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WATER-MODERATED U(4.31)0_2 FUEL RODS REFLECTED BY TWO LEAD, URANIUM, OR STEEL WALLS

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1.0 DETAILED DESCRIPTION

1.1 Overview of Experiment

A series of critical-approach experiments with clusters of aluminum clad U(4.31)O_2 fuel rods in a large water-filled tank was performed over the course of several years at the Critical Mass Laboratory at the Pacific Northwest Laboratories (PNL). Experiments included rectangular, square-pitched lattice clusters, with pitches of 2.54 cm or 1.892 cm (LEU-COMP-THERM-002 and -004). Some of these experiments were performed with absorber plates of various materials between clusters (LEU-COMP-THERM-009). Some circular, triangular-pitched lattices, with pitches of 2.398, 1.891, 1.801, or 1.598 cm, were used to measure the effect of gadolinium dissolved in the water (LEU-COMP-THERM-005).

This evaluation documents water-reflected clusters with reflecting walls of depleted uranium, lead, and steel on two opposite sides of the cluster array. A total of thirty experiments, performed in the late 1970's and early 1980's, were evaluated. All of these were judged to be acceptable as benchmark data.

Information in this section comes from References 1 - 10, which are the original PNL reports of these experiments. The primary references for this set of experiments at 2.54-cm or 1.892-cm pitch are References 3, 5, and 6. Over the course of performing experiments with this set of fuel rods, analyses were done which resulted in better characterization of the rods over time (Reference 5, p. x; Reference 6, p. xiii[a]). For example, the enrichment was originally reported at 4.29 wt.%, but later improved to 4.306 wt.%. Therefore, only the most recent fuel rod data is provided in this evaluation. References 11 - 14 provide supplemental information. Details which are from specific references are so noted.

[a] Confirmed by private communication, Sid Bierman, April 1994.

1.2 Description of Experimental Configuration

1.2.1 Experiment Tank and Surroundings - Experiments were performed in a 0.952-cm-thick, open-top, carbon-steel tank. Tank inside dimensions were 1.8 x 3.0 x 2.1 meters deep. The experiment was centered in the tank to within one-quarter inch. The reflecting walls were built or placed on the bottom of the tank. The control blade, the safety blade, and any control or safety rods were withdrawn above the top water reflector for the reported configurations. Other than radiation detectors and support structures (acrylic support plate, acrylic or polyethylene lattice plates, 6061 aluminum angle supports, and control/safety blade guides, all described in this section), no other apparatus was in the tank.[a] (see Figures 1 and 2.)

The experiment tank was located in one corner of the Critical Mass Laboratory at the Pacific Northwest Laboratories, Hanford, Washington. The tank sat upon a concrete floor, which was at least 40.6 cm thick (Reference 11, p. 32). The concrete walls of the room were 5 feet thick. The concrete ceiling was 2 feet thick and approximately 20 feet high. The tank is located approximately four feet from the two closest corner walls.[b]

1.2.2 Fuel Rod Support Plate - The bottoms of the fuel rods were supported by a 2.54-cm-thick, acrylic support plate. The width and length of the support plate were approximately the width and length of the clusters.[c] The acrylic support plate was supported by two 15.3 x 5.08 x 0.635-cm 6061 aluminum channel angles resting on the floor of the tank. The angles were oriented so that the bottom surface of the support plate was 15.3 cm above the bottom of the tank.

1.2.3 Lattice Plates and Supports - The pitch of the fuel rods was maintained by two levels of acrylic lattice plates. Holes for the fuel rods were no more than 5 mils (0.0127 cm) larger than the rod diameter.[d]

The top lattice plates were bolted to 5.08 x 5.08 x 0.635-cm aluminum angles, attached at their ends to the walls of the tank. In one experiment with 2.35% enriched UO_2 fuel rods, these aluminum lattice supports were doubled, with no effect on the critical separation between clusters (Reference 1, pp. 26 and 28).

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[a] Tank and water reflector dimensions were from the references. Other information was from private communication, Sid Bierman, July 1993.

[b] Sid Bierman, private communication, July 1993.

[c] Sid Bierman recalls that there may have been three separate support plates for the 3-cluster experiments. Exact dimensions of the support plates are not known. (Private communication, Sid Bierman, August 1993)

[d] Sid Bierman, private communication, August 1993.

Figure 1. Experiment Tank.

Figure 2. Arranging Fuel Rods.

The bottom lattice plates rested on the fuel-rod support plate. The lattice plates were acrylic for the 2.54-cm-pitch experiments reported in References 3 and 5, and top lattice plates were about 66 cm[a] above the fuel-rod support plate. The lattice plates were polypropylene for the 1.892-cm-pitch experiments reported in References 5 and 6, and the top lattice plates were about 79 cm[b] above the fuel-rod support plate. The lattice plates were 1.27-cm thick. The uncertainty in the thickness of the polypropylene is ±0.4 cm (Reference 4, p. 20).

In some 3-cluster experiments, the required horizontal separation between bottom lattice plates or between bottom lattice plates and the control/safety blade guides was maintained by shims. This was necessary in order to position the bottom lattice plates accurately. (The control and

[a] Estimated from Reference 3, p.3 (Figure 1).

[b] Reference 4, pp. 20 and 25.

safety blade guides could not, by themselves, be used for positioning since they were not fastened to anything below their attachment to the angles supporting the top lattice plates.) The shim was either Lucite or was made from the lattice plate material. The Lucite shim was approximately 1 inch thick.[a]

1.2.4 Radiation Detectors - The boron-lined proportional counters (usually three in number) were placed symmetrically around the experiments. The detectors were kept dry by being placed in aluminum tubes that extended above the top surface of the water. The elevation of the detectors varied, depending on the buoyancy of the tube holding the detector. The aluminum tubes were approximately 1.5 inches in diameter and were placed about 30 cm from the experimental assembly, always outside a 15-cm thickness of water.[b]

1.2.5 Water Reflector - The top water surface was always at least 15 centimeters above the top of the fuel region of the rods. (Reference 13, p. 132)[c] The bottom water reflector also was at least 15 cm thick, since the aluminum angle supporting the fuel-rod support plate above the bottom of the tank was 15.3 cm tall.

1.2.6 Reflecting Walls

Lead Walls. The lead walls (see Figure 3) are described in Reference 3, Appendix B: "Two walls were constructed, one on either side of the fuel clusters .... Each was constructed by stacking lead bricks into a free standing wall, 1640 ± 2 mm long by 1234 ± 2 mm high by 102 ± 0.3 mm thick. Each wall was 8 bricks long by 24 bricks high by 1 brick wide. The average 'stacked' dimensions per brick were:

length: 205.1 ± 0.4 mm
thickness: 51.4 ± 0.1 mm
width: 102.0 ± 0.3 mm"

Uranium Walls. The dimensions of the uranium wall are shown in Figure 4. Each wall was constructed by assembling ten tongue-and-groove slabs of uranium. Dimensions of each slab, including those for the tongues and grooves, are described in Appendix A of Reference 3. The tongues were about 1¼ inches long and the grooves were about 1⅓ inches deep.

The dimensions, weights, and enrichments of the slabs varied slightly. Major characteristics of each slab are shown in Table 1.

[a] Private communication, Sid Bierman, August 1993.

[b] Private communication, Sid Bierman, July 1993.

[c] Confirmed by private communication, Sid Bierman, July 1994.

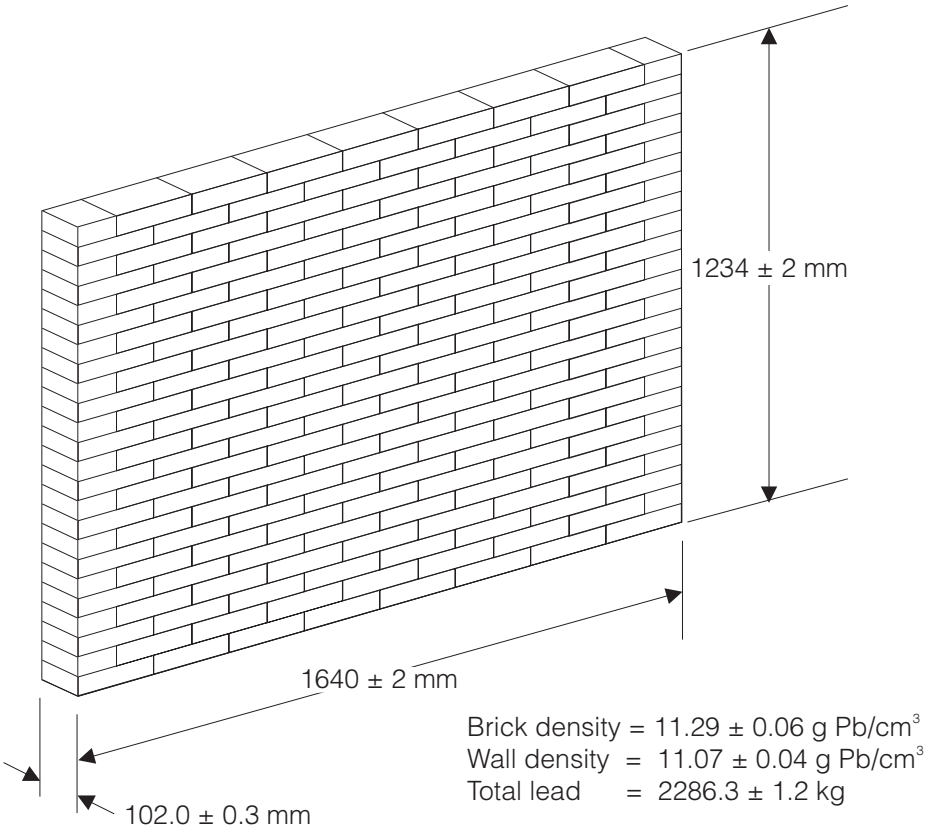

Figure 3. Assembled Lead Wall (Reference 3, Figure 6).

