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NEAMS FY20 Assessment Problem Draft

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Changing the World's Energy Future

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Idaho National Laboratory

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NEAMS Reactor Physics Assessment Problem

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Contents

1 Introduction

This report documents the physical configuration for required to model the assessment problem posed by the Reactor Physics focus area within the Department of Energy (DOE) Nuclear Energy Advanced Modeling and Simulation (NEAMS) program. This model is based on the *Empire* model [1] developed by staff at Los Alamos National Laboratory under the MEITNER (Modeling-Enhanced Innovations Trailblazing Nuclear Energy Reinvigoration) program. The reference report does not provide dimensions for development of computational models; those data are provided elsewhere in published. Thus, this report has been prepared to provide a single reference that can be used to create consistent models by assessment participants.

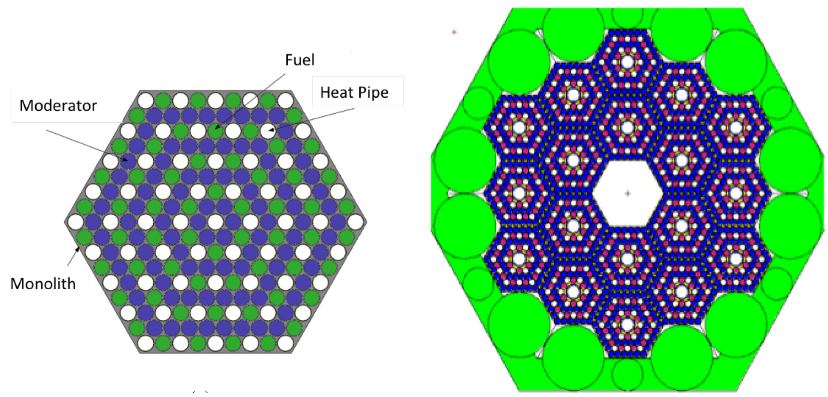

Figure 1: LANL Empire unit assembly (left) and core design (right) [1]

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The Empire concept is illustrated in Figure 1. A unit assembly is comprised of heat pipes, moderator pins made of yttrium hydride (YH_2), and fuel pins, placed in a monolithic stainless steel block with a triangular pitch. A full core consisting of 18 assemblies surrounded by a beryllium reflector was conceptualized but never modeled (right side of figure). The full core was envisioned to have a central void region that would accommodate a safety/shutdown rod and control drums located in the reflector regions. However, specifications for the full core were never generated. Hence, this report also provides the specifications for a simple full-core model based on the concept illustrated above.

The following section provides the geometrical description of the unit assembly and constituent parts (fuel pins, heat pipes and moderator, and enclosing the monolith. This specification is based on the Empire design, but with minor changes as will be described in that section. Initial assessment calculations will be performed with this assembly. Section 3 describes the extension of the assembly to a full core model. Because that full core was not described in the Empire design, this model is based on the configuration show on the right side of Fig. 1 with some assumptions on the exact composition and structure, including control drum placement and design. All materials to be used in this assessment are provided in Appendix A.

2 Unit Assembly Model

The Empire unit assembly consists of 60 fuel rods, 61 heat pipes, and 96 moderator rods, with parameters listed in Table 1. A Serpent 2 rendering of the assembly is provided in Fig. 2. Fuel rods are dark green, moderator pins are dark blue, heat pipes are shown as yellow, and the monolith is grey. Void space (between pins and monolith) is white. Monolith holes are placed on a regular triangular pitch of 2.15 cm center-to-center. Heat pipe and moderator holes have a 1 cm radius, fuel rod positions have a 0.975 cm radius. For fuel and moderator pins, no cladding is specified (the monolith serves as cladding), and have a 0.05 cm gap (assumed to be void) around the pin.

Table 1: Unit Assembly Parameters

Parameter	Value
Triangular pitch	2.15 cm
Fuel radius	0.925 cm
Fuel pin gap thickness	0.05 cm
Moderator radius	0.95 cm
Moderator gap thickness	0.05 cm
Heat pipe hole radius	1.0 cm
Monolith flat-to-flat	32.2739 cm
Unit assembly pitch	33.5 cm
Inter-assembly gap	1.2261 cm
Unit assembly height	60 cm
Bottom reflector axial thickness	20 cm
Top reflector axial thickness	10 cm
Total core height	90 cm
Radial boundary condition	Reflection
Axial boundary condition	Vacuum
Fuel enrichment	19.75 a/o U-235

The assembly has 1 cm of monolith material as reflector above and below the active core height. This means that fuel, moderator, heat pipe and containing monolith are 60 cm tall, with 20 cm of beryllium reflector material below and 10 cm above . In this model, there are no heat pipe penetrations through the top of the core. Vacuum boundary conditions are imposed at the top and bottom of the reflector material. Figures 3 and 4 show the axial configuration of the core in X-Z (Y = 0) and Y-Z (X = 0) cuts, respectively.

