector were surrounded by a shield of borated polyethylene. On top of the reflector was a steel plate.

The geometry of the experiment is depicted in Figure 1.

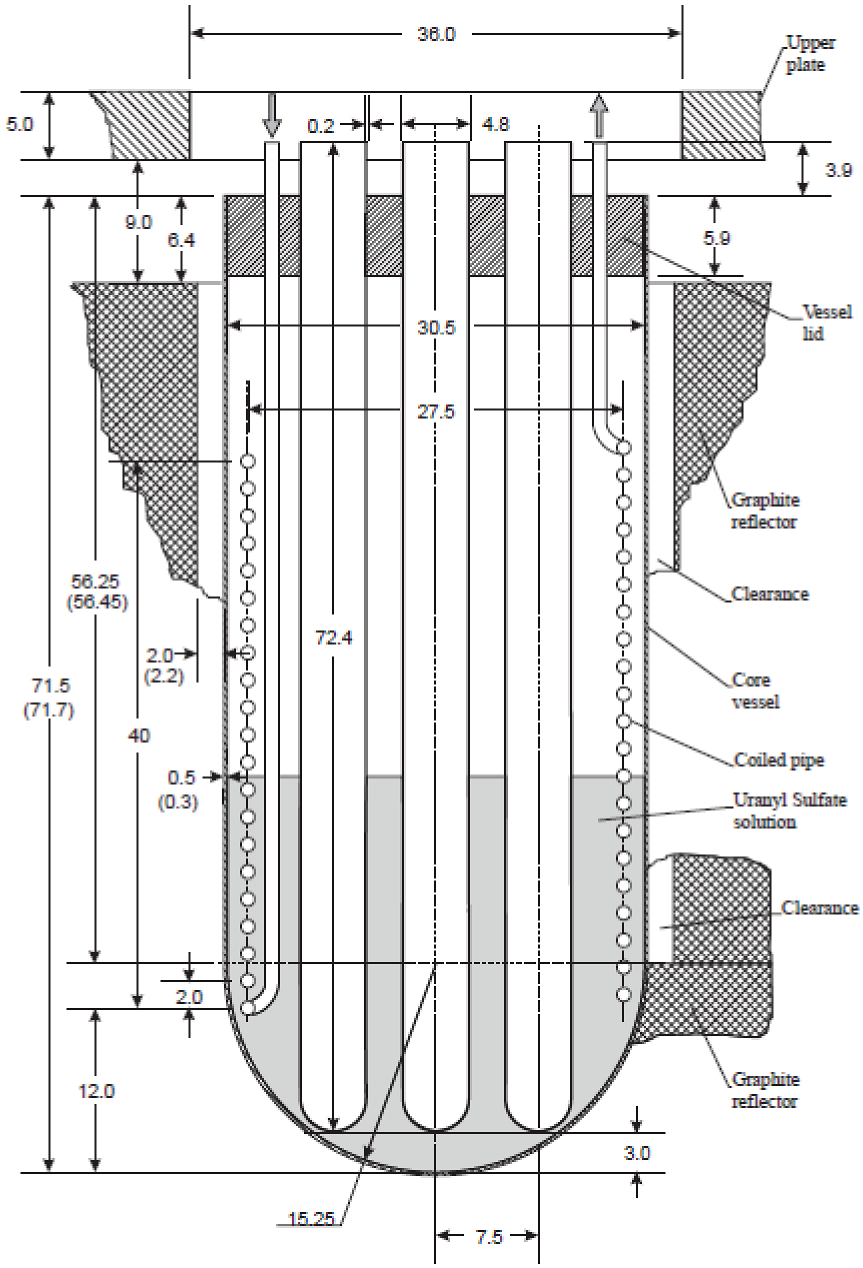

Figure 1 – IEU-SOL-THERM-001 Reactor

The benchmark model was developed from calculational models describing the actual critical experiments. In Reference 1, the model was simplified while preparing the benchmark specifications. The following components of the assembly, whose effects on criticality were found to be insignificant in Reference 1, were excluded:

- impurities in fissile solution and graphite
- some structural elements in the assembly and around it
- room reflection

The sample calculation results from the benchmark summary report, along with pertinent nuclear parameters for each case, are presented in Table 1. See Reference 1 for more detailed information.

Table 1 – IEU-SOL-THERM-001 Sample Calculations

Case	Case	Sample k_{EFF}	Sample σ	$H/^{235}U$*	g U/l	g ^{235}U/l
1	ist1-1	0.9855	0.0013	444.0	263.3	54.5
2	ist1-2	0.9807	0.0013	297.4	382.2	79.2
3	ist1-3	0.9777	0.0013	297.4	382.2	79.2
4	ist1-4	0.9735	0.0014	217.4	505.0	104.6

* This is the moderation ratio, the ratio of hydrogen atoms to 235U atoms in the fuel solution.