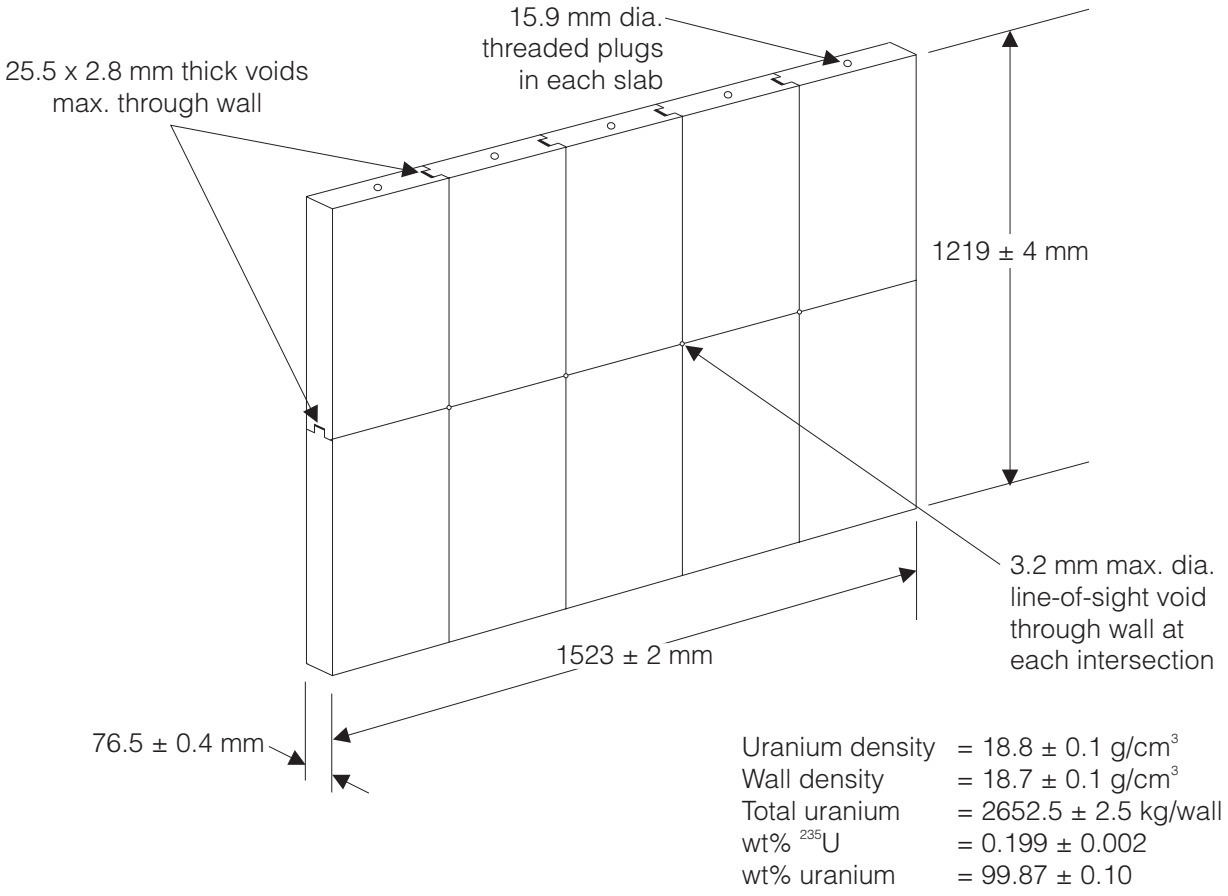

Figure 4. Assembled Depleted Uranium Wall (Reference 3, Figure 5).

Table 1. Dimensions of the Depleted Uranium Slabs.

Slab Number	Height (inches)[a]	Width (inches)[b]	Thickness (inches)[c]	Uranium Weight (lb)	Enrichment (wt.% ^{235}U)
1	24.063 24.063	12.000 12.000	3.023 3.026 3.010 2.994	556	0.197
2	23.938 23.938	11.938 12.063	3.012 3.037 3.017 2.985	571	0.199
3	24.000 24.000	11.938 12.000	2.990 3.019 3.022 3.000	575	0.198
4	23.938 24.063	12.000 11.938	3.000 3.015 3.021 3.005	573	0.203
5	24.063 24.063	12.000 12.000	2.993 3.010 3.026 3.009	577	0.198
6	24.000 24.000	12.000 12.063	2.985 3.013 3.025 3.002	574	0.199
7	24.125 24.125	11.938 12.000	3.008 3.040 3.038 3.002	577	0.198
8	24.125 24.188	11.938 11.938	2.991 3.023 3.040 3.018	577	0.203
9	24.000 24.125	12.000 12.000	3.000 3.030 3.055 3.007	570	0.198
10	24.125 24.188	12.000 12.000	3.000 3.018 3.035 2.998	575	0.254

Slab Number	Height (inches)[a]	Width (inches)[b]	Thickness (inches)[c]	Uranium Weight (lb)	Enrichment (wt.% ^{235}U)
11	24.000 24.125	12.000 12.063	2.989 3.026 3.020 2.996	597	0.199
12	24.000 24.000	11.938 12.000	2.998 3.018 3.027 3.007	594	0.198
13	23.938 23.938	11.938 12.000	2.998 3.024 3.029 3.025	594	0.201
14	23.938 23.938	11.938 12.000	2.994 3.028 3.049 3.010	594	0.199
15	23.938 23.938	11.938 12.000	2.994 3.011 3.022 2.994	592	0.195
16	23.750 23.750	12.000 12.000	3.005 3.020 3.023 3.005	593	0.199
17	23.938 23.938	12.000 12.000	2.990 3.010 3.024 3.014	594	0.201
18	23.938 23.875	12.000 12.000	2.993 3.009 3.038 3.022	592	0.189
19	23.938 23.938	12.000 12.000	2.994 3.018 3.030 3.020	592	0.199
20	23.938 23.938	12.063 12.000	3.022 3.016 3.003 3.001	617	0.200

(a) Measured at the two ends of the slab.
(b) Measured at top and bottom of the slab.
(c) Measured at the four corners of the slab.

Slab placement is given as the following: Slabs 15, 14, 13, 12, and 2 along the bottom of one wall, with slabs 6, 5, 4, 3, and 1 above them: and slabs 20, 19, 18, 17, and 16 along the bottom of the second wall, with slabs 11, 10, 9, 8, and 7 above them (Reference 3, pp. A-2 and A-3).

Steel Walls. The steel walls on either side of the fuel clusters, shown in Figure 5, were 1.473 ± 0.0032 m long by 1.219 ± 0.003 m high and were 0.1785 ± 0.004 m thick (Reference 5, p. 10).

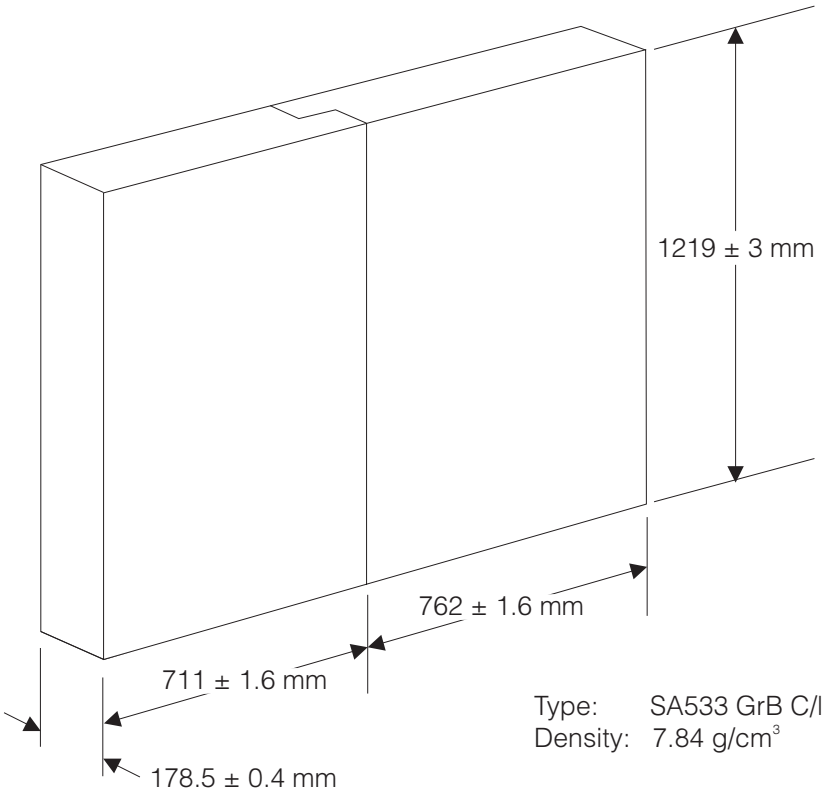

Figure 5. Steel Reflecting Walls (Reference 5, p. 10).

1.2.7 Others - A ^{252}Cf source of approximately 0.6 micrograms was placed near the center of each experimental assembly. The source was mounted in an open acrylic tube, 0.6 cm in diameter (Reference 8, p. 2.3) and two or three inches long.[a] During the triangular-pitched experiments, no measurable effect on critical size was detected with replacement-type reactivity worth measurements of the californium source (Reference 8, pp. 3.6 and 3.7).

The aluminum control and safety blade guides were located between clusters in multi-cluster experiments. The blade guides, two for the control blade and two for the safety blade, extended from the bottom of the fuel pin array to well above the water surface. Two slightly different sizes of guides were used throughout the series of experiments. Guides were 3.8 cm wide and were 2.54 cm thick (Reference 3, p. 5), with a slot that was 0.96 cm wide for the blades.[b]

During one experiment from a set of similar experiments using 2.35 wt.% enriched UO_2 rods, the aluminum of the control and safety blade guides was doubled. The results demonstrated "no change in the predicted critical separation between fuel rod clusters." (Reference 1, pp. 13 and 28) These experiments were not repeated with 4.31% enriched rods. However, the experimenters report, "Since the support structures are further from the fuel clusters in the experiments covered by this report, they would have even less of an effect on the data. Consequently, the measurements to determine the effect of the supports were not repeated for these current experiments." (Reference 2, p. 22)

1.2.8 Fuel Rods - Fuel rod dimensions are given in diagrams in References 3-10. Figure 6 is a reproduction of the diagram from Reference 10 (p. 2.3). UO_2 fuel pellets were taken from rods "originally fabricated for Core II of the N.S. Savannah . . . The fuel diameter (1.265 ± 0.003 cm) ... was checked repeatedly during the reloading operations and found to agree with that quoted in the document characterizing Core II of the N.S. Savannah." (Reference 10, p. 2.4)

Diagrams in some of the earlier references showed end plugs protruding from the ends of the rod beyond the aluminum cladding, with total rod length, including protruding plugs, of 96.52 cm. However, later references showed end plugs exactly filling the ends of the clad, which had a length of 96.52 cm.

One experimenter recalls that the experimenters carefully inserted rubber plugs in the bottoms of the rods, before filling, so that the rubber plug protruded approximately 1/16 inch uniformly for all rods. Some top end plugs protruded and some were recessed, depending on slight differences between thicknesses of UO_2 pellets. Differences in pellet thicknesses were also the reason for the reported

[a] Private communication, Sid Bierman, August 1993.