Details of heat pipes were not provided in the Empire specification. However, large void regions can cause numerical challenges. Hence, a homogenized material describing the anticipated contents of a sodium heat pipe were assumed. In an earlier study of micro-reactor design options [2], heat pipe contents were described. Based on those specifications, heat pipe material relative volumes were determined to be:

– Steel (wall and mesh material): 0.2625

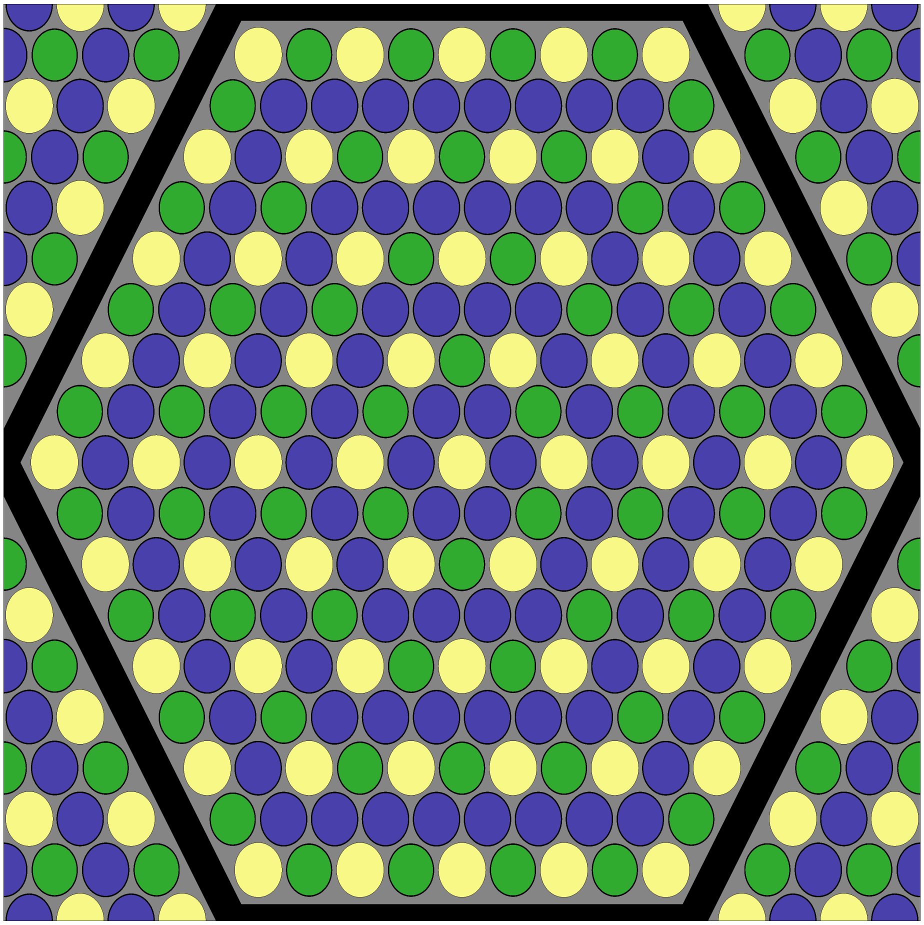

Figure 2: Single Empire assembly configuration.

– Sodium (liquid): 0.1936

– Sodium (vapor): 0.5439

Sodium vapor was assumed to be 1/2000$^{\text{th}}$ that of the liquid. Reference [2] specifies a density of 7900.0 kg/m^3 for Stainless Steel 316 and 802.0 kg/m^3 for liquid sodium. These properties were used to determine number densities, which were them combined by volume weighting according the the above volumes. This results in a homogenized mixture with an effective density of 2.267 g/cm^3. Although this is a very rough estimate, absorption in sodium and has a small but non-zero affect on neutron transport, while eliminating the effect of large void regions. Other material properties specified in Ref. [1] are provided in Table 2.