4.2 HEU-SOL-THERM-046

A series of subcritical high-multiplication approaches and critical experiments was performed with the Proserpine solution reactor in 1960 through 1961 at Saclay, France, using homogeneous aqueous solutions of uranium sulfate (89.84 wt. % ^{235}U), containing 0.1 N excess sulfuric acid. This benchmark includes thirteen subcritical approaches, with ^{235}U concentrations ranging between 36.588 to 56.51 g/liter. The experiments were performed to determine empirical critical-mass data for criticality safety guidance and for verification of calculational methods.

The core was comprised of the fissile solution inside a cylindrical tank of Zircaloy-2. The inner tank was 25 cm in diameter and 30 cm in height, with a conical bottom, surrounded by an outer aluminum-alloy tank, and reflected by a minimum of 27.5 cm of beryllium oxide followed by a layer of at least 50 cm of graphite. The reflectors contained structural plates of aluminum alloy, as well as several penetrations throughout to accommodate the fill tube, experimental channels, control rods, safety rods, etc.

Experiments performed with this reactor were either critical with the use of control and safety rods, or were subcritical approaches extrapolated to critical with the multiplication factor reached being very close to 1.0000. In these latter cases, the subcritical approach parameter was the solution height in the core, with the control and safety rods in positions outside the reactor.

The geometry of the experiment is depicted in Figure 2.

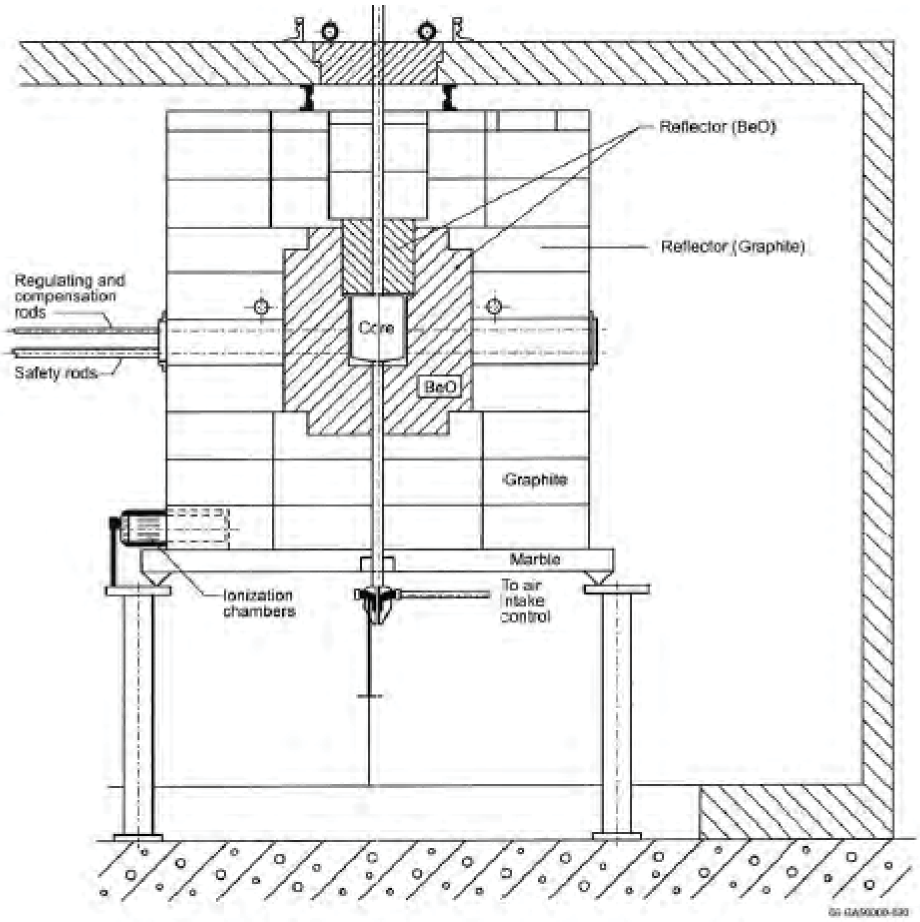

Figure 2 – HEU-SOL-THERM-046 Reactor

The benchmark model for the Proserpine experiments is an accurate representation of the actual assembly with the following simplifications (and their associated biases, if any) derived in Reference 1:

- Insignificant quantities of blotting paper (used for leak detection) between tanks are considered negligible and are omitted.
- The copper wire is omitted and a +0.00100 bias is introduced.
- The gaps between the aluminum alloy tubes in channels and the reflectors are negligible and are omitted.
- Trace impurities in the Zr-2 alloy are omitted and a +0.00008 bias is introduced.
- Iron buildup in the solution is omitted and a +0.00007 bias is introduced.
- The 3-mm gap between the inner (Zr-2) and outer (aluminum alloy) tanks is included; the gap between the outer tank and the inner BeO reflector surface is negligible and is omitted.
- Neutron-return from structures external to the graphite surface is negligible and is omitted (vacuum boundary).