[b] Different widths of control and safety blades were used for different experiments. (Private communication, Sid Bierman, August 1993)

maximum and minimum lengths of 92.71 cm and 91.44 cm for the fuel region. There were no problems with water leakage into the fuel region of the rods.[a]

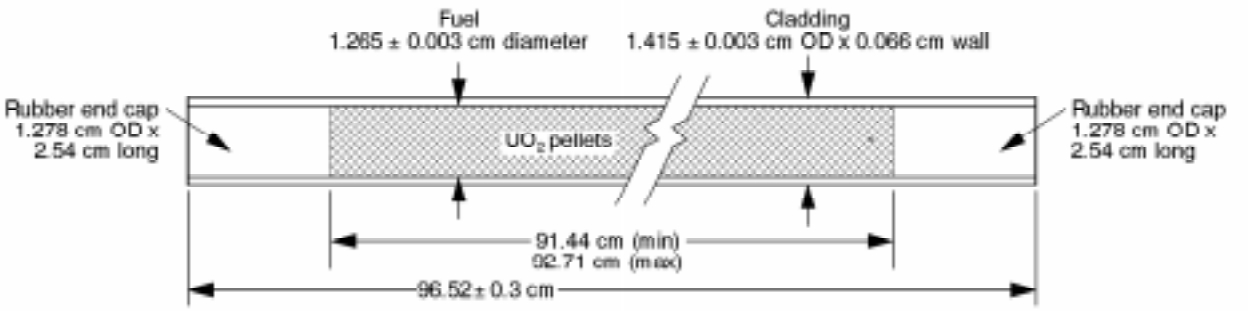

Figure 6. $U(4.31)O_2$ Fuel Rod.

Dimensions of the $U(4.31)O_2$ fuel rods are summarized in Table 2. To test the effects of small differences between rods, "experiments were repeated using alternate but identical (within the quality control applied during fabrication) fuel rods and different fuel loading arrangements on the approach to critical. ... the measurement data thus checked were reproduced to within a one sigma limit of 0.3%" in most cases (Reference 2, p. 19). The standard deviations of a few reported critical cluster separations were greater than 0.3%.

Table 2. 4.31 Wt.% Enriched UO_2 Fuel Rod Dimensions.

Component	Length (cm)	Diameter (cm)
UO_2 Fuel	91.44 - 92.71	1.265 ± 0.003
Rubber End Caps	2.54	1.278
Gap (not shown)	-	1.283 ± 0.003 OD
Clad (6061 Al)	96.52 ± 0.3	1.415 ± 0.003 OD (0.066 cm thick)

1.2.9 Experimental Method for Determining Critical Configuration - Critical configurations were determined by extrapolation to critical (see LEU-COMP-THERM-001), based on count rates of two or three detectors. Generally, the most reactive configuration measured was at least 99% of critical (M > 100).

1.2.10 Critical Cluster Dimensions and Separations - Cluster sizes and separations for the thirty critical configurations are listed in Table 3. Each configuration consists of three clusters. Typical arrangements of fuel clusters and reflecting walls are shown in Figures 7 and 8.

Table 3. $U(4.31)O_2$ Fuel Rod Critical Configurations.

Case No.	Pitch (cm)	Cluster Dimensions (number of rods)[a] (X x Y)	Separation Between Clusters (cm)[b]	Distance Between Reflecting Walls and Fuel Clusters (cm)[c]	Reflecting Wall Material	Ref. (pg)
1	2.540	13 x 8	19.495 ± .01[d]	0.0	lead	3 (14)
2	2.540	13 x 8	19.655 ± .02[d]	0.660 ± 0.102	lead	3 (14)
3	2.540	13 x 8	17.915 ± .02[d]	1.321 ± 0.076	lead	3 (14)
4	2.540	13 x 8	9.175 ± .02[d]	5.405 ± 0.102	lead	3 (14)
5	2.540	13 x 8	14.255 ± .01[d]	0.0	uranium	3 (14)
6	2.540	12 x 8	14.195 ± .01[d]	1.956 ± 0.102	uranium	3 (14)
7	2.540	13 x 8	16.925 ± .05[d]	3.912 ± 0.076	uranium	3 (14)
8	2.540	13 x 8	12.365 ± .02[d]	5.405 ± 0.102	uranium	3 (14)
9	2.540	13 x 8	11.765 ± .02	0.0	steel	5 (16)
10	2.540	13 x 8	13.125 ± .05	0.660 ± 0.102	steel	5 (16)
11	2.540	13 x 8	12.995 ± .01	1.321 ± 0.076	steel	5 (16)
12	2.540	13 x 8	11.315 ± .05	2.616 ± 0.107	steel	5 (16)
13	2.540	13 x 8	8.675 ± .05	5.405 ± 0.102	steel	5 (16)
14	1.892	12 x 16	14.393 ± .02	0.0	steel	5 (16)
15	1.892	12 x 16	15.263 ± .02	0.660 ± 0.102	steel	5 (16)
16	1.892	12 x 16	15.393 ± .01	1.321 ± 0.076	steel	5 (16)
17	1.892	12 x 16	15.363 ± .02	1.956 ± 0.102	steel	5 (16)
18	1.892	12 x 16	14.973 ± .01	2.616 ± 0.107	steel	5 (16)
19	1.892	12 x 16	13.343 ± .03	5.405 ± 0.102	steel	5 (16)
20	1.892	12 x 16	17.263 ± .03	0.0	lead	6 (13)
21	1.892	12 x 16	17.703 ± .05	0.660 ± 0.102	lead	6 (13)
22	1.892	12 x 16	16.953 ± .02	1.956 ± 0.102	lead	6 (13)
23	1.892	12 x 16	13.873 ± .03	5.001 ± 0.086	lead	6 (13)
24	1.892	12 x 16	14.853 ± .03	0.0	uranium	6 (13)

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Case No.	Pitch (cm)	Cluster Dimensions (number of rods)[a] (X x Y)	Separation Between Clusters (cm)[b]	Distance Between Reflecting Walls and Fuel Clusters (cm)[c]	Reflecting Wall Material	Ref. (pg)
25	1.892	12 x 16	16.233 ± .02	0.660 ± 0.102	uranium	6 (13)
26	1.892	12 x 16	17.793 ± .05	1.321 ± 0.076	uranium	6 (13)
27	1.892	12 x 16	18.763 ± .04	1.956 ± 0.102	uranium	6 (13)
28	1.892	12 x 16	18.893 ± .04	2.616 ± 0.107	uranium	6 (13)
29	1.892	12 x 16	18.303 ± .02	3.276 ± 0.148	uranium	6 (13)
30	1.892	12 x 16	15.923 ± .02	5.405 ± 0.102	uranium	6 (13)

(a) The first dimension is along the direction of cluster placement. Second dimension is the width of facing sides.
(b) Distance between outer fuel-rod cell boundaries of clusters.
(c) Distance between edge of outermost fuel rod cell boundary and inner surface of reflecting wall.
(d) Separations were reported as "between cell boundaries of the fuel clusters" (Reference 3, footnote d, p. 14), but the separations given were actually rod-surface-to-rod-surface (Sid Bierman, private communication, July, 1993). Therefore, the difference between pitch and rod diameter (2.54 - 1.415 = 1.125) is subtracted from the reported cluster separations to obtain these cell-boundary separations.

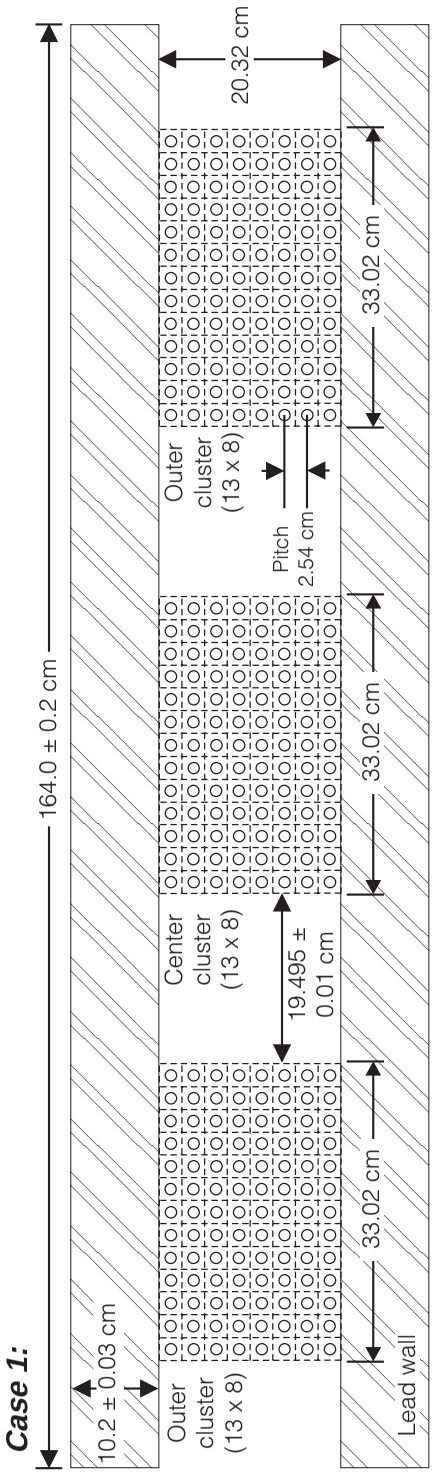

Figure 7. Critical Configuration of Case 1.

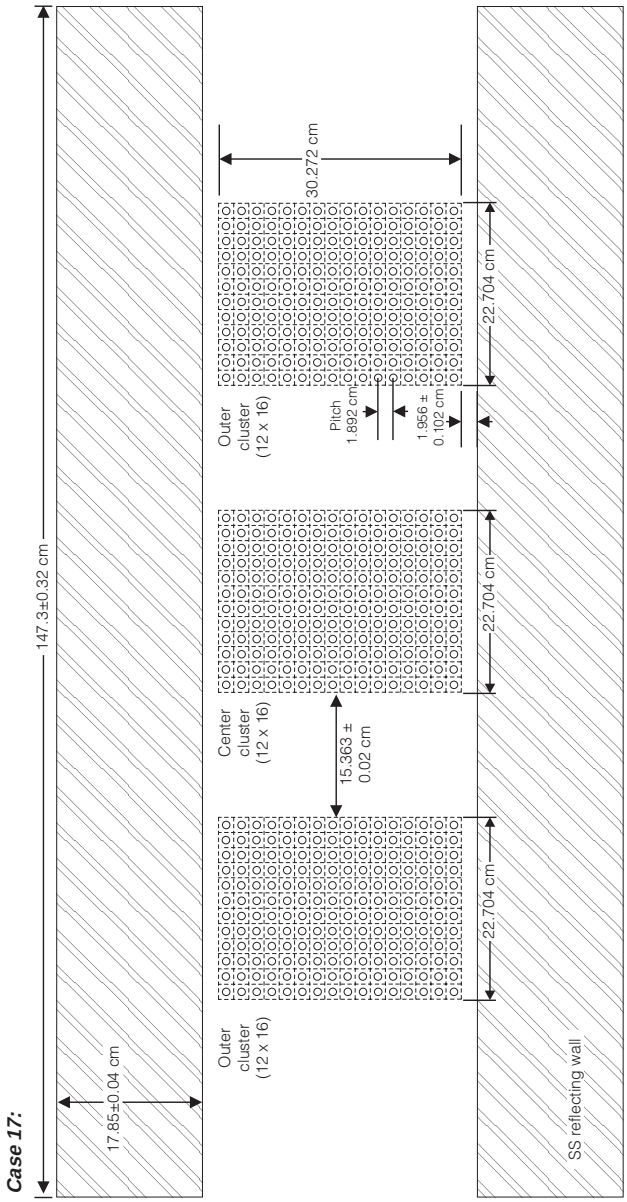

Figure 8. Critical Configuration of Case 17.