Based on these data, atomic number densities (with corresponding atom

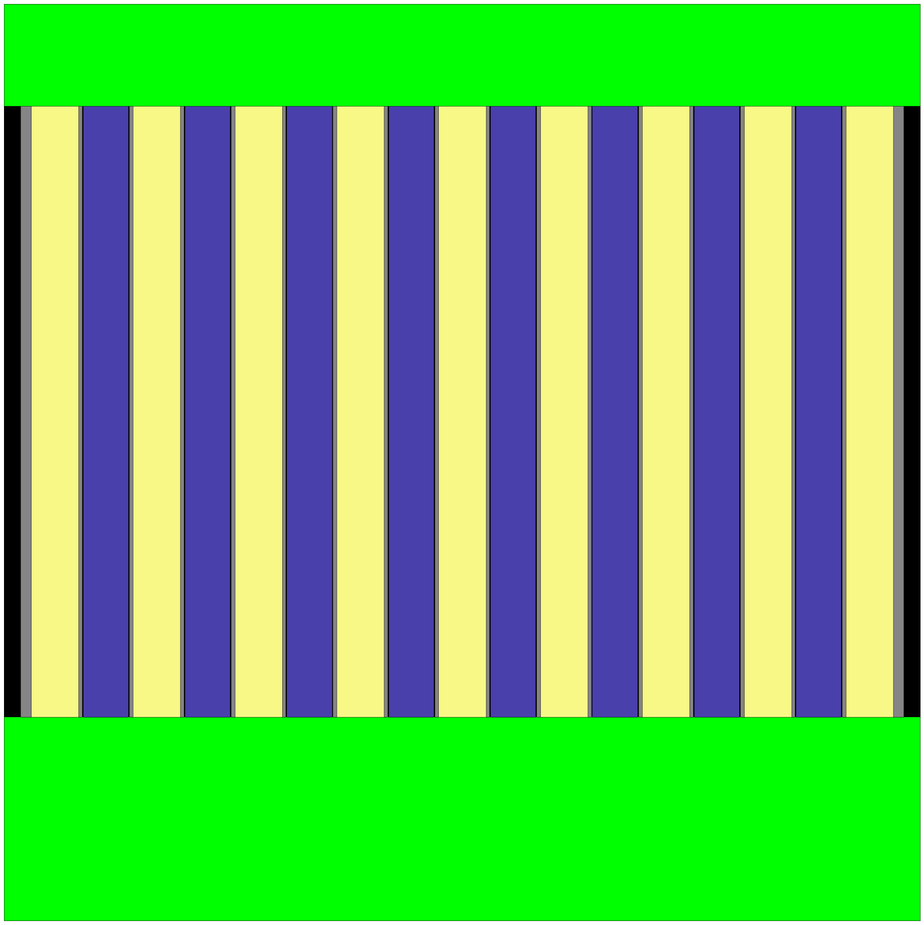

Figure 3: X-Z view of three-dimensional Empire assembly.

Table 2: Assembly Material Densities

Property	Fuel	Moderator	Monolith	Reflector	Heat Pipe
Material	UN	YH_2	SS-316	Beryllium	Homogenized Na/SS
Density (g/cm^3)	14.3	4.3	7.9	1.8538	2.267

fractions and mass fractions) have been calculated and are provided in Appendix A. Natural isotopic abundances were assumed for nitrogen, sodium and yttrium. As specified in Table 1, the uranium was assumed to be enriched to 19.75 wt.% ^{235}U. This is a departure from the Empire model, which assumed 16.05 wt.% enrichment. The increased enrichment was needed to be able to obtain a critical loading for the full core model.