- The aluminum alloy used for the tubes and support plates is assumed to also be Brillalumag 3.

The sample calculation results from the benchmark summary report, along with pertinent nuclear parameters for each case, are presented in Table 2. See Reference 1 for more detailed information.

Table 2 – HEU-SOL-THERM-046 Sample Calculations

Case	Case	Sample k_{EFF}	Sample σ	$H/^{235}U$	g U/l	g ^{235}U/l
1	pros1	1.0185	0.0003	708.2	40.7	36.6
2	pros2	1.0143	0.0003	689.1	41.8	37.6
3	pros3	1.0153	0.0003	677.7	42.5	38.2
4	pros4	1.0160	0.0003	661.2	43.6	39.2
5	pros5	1.0142	0.0003	652.9	44.1	39.7
6	pros6	1.0154	0.0003	641.1	44.9	40.4
7	pros7	1.0161	0.0003	622.3	46.3	41.6
8	pros8	1.0158	0.0003	601.0	47.9	43.1
9	pros9	1.0150	0.0003	592.7	48.6	43.7
10	pros10	1.0132	0.0003	560.5	51.4	46.1
11	pros11	1.0163	0.0003	530.9	54.2	48.7
12	pros12	1.0152	0.0003	487.5	59.0	53.0
13	pros13	1.0154	0.0003	456.7	62.9	56.5

5.0 MCNP5 Evaluation

5.1 Approach

Each of the four IEU-SOL-THERM-001 and thirteen HEU-SOL-THERM-046 cases are modeled in MCNP5-1.60 and executed with [Proprietary Information] cross-sections as listed in Table 3. In addition [Proprietary Information]. The MCNP model results are directly compared to the sample benchmark model results provided in Reference 1.

Table 3 – Library Designations for Modeled Nuclides

Proprietary Information

Proprietary Information

5.2 Results

The MCNP5 results are presented in Tables 4 and 5 for IEU-SOL-THERM-001 and HEU-SOL-THERM-046, respectively. Note that, with respect to the Δk/σ column in the two tables, σ represents the combined uncertainty, which is calculated as the square-root of the sum of the squared standard deviations of the sample and MCNP calculations.

Table 4 – IEU-SOL-THERM-001 Results

Case	Case	Sample k_{EFF}	Sample σ	MCNP k_{EFF}	MCNP σ	Δk	Δk/σ
1	ist1-1	0.9855	0.0013	Proprietary Information			
2	ist1-2	0.9807	0.0013				
3	ist1-3	0.9777	0.0013				
4	ist1-4	0.9735	0.0014				

Table 5 – HEU-SOL-THERM-046 Results

Case	Case	Sample k_{EFF}	Sample σ	MCNP k_{EFF}	MCNP σ	Δk	Δk/σ
1	pros1	1.0185	0.0003				
2	pros2	1.0143	0.0003				
3	pros3	1.0153	0.0003				
4	pros4	1.0160	0.0003				
5	pros5	1.0142	0.0003				
6	pros6	1.0154	0.0003	Proprietary Information			
7	pros7	1.0161	0.0003				
8	pros8	1.0158	0.0003				
9	pros9	1.0150	0.0003				
10	pros10	1.0132	0.0003				
11	pros11	1.0163	0.0003				
12	pros12	1.0152	0.0003				
13	pros13	1.0154	0.0003				

The results demonstrate that the MCNP5 calculations agree very well with the two sets of benchmark sample calculations, with reactivity differences ranging from [Proprietary Information] Δk or [Proprietary Information]. The average reactivity difference is [Proprietary Information]. If the average reactivity differences are calculated separately for each benchmark data set, the results demonstrate a lower average reactivity difference for HEU-SOL-THERM-046 [Proprietary Information] than for IEU-SOL-THERM-001 [Proprietary Information].

6.0 Area of Applicability

Table 6 presents the combined area of applicability for the two benchmark data sets, as well as a nominal area of applicability for the SHINE system.