1.3 Description of Material Data

1.3.1 UO_2 Fuel Rods - Over the course of performing the experiments, the experimenters improved their analyses of the fuel rods. In Reference 5 (p. x), the experimenters state:

> The same UO_2 fuel, lattice grid plates, neutron absorber plates, and reflecting walls have been used throughout these experiments. However, during this period of time some of these parameters have become better defined as a result of repeated analysis. For example, the 4.31 wt.% ^{235}U enriched UO_2 rods were originally identified as having a ^{235}U enrichment of 4.29 wt.%. Multiple analysis of the rods during the course of these five sets of experiments have resulted in the more correct average of 4.31 wt.% quoted in this and some of the more recent reports. . . . the values quoted in this report should be considered the latest and, hopefully, the more correct values to use.

A similar statement is given in Reference 6 (p. xiii).

The latest reported values (Reference 10, p. 2.3) are assumed to be most accurate. In Reference 10, measurement methods are described. The experimenters state (Reference 10, p. 2.4):

> The uranium assay (1059.64 ± 4.80 g/rod) and the ^{235}U enrichment (4.306 ± 0.013%) . . . are the average of six assays and six spectrographic analyses made on fuel pellets chosen at random during the reloading. The oxide density (10.40 ± 0.06 g UO_2/cm^3) . . . is based on individual volume displacement measurements with 20 pellets selected at random during the reloading operations. The mass of UO_2 per rod (1203.38 ± 4.12 g) is the average mass of the 1865 rods of this type available for use in the experiments. . . . The rubber end cap density (1.321 g/cm^3) . . . is the result of a single mass-volume measurement with six end caps selected at random. The composition of the end caps is the result of four analyses on randomly selected end caps.

Uranium isotopic composition is summarized in Table 4.

Table 4. Isotopic Composition of Uranium in 4.31% Enriched UO_2 Fuel Rods (Reference 10, p. 2.3).

Uranium Isotope	Wt.%
^{234}U	0.022 ± 0.002
^{235}U	4.306 ± 0.013
^{236}U	0.022 ± 0.002
^{238}U	95.650 ± 0.017
Total	100.000

Rubber end cap data[a] and 6061 aluminum tubing (clad) data are given in Table 5. The 6061 aluminum data includes the measured density and the ASTM Standard chemical composition.[b]

[a] Reference 10, p. 2.3.

[b] Reference 10, p. A.2, and from *Alcoa Aluminum Handbook*, Aluminum Company of America, pp. 46-50, 1967.

Table 5. Rubber End Cap and 6061 Aluminum Clad Data.

Element	Wt.%
Rubber End Cap (density - 1.321 g/cm^3)	
C	58.0 ± 1
H	6.5 ± 0.3
Ca	11.4 ± 1.8
S	1.7 ± 0.2
Si	0.3 ± 0.1
O	22.1 (balance)
6061 Aluminum[(a)] (density - 2.69 g/cm^3)	
Si	0.40-0.80 (0.6 nominal)
Fe	0.7 (maximum)
Cu	0.15-0.40 (0.25 nominal)
Mn	0.15 (maximum)
Mg	0.8-1.2 (1.0 nominal)
Cr	0.04-0.35 (0.2 nominal)
Zn	0.25 (maximum)
Ti	0.15 (maximum)
Al	remainder (96.00-98.61)

(a) Impurities are limited to maximums of 0.05 wt.% each and 0.15 wt.% total.

1.3.2 Reflecting Walls

Assembled Lead Wall. The reported lead wall density is 11.07 ± 0.04 g/cm^3 (Reference 3, p. 12). The lead bricks are 99.87% pure. Chemical composition of the lead is given in Table 6 (Reference 3, B-3).

Table 6. Material Composition of Lead Wall.

Element	Wt.%
Pb	99.870 ± 0.160
Cu	0.014 ± 0.017
Sb	0.071 ± 0.134
All Others	0.045 (Balance)

Assembled Uranium Wall. The reported depleted uranium wall density is 18.7 ± 0.1 g/cm^3 (Reference 3, p. 10). The weight percent of uranium is 99.87 ± 0.10%, and the weight percent of ^{235}U is 0.199 ± 0.002.

Steel Wall. The reported density of the steel wall is 7.84 g/cm^3. The material composition of the steel wall (Reference 5, p. 10) is given in Table 7.

Table 7. Material Composition of Steel Wall.

Element	Wt.%
Fe	96.77 ± 0.13
C	0.19
Mn	1.28 ± 0.03
P	0.004
S	0.006
Si	0.22
Ni	0.79 ± 0.14
Mo	0.49 ± 0.05
Cr	0.12 ± 0.01
Cu	0.13 ± 0.01

1.3.3 Water - Laboratory analyses of the water in the tank were done. The reported impurity concentrations are given in Table C.1 of Appendix C. The approximate average water temperature was 22°C.[a] This corresponds to a density of 0.997766 g/cm^3.[b]

1.3.4 Lattice Plates and Fuel Rod Support Plates - The acrylic fuel rod support plates and lattice plates had a density of 1.185 g/cm^3 and were 8 wt.% hydrogen, 60 wt.% carbon, and 32 wt.% oxygen. (Reference 4, pp. 11 and 20; Reference 10, p. 2.5; Reference 13, p. 133) Uncertainties and methods of determination were not given. Polypropylene (C_3H_6) lattice plates had a density of 0.904 g/cm^3 (Reference 6, p. 3).

1.3.5 Support Structures and Tank - Experiment support structures, including lattice plate supports and spacer rods, control/safety blade guides, and tubes housing the proportional counters were 6061 aluminum alloy. (Constituents of 6061 aluminum are given in Table 5.) As mentioned in Section 1.2, doubling the aluminum grid plate supports and the control and safety blade guides did not have a measurable effect on predicted critical separation.

The experiment tank was carbon steel, which is approximately 1 wt.% Mn, 0.9 wt.% C, and the remainder, 98.1 wt.% Fe.[c]

1.4 Supplemental Experimental Measurements

No supplemental experimental measurements were reported.

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[a] Estimated from logbook values, which were recorded for approximately 10 percent of the experiments and ranged from 18°C to 26°C.

[b] Interpolated from densities at 20 and 25°C, Robert C. Weast, ed., *CRC Handbook of Chemistry and Physics, 68th Edition*, p. F-10.

[c] Robert C. Weast, ed., *CRC Handbook of Chemistry and Physics, 68th Edition*, CRC Press, p. E-114, 1987.

2.0 EVALUATION OF EXPERIMENTAL DATA

Experiments were well documented and carefully performed. There were no significant omissions of data. However, uncertainties in measurement data contribute to an uncertainty in the benchmark-model k_{eff}. Descriptions of calculations of the effect of the uncertainties on k_{eff} are given below. Results are summarized in Table 8.

2.1 Fuel Rod Characterization

The average length of the fuel region was not given. Rather, a maximum fuel length of 92.71 cm and a minimum fuel length of 91.44 cm were reported. However, using the average of the reported maximum and minimum lengths, the reported fuel diameter, and the reported average mass of UO_2 per rod does give the reported average UO_2 density of 10.40 g/cm^3. A sensitivity study, with mass of UO_2 per rod held constant over this range in fuel length, gave Δk_{eff}'s of from -0.02 to +0.08%,[a] as shown in Table 8. Therefore uncertainty in the fuel length contributes a small uncertainty to the benchmark-model k_{eff} value.

Reported end plug dimensions and density were for uncompressed plugs. Uncompressed plugs were slightly thinner and longer than the space inside the clad at the ends of the fuel rod. Plugs were, therefore, compressed in order to hold the fuel in the rods. A sensitivity study was performed with compressed plugs that exactly filled the clad on both ends of the centered 92.075-cm-long fuel region. In order to conserve plug mass, density increased. Compressing the plugs in this manner increased k_{eff} by 0.0007% for both 2.54-cm-pitch rods and 1.892-cm-pitch rods. Replacing the plugs with water changed k_{eff} by -0.011% for 2.54-cm-pitch rods and by -0.014% for 1.892-cm-pitch rods. Since compression of the plugs has such a small effect on k_{eff}, this uncertainty may be neglected.

The uncertainty in fuel diameter was ± 0.003 cm. Varying the fuel diameter by this amount, with a corresponding change in UO_2 density, gave a maximum Δk_{eff} of 0.02% The maximum reported uncertainty in pitch was ± 0.003 inch (0.0076 cm).[b] The maximum Δk_{eff}'s calculated were 0.103% for 2.54-cm-pitch rods and 0.127% for 1.892-cm-pitch rods.

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[a] Sensitivity studies described in this section used ONEDANT models, with ENDF/B 27-group cross sections, of a homogenized mixture representing an infinite slab of fuel rods. The calculations were P_3, S_{16}, with a convergence criterion of 10^{-6}. The mesh spacing was approximately one mean-free-path (~0.2 cm) within approximately one centimeter of material boundaries and approximately 2 mean-free-paths elsewhere. (Occasional check calculations with double mesh were performed to verify calculated k_{eff} values.)

Cross sections for the homogenized mixture were generated by XSDRNPM-S for rods of the specified materials, radial dimensions, and pitch. The thickness of the slab was equal to the oxide length in the rods. The plugged ends of the rods were represented by a homogeneous mixture of plug material, clad, and water.

[b] Reference 8, p. E.4, bottom plate, corrected.