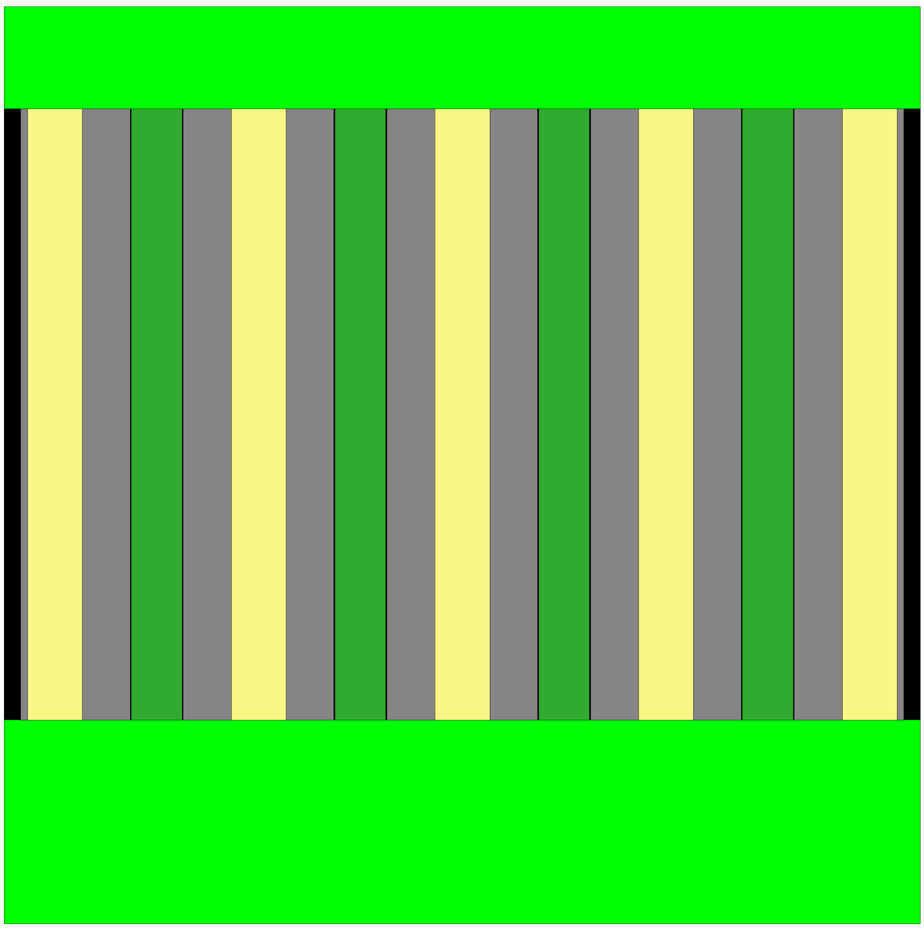

Figure 4: Y-Z view of three-dimensional Empire assembly.

3 Full Core Model

The Empire design was never advanced to a full core design, beyond the illustration provided in Fig. 1. For the purposes of this assessment, a core design has be developed based on an 18 fuel element lattice surrounded by beryllium blocks, illustrated in Fig. 5. The center of the core is unoccupied, providing room for the insertion of a single safety rod, which is not included in this model. The fueled region of the core is surrounded by 12 full hexagon beryllium blocks, each containing a control drum. The central region is empty (void or air); this location is to be used for the insertion of a safety/shutdown rod, which would be fully withdrawn during core operation. The safety rod, like heat pipes exiting above the core, are not included in this model. The core also contains six ½-blocks, located at 0, 60, 120, 180, 240 and 300 degrees from the center of the core. Six ⅓-block elements are located at the six corners of the core hexagon. All blocks are 60 cm in height, aligned with the 60 height of the fuel. Assemblies are spaced with a 32.553 cm pitch, with a 4 mm gap between all assemblies and beryllium blocks. Control drums are 14.8 cm radius beryllium cylinders, 60 cm tall, and are centered in their containing hexagonal beryllium blocks, also centered in 15.0 cm holes in the blocks. Each control drum has a 90°arc of EuB_6 alloy, one cm in thickness. EuB_6 was selected as the control drum poison as it is an effective fast spectrum absorber. The core specifications are summarized in Table 5.

Table 3: Full Core Parameters

Parameter	Value
Fuel assembly flat-to-flat	32.153 cm
Beryllium block flat-to-flat	32.153 cm
Assembly/block pitch	32.553 cm
Inter-block gap	0.4 cm
Beryllium block height (bottom aligned with bottom of fuel)	60 cm
Beryllium control drum hole radius (centered in hexagon)	15 cm
Control drum radius	14.8 cm
Control poison outer radius	14.8 cm
Control poison inner radius	13.8 cm
Control poison thickness	1.0 cm
Control poison arc width	90 degrees
Control drum height (bottom aligned with bottom of fuel)	60 cm

Figure 5 shows control drums in the zero rotation position. Drums are assumed to be all ganged together, but with each pair of drums rotating in opposite directions. Figure 6 identifies each drum by number for later identification, and shows the rotation direction for each drum. Odd numbered drums rotate in a