Table 6 – Area of Applicability Comparison

Parameter	SHINE Nominal	Benchmarks
Fissile Material	UO_2SO_4	UO_2SO_4
Fissile Material Form	Solution	Solution
$H/^{235}U$ Ratio	[Proprietary Information]	$217 \leq H/^{235}U \leq 708$
Concentration (g U/l)	[Proprietary Information]	40.7 to 505.0
Average Neutron Energy Causing Fission (MeV)	[Proprietary Information]	0.0036 < ANECF < 0.0272
Enrichment	19.75 wt.% ^{235}U	20.71 to 89.84 wt.% ^{235}U
Reflecting/Absorbing Materials	Water, [Proprietary Information] Tritium, Aluminum, Zircaloy-4, Concrete, Boron	Water, Graphite, BeO, Polyethylene, Stainless Steel, Zircaloy-2, Aluminum, Boron, Teflon
Geometry	Annular Cylindrical Solutions	Cylindrical Solutions

Given the unique design parameters of the SHINE system, it is not possible to find reactor physics benchmarks that precisely correspond to all aspects of the SHINE AoA. With respect to moderation ratio, ANECF[1], select reflecting/absorber materials (e.g., [Proprietary Information] multiplier[2] and tritium), and geometry (i.e., an annular system with central tritium region versus the benchmark cylindrical systems), there are discontinuities between the benchmark and SHINE AoAs. However, with respect to significant nuclear parameters such as fissile material/form (i.e., uranyl sulfate solutions), uranium concentrations, and enrichment[3], the benchmark and SHINE AoAs correspond very well. Therefore, it is judged that the AoA of the validation results is sufficiently representative of the SHINE system.

7.0 CONCLUSIONS

The following conclusions can be drawn from the above results:

- The MCNP5 calculations agree very well with the benchmark sample calculations, with the average reactivity difference equivalent to [Proprietary Information].
- It is judged that, despite differences between the SHINE and benchmark experiment AoAs, the AoA of the validation results is sufficiently representative of the SHINE system, given the close correspondence with respect to uranyl sulfate composition, enrichment, and concentration.

1 Note that the ANECF value listed for the SHINE system represents the ANECF averaged over the entire SHINE system (i.e., TSV and neutron multiplier region). The ANECF for the TSV alone is approximately 0.008 MeV.

2 Although the [Proprietary Information].

3 With respect to enrichment, most of the benchmark cases have a significantly higher enrichment than the SHINE system, but the IEU-SOL-THERM-001 cases involve enrichments well within the extrapolation limit recommended by Reference 6 (± 5 wt% ^{235}U).

Based on the above points, it is judged that the MCNP5 calculational techniques employed for SHINE neutronics calculations are sufficiently accurate to establish the SHINE safety basis, with the use of suitably conservative modeling conventions and assumptions.

8.0 REFERENCES

1. *International Handbook of Evaluated Criticality Safety Benchmark Experiments*, NEA/NCS/DOC (95)03, Organization for Economic Cooperation and Development, September 2011.

2. *MCNP – A General Monte Carlo N-Particle Transport Code, Version 5.0*, LA-UR-03-1987, Los Alamos National Laboratory.

3. Revolinski, S. M., *Core i7 Linux Computer with Scale 6.0, MCNP 5 1.50 and MCNP 5 1.60*, NSA-SMR-11-02, May 2011

4. ORNL/TM-2005/39, *ORIGEN-S: Depletion Module to Calculate Neutron Activation, Actinide Transmutation, Fission Product Generation, and Radiation Source Terms*, Version 6.1, Section F7, June 2011.

5. Revolinski, S. M., *Installation and Verification of Scale 6.1 on the Linux Computers*, NSA-SMR-12-08, May 2012.

6. *Forecast of Criticality Benchmark Experiments and Experimental Programs Needed to Support Nuclear Operations in the United States of America: 1994-1999*, LA-12683 (Appendix E), Los Alamos, March, 1994.

7. NSA-TR-SHN-12-01, *Initial Hazard Analysis for the SHINE Medical Isotope Production Facility*, Rev. A, June 2012.

8. *Steady-state Neutronics Methods for Power Reactor Analysis*, ANSI/ANS-19.3(2011), American Nuclear Society.

APPENDIX A: MCNP5 INPUT FILES

Case ist1-1

Proprietary Information

[Proprietary Information]

[Proprietary Information]

Case ist1-2

[Proprietary Information]

Proprietary Information

[Proprietary Information]

[Proprietary Information]

Case ist1-3

[Proprietary Information]

Proprietary Information

Proprietary Information

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Case ist1-4

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