Uncertainties were also reported in average mass of UO_2 per rod (± 4.12 g), in average mass of uranium per rod (± 4.80 g), and in enrichment (± 0.013 wt.%). Eight cases for each of the two pitches were calculated for all possible combinations of the extremes of these three variables. A decrease in ^{235}U wt.% was accompanied by an equal increase in ^{238}U wt.% in the calculational model. The highest calculated k_{eff}'s were for the minimum UO_2 mass, the maximum U mass, and the maximum enrichment. The calculated Δk_{eff}'s, as compared to models having the average amounts of these variables, was +0.083% for 2.54-cm-pitch rods and +0.070% for 1.892 cm pitch. The lowest calculated k_{eff} for 2.54-cm-pitch rods was for maximum UO_2, minimum U, and minimum enrichment, with a Δk_{eff} of -0.147%. For rods at 1.892 cm pitch, the lowest calculated k_{eff} was for minimum UO_2, maximum U, and minimum enrichment, with a Δk_{eff} of -0.054%. These four worst-case results should also contribute to the uncertainty in the benchmark model k_{eff}.

In the last two rows of Table 6 are results from a model that simultaneously combines all modifications that contribute to a change in k_{eff} in the same sense, either positive or negative. For example, all changes that produce negative effects on rods at 1.892-cm pitch are: decreased fuel length, compressed plug, increased fuel diameter, decreased pitch, with minimum UO_2, maximum U, and minimum enrichment. (Dimensions and atom densities of the model are modified accordingly.)

Results indicate that an uncertainty of ± 0.18% for 2.54-cm-pitch rods and ± 0.26% for 1.892-cm-pitch rods should be included in the benchmark-model k_{eff} to account for fuel rod measurement uncertainties. This estimate of the effect on k_{eff} is conservative because it is assumed that all rods differ from the average in all respects that affect k_{eff} in the same sense, which is unlikely. The estimate for the uncertainty in pitch is especially conservative. (See footnote c of Table 8).

Table 8. Sensitivity of k_{eff} to Uncertainties in Fuel Rod Characterization.

Quantity (Amount of Change)	% Δk_{eff} (ONEDANT)[a] for Increase in the Quantity		% Δk_{eff} (ONEDANT)[a] for Decrease in the Quantity	
Pitch →	2.54 cm	1.892 cm	2.54 cm	1.892 cm
Fuel Length (± 0.635 cm)	-0.020	+0.076	-0.026	-0.057
Plug Compression (± 0.3175 cm change in length)	+0.0007	+0.0007	-0.0007[b]	-0.0007[b]
Fuel Diameter (± 0.003 cm)	+0.021	-0.004	+0.005	+0.023
Pitch (± 0.0076 cm[c])	-0.103	+0.127	+0.074	-0.122
Combination of Enrichment (± 0.013 wt.%), UO_2 Mass Per Rod (± 4.12 g), U Mass Per Rod (± 4.80 g)	+0.083[d]	+0.070[d]	-0.147[e]	-0.054[f]
Pitch →	2.54 cm		1.892 cm	
Combine all changes that individually increase k_{eff}	Δk_{eff} = +0.13%		Δk_{eff} = +0.26%	
Combine all changes that individually decrease k_{eff}	Δk_{eff} = -0.18%		Δk_{eff} = -0.21%	

(a) 27-group cross sections with homogenized lattice-cell fuel region (CSASIX); infinite slab geometry; sample input given in Appendix D.
(b) Not calculated; estimated from result for increase in compression.
(c) The largest standard deviation for sets of center-to-center spacing measurements for triangular pitch lattice plates of Reference 8 (Appendix E) was 0.003 inch (0.0076 cm). References 7 (p.2) and 8 (p.36) give the uncertainty in pitch as ± 0.005 cm. References 9 (p. 3.2) and 10 (Appendix D) give the uncertainty in pitch as ± 0.001 cm. Therefore, the calculated uncertainty is conservative.
(d) Highest k_{eff} value; for a model with minimum UO_2, maximum U, and maximum enrichment.
(e) Lowest k_{eff} value; for a model with maximum UO_2, minimum U, and minimum enrichment.
(f) Lowest k_{eff} value; for a model with minimum UO_2, maximum U, and minimum enrichment.

2.2 Reflector

2.2.1 Top Water Reflector - The minimum thickness of the top water reflector was 15 cm above the fuel region. Since the end plug is slightly less than 1 inch long (2.2225 cm), the minimum water reflector thickness above the rods is 12.7775 cm.

ONEDANT (27-group, ENDF/B-IV) calculations were performed for an infinite-slab fuel region with a water reflector on both sides. The reflector thickness was varied from 15 to 30 centimeters. The effect on k_{eff} of the outermost 15 centimeters of water was less than 0.001%. Replacing the outermost 15 centimeters of water with 40 centimeters of full-density stainless steel or concrete gave similar results: the effect on k_{eff} was 0.002% or less.

These calculations indicate that a top water reflector with a thickness of 15 centimeters may be considered as "effectively infinite" and the effects of materials beyond the top and bottom reflectors may be neglected. Therefore, the lack of data about material above the 15-cm-thick top water reflector does not affect the acceptability of these experiments as benchmark critical experiments.

2.2.2 Side Water Reflector - Additionally, ONEDANT was used to determine the effect of a radial water reflector outside of lead, stainless steel, or uranium walls for a cylindrical, XSDRN-homogenized array of pins. The difference in k_{eff} between a 15-cm-thick water reflector and a 30-cm-thick water reflector is 0.002%. Replacing the outermost 8 centimeters of the 15-cm-thick water reflector with 20% stainless steel in water affects k_{eff} by less than 0.01%. Therefore, lack of specifications about detectors, which were placed in the water reflector more than 15 centimeters away from the reflecting walls, does not affect the acceptability of these experiments.

2.3 Water Impurities

Water impurity sensitivity studies in Appendix C and Section 3.3 indicate that only boron and gadolinium impurities significantly affect k_{eff}. No boron or gadolinium impurities were reported in References 3, 5, and 6, which describe all of Cases 1 - 30.

2.4 Temperature Data

Water temperatures were recorded in logbooks for approximately ten percent of the experiments. Measured temperatures ranged from 18°C to 26°C. Calculations gave a change in k_{eff} of 0.072% between these two extremes of temperature for a pitch of 2.54 cm and 0.023% for a pitch of 1.892 cm. Therefore, estimates of the uncertainty in k_{eff} due to the effects of temperature are half of these amounts, namely 0.04% for 2.54-cm pitch and 0.01% for 1.892-cm pitch.

2.5 Cluster Separations

The measurement uncertainties in cluster separation for Cases 1 through 30 (see Table 3) range from 0.01 cm to 0.05 cm. To calculate the effect on k_{eff} of this uncertainty, cluster separations were reduced for all of the 30 cases. Results are summarized in Table 9. The largest effect was 0.03% for Cases 13 and 23. This, then, is a conservative estimate of the effect on k_{eff} of cluster separation uncertainty.

Table 9. Uncertainties in Benchmark-Model k_{eff} Due to Cluster Separation Measurement Uncertainty.

Case No.	Pitch (cm)	Reflecting Wall Material	Uncertainty in Cluster Separation Measurement (cm)	$\%\Delta k_{eff}$ in Uncertainty of Benchmark-Model k_{eff} [(a)]
1	2.540	lead	0.01	0.001
2	2.540	lead	0.02	0.003
3	2.540	lead	0.02	0.002
4	2.540	lead	0.02	0.012
5	2.540	uranium	0.01	0.002
6	2.540	uranium	0.01	0.002
7	2.540	uranium	0.05	0.012
8	2.540	uranium	0.02	0.005
9	2.540	steel	0.02	0.007
10	2.540	steel	0.05	0.014
11	2.540	steel	0.01	0.007
12	2.540	steel	0.05	0.010
13	2.540	steel	0.05	0.026
14	1.892	steel	0.02	0.008
15	1.892	steel	0.02	0.008
16	1.892	steel	0.01	0.003
17	1.892	steel	0.02	0.007
18	1.892	steel	0.01	0.002
19	1.892	steel	0.03	0.017
20	1.892	lead	0.03	0.008
21	1.892	lead	0.05	0.013
22	1.892	lead	0.02	0.004
23	1.892	lead	0.03	0.026
24	1.892	uranium	0.03	0.013

Case No.	Pitch (cm)	Reflecting Wall Material	Uncertainty in Cluster Separation Measurement (cm)	$\%\Delta k_{eff}$ in Uncertainty of Benchmark-Model k_{eff} [(a)]
25	1.892	uranium	0.02	0.007
26	1.892	uranium	0.05	0.012
27	1.892	uranium	0.04	0.007
28	1.892	uranium	0.04	0.007
29	1.892	uranium	0.02	0.004
30	1.892	uranium	0.02	0.004

(a) TWODANT with 27-group ENDF/B-IV cross sections.

2.6 Reflecting Wall Separations

The measurement uncertainties in separation of the reflecting walls from the clusters (see Table 3) vary from 0.076 cm to 0.148 cm. To calculate the effect on k_{eff} of this uncertainty, reflecting wall separations were varied by the amount of the uncertainty. Results are summarized in Table 10. The largest effect, 0.08% for Case 25, can be used as a conservative estimate of the effect on k_{eff} of the uncertainty in separation between reflecting walls and clusters.

Table 10. Uncertainties in Benchmark-Model k_{eff} Due to Wall Separation Measurement Uncertainty.

Case No.[a]	Pitch (cm)	Reflecting Wall Material	Uncertainty in Wall Separation Measurement (cm)	$\%\Delta k_{eff}$ in Uncertainty of Benchmark-Model k_{eff}[b]
2	2.540	lead	0.102	0.030
3	2.540	lead	0.076	0.053
4	2.540	lead	0.102	0.056
6	2.540	uranium	0.102	0.009
7	2.540	uranium	0.076	0.061
8	2.540	uranium	0.102	0.067
10	2.540	steel	0.102	0.009
11	2.540	steel	0.076	0.040
12	2.540	steel	0.107	0.075
13	2.540	steel	0.102	0.041
15	1.892	steel	0.102	0.011
16	1.892	steel	0.076	0.013
17	1.892	steel	0.102	0.036
18	1.892	steel	0.107	0.047
19	1.892	steel	0.102	0.029
21	1.892	lead	0.102	0.004
22	1.892	lead	0.102	0.043
23	1.892	lead	0.086	0.016
25	1.892	uranium	0.102	0.083
26	1.892	uranium	0.076	0.039
27	1.892	uranium	0.102	0.019

Case No.[a]	Pitch (cm)	Reflecting Wall Material	Uncertainty in Wall Separation Measurement (cm)	$\%\Delta k_{eff}$ in Uncertainty of Benchmark-Model k_{eff}[b]
28	1.892	uranium	0.107	0.004
29	1.892	uranium	0.148	0.033
30	1.892	uranium	0.102	0.041

(a) Distance between reflecting walls and fuel clusters for Cases 1, 5, 9, 14, and 24 is 0 cm, with no uncertainty reported. Therefore, these cases are not included.
(b) TWODANT with 27-group ENDF/B-IV cross sections.