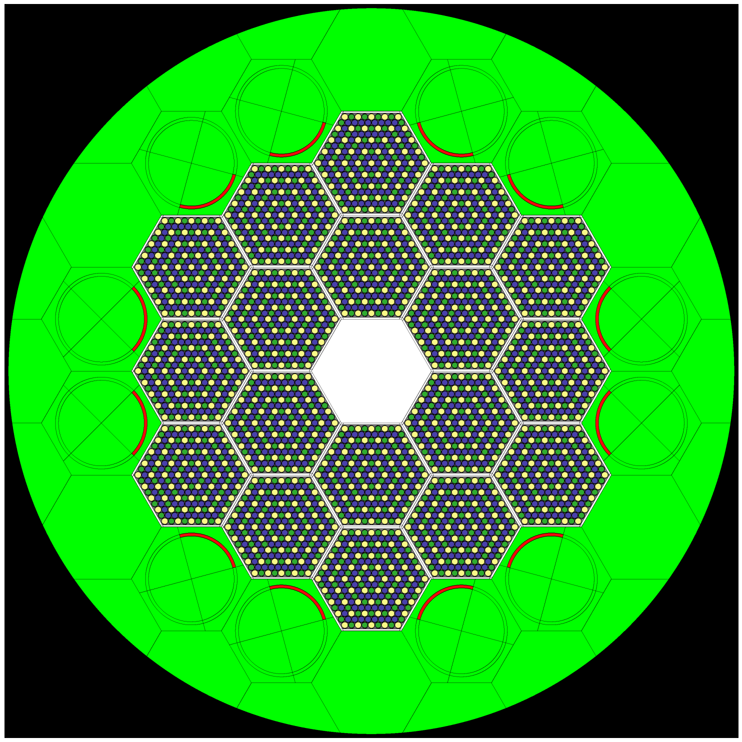

Figure 5: Empire core configuration.

clockwise direction, while even-numbered drums rotate in a counter-clockwise direction.

Zero rotation is considered to be when the poison region of a drum faces the two adjacent fuel assemblies in equal measure. More formally, when a line from the center of a drum bisects the poison region arc (45°of arc on either side) with an outward angle as provided in Table

Note that while a stainless steel reflector is present above and below the fuel assemblies, no reflector exists above the beryllium regions. Ref. [1] does not provide such details; however, other micro-reactor designs evaluated in relation to the MEITNER program [2] did not use additional reflector above and below outer beryllium regions.

Boundary conditions are assumed to be vacuum on all core boundaries.

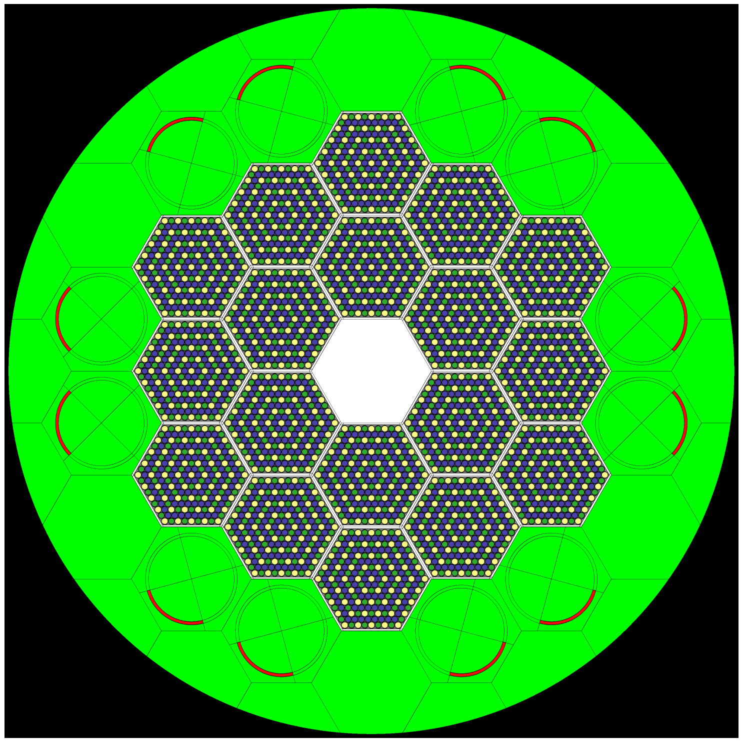

Figure 6: Empire core rotated configuration.