3.0 BENCHMARK SPECIFICATIONS

3.1 Description of Model

The calculational models consist of square-pitched, aluminum-clad cylindrical fuel pins in water arranged in rectangular clusters. Descriptions of the benchmark critical configurations, including cluster dimensions, separations, and fuel rod pitch, are given in Table 3.

The results of sensitivity studies were used to simplify the model. They are described below.

3.1.1 Reflecting Wall Compositions - Three cases were chosen, based on apparent maximum effect of the wall, to determine the influence, if any, of wall impurities and wall density and composition uncertainties on k_{eff}. For Case 1 of Table 3, maximum wall density and lead wt.% was compared to minimum wall density and lead wt.% and to minimum wall density and lead wt.% with impurities added. Results are shown in Table 11. Similarly, for Case 6 of Table 3, uranium at maximum wall density and uranium wt.% was compared to minimum wall density and uranium wt.%, with and without typical impurities. Results are shown in Table 12. For Case 18 of Table 3, maximum and minimum wt.% Fe, compensated by decreased Ni and increased Ni, respectively, were compared, with results given in Table 13. Results indicate that the uncertainty in k_{eff} due to uncertainty in reflecting wall density and composition is less than 0.040 $\%\Delta k_{eff}$. This should be included in the total uncertainty of the benchmark-model k_{eff}.

Table 11. Calculated Effect of Lead Wall Composition Uncertainties on k_{eff} (Case 1).

Description	$\%\Delta k_{eff}$
11.11 g/cm^3, 100 wt.% Pb	+0.040
11.03 g/cm^3, 99.71 wt.% Pb	-0.025
11.03 g/cm^3, 99.71 wt.% Pb with 0.29 wt.% Impurities[(a)]	-0.025
Lead Walls Replaced with Water	-4.458

(a) based on Material Handbook, Vol. 1, p 1055, 8th Edition, American Society for Metals, 1961. Cu:0.031, Si:0.02, Sn:0.235, Fe:0.002, Zn:0.002 wt.%.

Table 12. Calculated Effect of Uranium Wall Composition Uncertainties on k_{eff} (Case 6).

Description	$\%\Delta k_{eff}$
18.8 g/cm^3, 99.97 wt.% Uranium	+0.017
18.6 g/cm^3, 99.77 wt.% Uranium	-0.018
18.6 g/cm^3, 99.87 wt.% Uranium with Impurities[(a)]	+0.008
Uranium Walls Replaced with Water	-4.436

(a) Based on Reference 3. C:679, N:43, Fe:297, H:0.85, O:42, Si:199 ppm.

Table 13. Calculated Effect of Steel Wall Composition Uncertainties on k_{eff} (Case 18).

Case No.	Description	$\%\Delta k_{eff}$
1	7.84 g/cm^3 SS with 96.9 wt.% Fe, all other constituents, & 0.66 wt.% Ni	+0.001
2	7.84 g/cm^3 SS with 96.64 wt.% Fe, all other constituents, & 0.92 wt.% Ni	+0.001
3	Steel Walls Replaced with Water	-1.761

3.1.2 Lattice Plates - ONEDANT calculations of an infinite slab of fuel pins, with and without lattice plates present (using two fuel mixtures, one with acrylic or polypropylene moderator and one with water moderator) and reflected by 15 centimeters of water, were performed. The effect on k_{eff} of the lattice plates of the specified thickness and at the specified locations was 0.03% for rods at 2.54-cm pitch and acrylic lattice plates and was 0.02% for rods at 1.892-cm pitch with polypropylene lattice plates. This estimate of the effect of omitting the lattice plates is small and can be included in the total k_{eff} uncertainty.

3.1.3 Bottom Reflector - The effects on k_{eff} of the one-inch-thick acrylic support plate directly beneath an infinite slab of fuel rods and of the carbon-steel tank 17.84 cm below the fuel rods was calculated using ONEDANT. Results are shown in Table 14. As expected, the carbon-steel tank had practically no effect on k_{eff}, while the acrylic support plate had a small measurable effect (0.02% for one support plate). Therefore, the acrylic support plate is retained in the benchmark model. As discussed in Section 2.2, concrete or stainless steel beyond 15 centimeters of water

reflector have a negligible effect on k_{eff}. Therefore, the model of the bottom reflector is 2.54 cm of acrylic followed by 15.3 cm of water.

Table 14. Effect of Reflector Materials on k_{eff}.[(a)]

Reflector			Δk_{eff} (%)
Inner 2.54 cm	Middle 15.3 cm	Outer 0.952 cm	
acrylic	water	carbon steel	-
acrylic	water	water	+0.001
water	water	water	-0.04

(a) ONEDANT infinite slab of fuel pins with reflector materials on both sides. CSAS 27-group ENDF/B-IV cross sections and homogeneous fuel region mixture created by XSDRNPM are used.

3.2 Dimensions

Fuel rod dimensions are shown in Figure 9. The rod has an outer diameter of 1.415 cm and is 96.52 cm long. The UO_2 fuel region has a diameter of 1.265 cm and is 92.075 cm long. The clad is 0.066 cm thick. Therefore, the gap between UO_2 and clad is 0.009 cm thick with an outer radius of 0.6415 cm. The compressed rubber end plugs are 2.2225 cm long with a radius of 0.6415 cm, to fit exactly within the ends of the fuel rod.

The bottom reflector is a single 2.54-cm-thick acrylic plate, which extends horizontally to the outermost cell-boundary edges of the clusters, followed by 15.3 cm of water. The four side reflectors are 30.5-cm-thick water including reflecting walls on two sides, and extending beyond the ends of the reflecting walls at the ends. The top reflector is 15.2 cm of water above the tops of the fuel rods.

The lead, depleted uranium, or steel reflecting walls were positioned on either side of the fuel clusters within the 30.5-cm-thick side reflector. The bottom surface of the walls was 15.3 cm below the bottom surface of the acrylic fuel rod support plate. The walls were centered horizontally beside the clusters. The lead walls were 1.64 m long by 1.234 m high and were 0.102 m thick. The uranium walls were 1.523 m long by 1.219 m high and were 0.0765 m thick. The steel walls were 1.473 m long by 1.219 m high and were 0.1785 m thick.

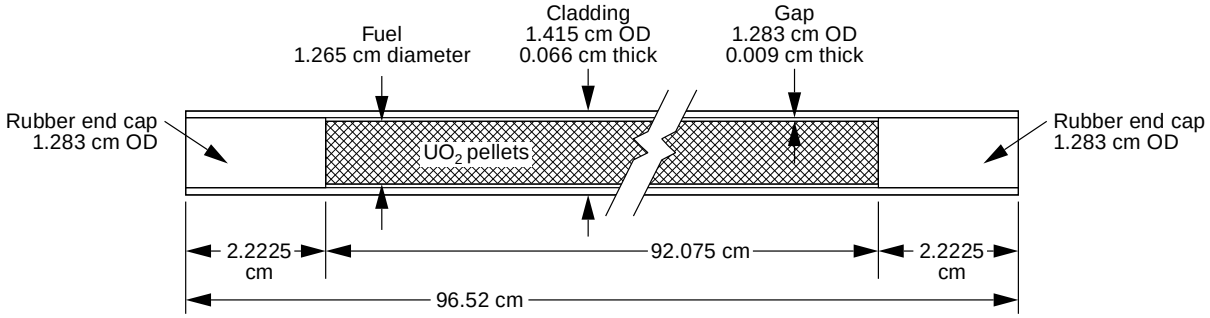

Figure 9. Fuel Rod Model.

3.3 Material Data

3.3.1 Fuel Rods - The fuel region consists of 1203.38 g of UO_2. The mass of uranium in each rod is 1059.64 g. The isotopic composition of the uranium is 0.022 wt.% ^{234}U, 4.306 wt.% ^{235}U, 0.022 wt.% ^{236}U, and 95.650 wt.% ^{238}U. Fuel rods have 6061 aluminum clad and compressed rubber end plugs of density 1.498 g/cm^3.[a] Atom densities are given in Table 15.

[a] This density is more than the reported density of the plugs in Table 5 because of the compression of the plugs.

Table 15. Fuel Rod Atom Densities.

Material	Isotope	Atom Density (barn-cm)$^{-1}$
$U(4.306)O_2$ Fuel	^{234}U	5.1835×10^{-6}
	^{235}U	1.0102×10^{-3}
	^{236}U	5.1395×10^{-6}
	^{238}U	2.2157×10^{-2}
	O	4.6753×10^{-2}
6061 Aluminum Clad (2.69 g/cm^3)	Al	5.8433×10^{-2}
	Cr	6.2310×10^{-5}
	Cu	6.3731×10^{-5}
	Mg	6.6651×10^{-4}
	Mn	2.2115×10^{-5}
	Ti	2.5375×10^{-5}
	Zn	3.0967×10^{-5}
	Si	3.4607×10^{-4}
	Fe	1.0152×10^{-4}
Rubber End Plug (1.498 g/cm^3)	C	4.3562×10^{-2}
	H	5.8178×10^{-2}
	Ca	2.5660×10^{-3}
	S	4.7820×10^{-4}
	Si	9.6360×10^{-5}
	O	1.2461×10^{-2}

3.3.2 Reflecting Walls - Lead, uranium, and steel wall atom densities are given in Table 16.

Table 16. Reflecting Wall Atom Densities.

Material	Isotope	Wt.%	Atom Density $(barns\text{-}cm)^{-1}$
Lead	Pb	99.87	3.2132×10^{-2}
Depleted Uranium	^{235}U	00.20	9.5220×10^{-5}
	^{238}U	99.67	4.7151×10^{-2}
Steel	Fe	96.77	8.1810×10^{-2}
	C	.19	7.4686×10^{-4}
	Mn	1.28	1.1000×10^{-3}
	P	.004	6.0971×10^{-6}
	S	.006	8.8332×10^{-6}
	Si	.22	3.6983×10^{-4}
	Ni	.79	6.3552×10^{-4}
	Mo	.49	2.4114×10^{-4}
	Cr	.12	1.0896×10^{-4}
	Cu	.13	9.6587×10^{-5}

3.3.3 Moderator-Reflector - Fuel rods rest on an acrylic support plate. The support plate density is 1.185 g/cm^3 and is composed of 8 wt.% hydrogen, 60 wt.% carbon, and 32 wt.% oxygen. The moderator-reflector is water at a temperature of 22°C. Atom densities are given in Table 17.

Table 17. Moderator-Reflector Atom Densities.

Material	Isotope	Atom Density $(barns\text{-}cm)^{-1}$
Water[(a)]	H O	6.6706×10^{-2} 3.3353×10^{-2}
Acrylic	H C O	5.6642×10^{-2} 3.5648×10^{-2} 1.4273×10^{-2}

(a) This is 0.997766 g/cm^3, interpolated from densities at 20°C and 25°C (CRC Handbook of Chemistry and Physics, 68th edition, p F-10.)

3.4 Temperature Data

Temperature data for the individual experiments were not published.

Logbook records give temperature data for approximately every tenth experiment. Recorded values vary between 18° and 26°C, with most values between 20°C and 25°C. An approximate temperature of 22°C (295 K) was used in the models.

A sensitivity study in Section 2.4 demonstrated that the effect on k_{eff} of half the temperature range is small. Therefore, any reasonable approximation to room temperature may be used in the model. (Temperature uncertainty is included in the uncertainty in benchmark-model k_{eff}.)

3.5 Experimental and Benchmark-Model k_{eff}

The reported configurations were extrapolations to critical configurations. Therefore, the experimental k_{eff} was 1.000.

Some model simplifications (no aluminum support structures; no reflection beyond 30 cm of water on the sides, 15 cm of water above, and 15.3 cm of water below; no measurement devices in the reflector beyond 15 cm; uniform end plugs filling the ends of the clad) were judged to have negligible effects on k_{eff}. However, other experimental uncertainties or model simplifications whose effects were calculated in sensitivity studies, contribute to an estimated uncertainty in the benchmark model k_{eff}. Uncertainties included are listed in Table 18.

Table 18. Uncertainty in Benchmark-Model k_{eff}.

Measurement Uncertainty or Model Simplification	Δk_{eff}	
	2.54-cm pitch	1.892-cm pitch
Fuel Rod Characterization	0.0018	0.0026
No Lattice Plates	0.0003	0.0002
Temperature	0.0004	0.0001
Cluster Separation	0.0003	
Reflecting Wall Composition/Density	0.0004	
Reflecting Wall Separation	0.0008	
Total Uncertainty in k_{eff} [(a)]	0.0021	0.0028

(a) Square root of sum of squares of individual Δk_{eff} values.

Therefore, the benchmark model k_{eff} is 1.0000 ± 0.0021 for Cases 1 - 13 and is 1.0000 ± 0.0028 for Cases 14 - 30.

4.0 RESULTS OF SAMPLE CALCULATIONS

Results of calculations representing the thirty critical configurations are presented in Tables 19 and 20. Code versions and modeling options are discussed briefly in paragraphs preceding the input listings in Appendix A.

For cases at 2.54-cm pitch (Cases 1 - 13), one-third of the results are below the range of k_{eff} that includes the estimated uncertainty, one-third of the results are above the range, and one-third are within the estimated uncertainty of the benchmark-model k_{eff}. For the remaining cases, at 1.892-cm pitch (Cases 14 - 30), KENO with Hansen-Roach cross sections underestimates k_{eff} by 2 - 3%. For the smaller pitch cases (Cases 14 - 30), KENO with Hansen-Roach cross sections predicts k_{eff} about 2% less than the larger pitch cases (Cases 1 - 13). About two-thirds of the KENO with 27-group cross sections and the MCNP results are below the range of k_{eff} that includes the estimated uncertainty. Nine results are within the range. Two KENO 27-group and two MCNP results are above the range that includes the estimated uncertainty.

Table 19. Sample Calculation Results for $U(4.31)O_2$ Fuel Rods, 2.54-cm Pitch in Water (United States).

Code (Cross Sections Set)--> Case Number	KENO (Hansen-Roach)[(a)]	KENO (27-Group ENDF/B-IV)	MCNP (Continuous-Energy ENDF/B-V)
1	1.0063 ± .0018	1.0060 ± .0014	1.0055 ± .0018
2	1.0023 ± .0017	1.0066 ± .0017	1.0085 ± .0019
3	1.0043 ± .0020	1.0047 ± .0017	1.0076 ± .0019
4	1.0005 ± .0019	0.9872 ± .0019	1.0008 ± .0019
5	0.9841 ± .0017	0.9946 ± .0017	0.9974 ± .0016
6	0.9900 ± .0019	0.9965 ± .0015	0.9989 ± .0016
7	0.9969 ± .0015	0.9963 ± .0017	1.0008 ± .0017
8	0.9950 ± .0017	0.9910 ± .0015	0.9977 ± .0018
9	0.9999 ± .0017	1.0064 ± .0018	1.0027 ± .0017
10	0.9984 ± .0017	1.0029 ± .0016	0.9991 ± .0018
11	1.0013 ± .0019	1.0025 ± .0018	1.0000 ± .0016
12	1.0004 ± .0017	0.9981 ± .0019	0.9984 ± .0020
13	0.9980 ± .0020	0.9997 ± .0019	1.0002 ± .0020

(a) Cross sections were the original Hansen-Roach 16-group set, except for the following: ^{234}U and ^{236}U (Mihalczo Mod of H-R U-238); Cr (AEROJET); Cu, Mn, Si, and S (XSDRN); Ti, Zn, and Ca (GAM-2).

Table 20. Calculated Results for U(4.31)O_2 Fuel Rods, 1.892-cm Pitch in Water (United States).

Code (Cross Sections Set)--> Case Number	KENO (Hansen-Roach)[a]	KENO (27-Group ENDF/B-IV)	MCNP (Continuous-Energy ENDF/B-V)
14	0.9756 ± .0017	1.0035 ± .0020	0.9965 ± .0018
15	0.9804 ± .0018	0.9991 ± .0017	0.9958 ± .0018
16	0.9773 ± .0018	1.0010 ± .0018	0.9989 ± .0020
17	0.9805 ± .0017	1.0006 ± .0019	0.9966 ± .0019
18	0.9753 ± .0017	0.9958 ± .0019	0.9988 ± .0021
19	0.9801 ± .0018	0.9927 ± .0020	0.9971 ± .0017
20	0.9808 ± .0019	0.9991 ± .0017	1.0025 ± .0020
21	0.9809 ± .0018	0.9951 ± .0019	1.0034 ± .0020
22	0.9754 ± .0020	0.9947 ± .0017	1.0045 ± .0017
23	0.9773 ± .0020	0.9941 ± .0017	0.9912 ± .0022
24	0.9664 ± .0017	0.9929 ± .0018	0.9949 ± .0018
25	0.9718 ± .0018	0.9951 ± .0015	0.9996 ± .0018
26	0.9712 ± .0018	0.9969 ± .0018	0.9952 ± .0017
27	0.9696 ± .0018	0.9910 ± .0015	0.9930 ± .0017
28	0.9742 ± .0018	0.9939 ± .0018	1.0000 ± .0018
29	0.9775 ± .0015	0.9982 ± .0016	0.9957 ± .0020
30	0.9768 ± .0017	0.9918 ± .0018	0.9932 ± .0020

(a) Cross sections were the original Hansen-Roach 16-group set, except for the following: ^{234}U and ^{236}U (Mihalczo Mod of H-R U-238); Cr (AEROJET); Cu, Mn, Si, and S (XSDRN); Ti, Zn, and Ca (GAM-2).

5.0 REFERENCES

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2. S. R. Bierman, B. M. Durst, and E. D. Clayton, "Critical Separation Between Subcritical Clusters of 4.29 Wt.% ^{235}U Enriched UO_2 Rods in Water with Fixed Neutron Poisons," NUREG/CR-0073, Battelle Pacific Northwest Laboratories, Richland, Washington, May 1978.

3. S. R. Bierman, B. M. Durst, and E. D. Clayton, "Criticality Experiments with Subcritical Clusters of 2.35 Wt.% and 4.29 Wt.% ^{235}U Enriched UO_2 Rods in Water with Uranium or Lead Reflecting Walls, Near Optimum Water-to-Fuel Volume Ratio," NUREG/CR-0796, Vol. 1, PNL-2827, Battelle Pacific Northwest Laboratories, Richland, Washington, April 1979.

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6. S. R. Bierman, B. M. Durst, and E. D. Clayton, "Criticality Experiments with Subcritical Clusters of 2.35 Wt.% and 4.31 Wt.% ^{235}U Enriched UO_2 Rods in Water with Uranium or Lead Reflecting Walls, Undermoderated Water-to-Fuel Volume Ratio of 1.6," NUREG/CR-0796, PNL-3926, Vol. 2, Battelle Pacific Northwest Laboratories, Richland, Washington, December 1981.

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8. S. R. Bierman, E. S. Murphy, E. D. Clayton, and R. T. Keay, "Criticality Experiments with Low Enriched UO_2 Fuel Rods in Water Containing Dissolved Gadolinium," PNL-4976, Battelle Pacific Northwest Laboratories, Richland, Washington, February 1984.

9. S. R. Bierman, "Criticality Experiments to Provide Benchmark Data on Neutron Flux Traps," PNL-6205, UC-714, Battelle Pacific Northwest Laboratories, Richland, Washington, June 1988.

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11. B. M. Durst, S. R. Bierman, E. D. Clayton, J. F. Mincey, and R. T. Primm III, "Summary of Experimental Data for Critical Arrays of Water Moderated Fast Test Reactor Fuel," PNL-3313, ORNL/Sub-81/97731/1, Battelle Pacific Northwest Laboratories, Richland, Washington, May 1981.

12. S. R. Bierman, B. M. Durst, and E. D. Clayton, "Critical Separation between Subcritical Clusters of Low Enriched UO_2 Rods in Water with Fixed Neutron Poisons," Nuc. Technol., **42**, pp. 237-249, March 1979.

13. S. R. Bierman and E. D. Clayton, "Criticality Experiments with Subcritical Clusters of 2.35 and 4.31 Wt.% ^{235}U-Enriched UO_2 Rods in Water with Steel Reflecting Walls," Nuc. Technol., **54**, August 1981.

14. S. R. Bierman, B. M. Durst, and E. D. Clayton, "Criticality Experiments with Subcritical Clusters of Low Enriched UO_2 Rods in Water with Uranium or Lead Reflecting Walls," Nuc. Technol., **47**, January 1980.

APPENDIX A: TYPICAL INPUT LISTINGS

A.1 KENO Input Listings

The version of KENO V.a used was SCALE 4.0 (creation date 08/09/91, for standalone KENO V.a with Hansen-Roach cross sections, provided by the Radiation Shielding Information Center; creation date 07/20/92, for KENO V.a with CSAS 27-group ENDF/B-IV cross sections).