Table 4: Zero Rotation Position for Control Drums

Control Drum No.	Angle Between Arc Bisector and Vertical (degrees)
1	210
2	210
3	270
4	270
5	330
6	330
7	30
8	30
9	90
10	90
11	150
12	150

References

[1] Christopher Matthews, Robert Blake Wilkerson, Russell Craig Johns, Holly Renee Trellue, and Richard C. Martineau. Task 1: Evaluation of m&s tools for micro-reactor concepts. 3 2019.

[2] James W. Sterbentz, James E. Werner, Andrew J. Hummel, John C. Kennedy, Robert C. O'Brien, Axel M. Dion, Richard N. Wright, and Krishnan P. Ananth. Preliminary assessment of two alternative core design concepts for the special purpose reactor. Technical Report INL/EXT-17-43212, Idaho National Laboratory, Idaho Falls, ID, May 2018.

A Material Specifications

As described earlier, two models are provided for both the single assembly and full core configurations; the first is the explicit model with gaps, the second is a simplified model with voids homogenized into adjacent materials. This appendix lists the number densities used in each model. Hence, it is important to use the appropriate set of number densities for any geometric approximations.

Tables A1-A6 provide nuclide compositions for nominal fuel, moderator, heat pipe, monolith, beryllium and EuB_6 materials.

Table A1: UN Fuel Composition Data
(Nominal density: 14.3 g/cm^3)

Nuclide	Atomic Weight	Atomic Density	Atomic Fraction	Mass Fraction
92235	235.04394	6.76350E-03	9.87500E-02	0.184604
92238	238.05080	2.74821E-02	4.01250E-01	0.759694
7014	14.00307	3.41086E-02	4.98000E-01	0.0554635
7015	14.99986	1.36982E-04	2.00000E-03	0.0002386
sum		6.84911E-02	1.00000E+00	1.00000E+00

Table A2: YH_2 Moderator Composition Data
(Nominal density: 4.3 g/cm^3)

Nuclide	Atomic Weight	Atomic Density	Atomic Fraction	Mass Fraction
39089	88.90585	2.84804E-02	3.33333E-01	9.78E-01
1001	1.00782	5.69608E-02	6.66667E-01	2.22E-02
sum		8.54411E-02	1.00000E+00	1.00E+00

Table A3: Homogenized Heat Pipe Composition Data
(Nominal density: 2.267 g/cm^3)

Nuclide	Atomic Weight	Atomic Density	Atomic Fraction	Mass Fraction
14028	27.97693	4.11552E-04	1.49701E-02	8.43E-03
14029	28.97693	2.08976E-05	7.60143E-04	4.44E-04
14030	29.97349	1.37758E-05	5.01090E-04	3.02E-04
24050	49.94606	1.77806E-04	6.46763E-03	6.51E-03
24052	51.94019	3.42886E-03	1.24724E-01	1.30E-01
24053	52.94079	3.88795E-04	1.41423E-02	1.51E-02
24054	53.93888	9.67787E-05	3.52029E-03	3.82E-03
25055	54.93805	4.56726E-04	1.66133E-02	1.84E-02
26054	53.93961	8.58252E-04	3.12186E-02	3.39E-02
26056	55.93451	1.34726E-02	4.90061E-01	5.52E-01

26057	56.93540	3.11151E-04	1.13180E-02	1.30E-02
26058	57.93368	4.14072E-05	1.50617E-03	1.76E-03
28058	57.93570	1.74225E-03	6.33738E-02	7.39E-02
28060	59.93079	6.71125E-04	2.44119E-02	2.95E-02
28061	60.93143	2.91727E-05	1.06115E-03	1.30E-03
28062	61.92799	9.30147E-05	3.38338E-03	4.22E-03
28064	63.92818	2.36883E-05	8.61654E-04	1.11E-03
42092	91.90682	4.83027E-05	1.75699E-03	3.25E-03
42094	93.90510	3.01072E-05	1.09514E-03	2.07E-03
42095	94.90585	5.18174E-05	1.88484E-03	3.60E-03
42096	95.90467	5.42900E-05	1.97478E-03	3.81E-03
42097	96.90597	3.10836E-05	1.13066E-03	2.21E-03
42098	97.90541	7.85385E-05	2.85681E-03	5.63E-03
42100	99.90726	3.13435E-05	1.14011E-03	2.29E-03
11023	22.98949	4.92833E-03	1.79266E-01	8.30E-02
sum		2.74917E-02	1.00000E+00	1.00E+00

Table A4: Monolith Composition Data
(Nominal density: 7.9 g/cm^3)

Nuclide	Atomic Weight	Atomic Density	Atomic Fraction	Mass Fraction
6000	12.01104	1.62484E-04	1.90102E-03	4.10E-04
14028	27.97693	7.92259E-04	9.26926E-03	4.66E-03
14029	28.97693	4.03866E-05	4.72515E-04	2.46E-04
14030	29.97349	2.66379E-05	3.11658E-04	1.68E-04
15031	30.97408	3.53188E-05	4.13223E-04	2.30E-04
16032	31.97207	2.11203E-05	2.47103E-04	1.42E-04
16033	32.97104	1.66760E-07	1.95105E-06	1.16E-06
16034	33.96800	9.44971E-07	1.10560E-05	6.75E-06
16036	35.96697	2.56553E-09	3.00162E-08	1.94E-08
24050	49.94606	6.76214E-04	7.91156E-03	7.10E-03
24052	51.94019	1.30401E-02	1.52566E-01	1.42E-01
24053	52.94079	1.47864E-03	1.72998E-02	1.65E-02
24054	53.93888	3.68066E-04	4.30629E-03	4.17E-03
25055	54.93805	8.78610E-04	1.02795E-02	1.01E-02
26054	53.93961	3.33588E-03	3.90290E-02	3.78E-02
26056	55.93451	5.23197E-02	6.12129E-01	6.15E-01
26057	56.93540	1.20891E-03	1.41440E-02	1.45E-02
26058	57.93368	1.14047E-04	1.33432E-03	1.39E-03
28058	57.93570	6.62538E-03	7.75155E-02	8.07E-02
28060	59.93079	2.55206E-03	2.98586E-02	3.21E-02
28061	60.93143	1.10951E-04	1.29810E-03	1.42E-03
28062	61.92799	3.53761E-04	4.13893E-03	4.60E-03

28064	63.92818	9.01186E-05	1.05437E-03	1.21E-03
42092	91.90682	1.81708E-04	2.12595E-03	3.51E-03
42094	93.90510	1.13670E-04	1.32992E-03	2.24E-03
42095	94.90585	1.96845E-04	2.30304E-03	3.93E-03
sum		8.54717E-02	1.00000E+00	1.00000E+00

Table A5: Beryllium Composition Data
(Nominal density: 1.854 g/cm^3)

Nuclide	Atomic Weight	Atomic Density	Atomic Fraction	Mass Fraction
4009	9.01220	1.23870E-01	1.00000E+00	1.00000E+00
sum		1.23870E-01	1.00000E+00	1.00000E+00

Table A6: EuB_6 Absorber Composition Data
(Nominal density: 4.895 g/cm^3)

Nuclide	Atomic Weight	Atomic Density	Atomic Fraction	Mass Fraction
5010	10.01294	1.62323E-02	1.70571E-01	5.51E-02
5011	11.00928	6.53371E-02	6.86571E-01	2.44E-01
63151	150.91986	6.49972E-03	6.83000E-02	3.33E-01
63153	152.92168	7.09518E-03	7.45571E-02	3.68E-01
sum		9.51643E-02	1.00000E+00	1.00E+00

Table A7: Homogenized UN Fuel/Void Composition Data
(Nominal density: 12.870 g/cm^3)

Nuclide	Atomic Weight	Atomic Density	Atomic Fraction	Mass Fraction
92235	235.04394	4.94497E-03	8.02500E-02	1.49953E-01
92238	238.05080	2.58648E-02	4.19750E-01	7.94369E-01
7014	14.00307	3.06865E-02	4.98000E-01	5.54389E-02
7015	14.99986	1.23239E-04	2.00000E-03	2.38495E-04
sum		6.16195E-02	1.00000E+00	1.00000E+00

Table A8: Homogenized YH_2 Moderator/Void Composition Data
(Nominal density: 3.881 g/cm^3)

Nuclide	Atomic Weight	Atomic Density	Atomic Fraction	Mass Fraction
39089	88.90585	2.57052E-02	3.33333E-01	9.77831E-01
1001	1.00782	5.14104E-02	6.66667E-01	2.21691E-02
sum		7.71156E-02	1.00000E+00	1.00000E+00