KENO V.a input files were created with arrays of fuel rod units. Cuboids of water provided the separation between clusters of rods.

KENO V.a was run using 110 active generations of 1500 neutrons each, after skipping 50 generations.

The resonance correction used to determine the Hansen-Roach cross section IDs for ^{235}U and ^{238}U were calculated using the formula

$$\sigma_{pj} = \sum_{i}^{n} \frac{\sigma_{si} N_i}{N_j} + \frac{1 - C}{2 r_f N_j}$$

σ_{pj} is the resonance correction for the j^{th} fissile nuclide. N_i is the atom density of the i^{th} nuclide in the fuel mixture, n is the number of different nuclides in the fuel mixture, and σ_{si} is the scattering cross section in the resonance region for the i^{th} component of the mixture. Values used for σ_{si} were 12 for uranium and 3.7 for oxygen. Linear interpolation was used to apportion atom densities between the two uranium cross section sets with σ_p values closest to the calculated σ_p.

The last term is the Wigner-Rational correction. C is the Dancoff correction factor and r_f is the radius of the cylindrical fuel region of the fuel rod. (The value of C, the Dancoff correction factor, calculated by CSAS, was 0.03894.)

```
KENO-V.a Input Listing for Case 1 of Table 19 (16-Energy-Group
Hansen-Roach Cross Sections).
phrld41 THREE 13X8  CLUSTERS, 2.540 CM PITCH, 20.62  CM
SEPARATION
READ PARA TME=200 GEN=160 NPG=1500 NSK=50
NUB=YES LIB=41 XS1=YES RUN=YES
LNG=60000   END PARA
READ MIXT SCT=3 MIX=1
' U(4.31)02
92400 5.1835-6 92508 9.1530-4 92509 9.4904-5
92600 5.1395-6 92857 1.1216-2 92858 1.0941-2 8100 4.6753-2
MIX=2
' water
1102 6.6706-2  8100 3.3353-2
MIX=3
' 6061 Al (clad)
13100 5.8433-2  24100 6.2310-5  29100 6.3731-5
12100 6.6651-4  25100 2.2115-5  22100 2.5375-5
30100 3.0967-5  14100 3.4607-4  26100 1.0152-4
MIX=4
'  rubber (end plug)
6100 4.3562-2  1102 5.8178-2  20100 2.5660-3
16100 4.7820-4 14100 9.63560-5  8100 1.2461-2
MIX=5
'acrylic
1102 5.6642-2  6100 3.5648-2  8100 1.4273-2
MIX=6
' lead
82100  3.2132-2
END MIXT
READ GEOM
UNIT 1
 COM=* FUEL PIN *
 CYLINDER  1 1  0.6325 92.075 0.0
 CYLINDER  0 1  0.6415 92.075 0.0
 CYLINDER  4 1  0.6415 94.2975 -2.2225
 CYLINDER  3 1  0.7075 94.2975 -2.2225
 CUBOID  2 1  4P1.27 94.2975 -2.2225
UNIT 2
 COM=* ARRAY OF FUEL PINS *
 ARRAY 1 0 0 -2.2225
UNIT 3
 COM=* WATER BETWEEN CLUSTERS *
 CUBOID  2 1  19.495   0 20.320 0 94.2975 -2.2225
GLOBAL
UNIT 4
 COM=* CLUSTERS WITH WATER BETWEEN *
 ARRAY 2 0 0 -2.2225
 CUBOID  5 1  138.050 0.0 20.320 0 94.2975 -4.7625
 CUBOID  2 1  151.025 -12.975 20.320 0 103.3375 -20.0625
 REPLICATE 6 1  2R0.0 2R10.2 2R0.0  1
 REPLICATE 2 1  2R30.5  2R20.3 6.16   0 1
END GEOM
READ ARRAY  ARA=1 NUX=13 NUY=8  FILL F1 END FILL
          ARA=2 NUX=5 NUY=1
          FILL  2 3 2 3 2
               END FILL
END ARRAY
READ PLOT
  XUL=-4 YUL=34 ZUL=20 XLR=97 YLR=-4
  ZLR=20  UAX=1  VDN=-1 NAX=120 NCH=' *~ctla~' END
END PLOT
END DATA
END
```

```
KENO-V.a Input Listing for Case 8 of Table 19 (16-Energy-Group
Hansen-Roach Cross Sections).
phru44 THREE 13X8  CLUSTERS, 2.54 CM PITCH, 13.49  CM
SEPARATION
READ PARA TME=200 GEN=160 NPG=1500 NSK=50
NUB=YES LIB=41 XS1=YES RUN=YES
LNG=60000   END PARA
READ MIXT SCT=3 MIX=1
' U(4.31)02
92400 5.1835-6 92508 9.1530-4 92509 9.4904-5
92600 5.1395-6 92857 1.1216-2 92858 1.0941-2 8100 4.6753-2
MIX=2
' water
1102 6.6706-2  8100 3.3353-2
MIX=3
' 6061 Al (clad)
13100 5.8433-2  24100 6.2310-5  29100 6.3731-5
12100 6.6651-4  25100 2.2115-5  22100 2.5375-5
30100 3.0967-5  14100 3.4607-4  26100 1.0152-4
MIX=4
'  rubber (end plug)
6100 4.3562-2  1102 5.8178-2  20100 2.5660-3
16100 4.7820-4 14100 9.63560-5  8100 1.2461-2
MIX=5
'acrylic
1102 5.6642-2  6100 3.5648-2  8100 1.4273-2
MIX=6
' depleted uranium
92512 9.5220-5 92807 4.7151-2
END MIXT
READ GEOM
UNIT 1
 COM=* FUEL PIN *
 CYLINDER  1 1  0.6325 92.075 0.0
 CYLINDER  0 1  0.6415 92.075 0.0
 CYLINDER  4 1  0.6415 94.2975 -2.2225
 CYLINDER  3 1  0.7075 94.2975 -2.2225
 CUBOID  2 1  4P1.27 94.2975 -2.2225
UNIT 2
 COM=* ARRAY OF FUEL PINS *
 ARRAY 1 0 0 -2.2225
UNIT 3
 COM=* WATER BETWEEN CLUSTERS *
 CUBOID  2 1  12.365   0 20.320 0 94.2975 -2.2225
GLOBAL
UNIT 4
 COM=* CLUSTERS WITH WATER BETWEEN *
 ARRAY 2 0 0 -2.2225
 CUBOID  5 1  123.790 0.0 20.320 0 94.2975 -4.7625
 CUBOID  2 1  138.045 -14.255 20.320 0 101.8375 -20.0625
 REPLICATE 2 1  2R0.0   2R5.405 2R0.0    1
 REPLICATE 6 1  2R0.0 2R7.65 2R0.0  1
 REPLICATE 2 1  2R30.5  2R17.445 7.66   0 1
END GEOM
READ ARRAY  ARA=1 NUX=13 NUY=8  FILL F1 END FILL
          ARA=2 NUX=5 NUY=1
          FILL  2 3 2 3 2
               END FILL
END ARRAY
READ PLOT
  XUL=-4 YUL=34 ZUL=20 XLR=97 YLR=-4
  ZLR=20  UAX=1  VDN=-1 NAX=120 NCH=' *~ctla~' END
END PLOT
END DATA
END
```

KENO-V.a Input Listing for Case 17 of Table 20 (16-Energy-Group Hansen-Roach Cross Sections).

```
shr49 THREE 12x16 CLUSTERS, 1.892 CM PITCH, 15.84  CM
SEPARATION
READ PARA TME=200 GEN=160 NPG=1500 NSK=50
NUB=YES LIB=41 XS1=YES RUN=YES
LNG=60000   END PARA
READ MIXT SCT=3 MIX=1
' U(4.31)02
92400 5.1835-6 92508 9.1530-4 92509 9.4904-5
92600 5.1395-6 92857 1.1216-2 92858 1.0941-2 8100 4.6753-2
MIX=2
' water
1102 6.6706-2  8100 3.3353-2
MIX=3
' 6061 Al (clad)
13100 5.8433-2  24100 6.2310-5  29100 6.3731-5
12100 6.6651-4  25100 2.2115-5  22100 2.5375-5
30100 3.0967-5  14100 3.4607-4  26100 1.0152-4
MIX=4
'  rubber (end plug)
6100 4.3562-2  1102 5.8178-2  20100 2.5660-3
16100 4.7820-4 14100 9.63560-5  8100 1.2461-2
MIX=5
'acrylic
1102 5.6642-2  6100 3.5648-2  8100 1.4273-2
MIX=6
' steel walls
26100 8.1810-2  6100 7.4686-4  25100 1.1-3
16100 8.8332-6 14100 3.6983-4
28100 6.3552-4  42100 2.4114-4 24100 1.0896-4
29100 9.6587-5
END MIXT
READ GEOM
UNIT 1
 COM=* FUEL PIN *
 CYLINDER  1 1  0.6325 92.075 0.0
 CYLINDER  0 1  0.6415 92.075 0.0
 CYLINDER  4 1  0.6415 94.2975 -2.2225
 CYLINDER  3 1  0.7075 94.2975 -2.2225
 CUBOID  2 1  4P.946 94.2975 -2.2225
UNIT 2
 COM=* ARRAY OF FUEL PINS *
 ARRAY 1 0 0 -2.2225
UNIT 3
 COM=* WATER BETWEEN CLUSTERS *
 CUBOID  2 1  15.363   0 30.272 0 94.2975 -2.2225
GLOBAL
UNIT 4
 COM=* CLUSTERS WITH WATER BETWEEN *
 ARRAY 2 0 0 -2.2225
 CUBOID  5 1  98.838  0.0 30.272 0 94.2975 -4.7625
 CUBOID  2 1  123.069 -24.231 30.272 0 101.8375 -20.0625
 REPLICATE 2 1  2R0.0   2R1.956 2R0.0    1
 REPLICATE 6 1  2R0.0 2R17.85  2R0.0  1
 REPLICATE 2 1  2R30.5  2R10.694 7.66   0 1
END GEOM
READ ARRAY  ARA=1 NUX=12 NUY=16  FILL F1 END FILL
          ARA=2 NUX=5 NUY=1
          FILL  2 3 2 3 2
               END FILL
END ARRAY
READ PLOT
  XUL=-4 YUL=34 ZUL=20 XLR=97 YLR=-4
  ZLR=20  UAX=1  VDN=-1 NAX=120 NCH=' *~ctla~' END
END PLOT
END DATA
END
```

KENO-V.a Input Listing for Case 1 of Table 19 (27-Energy-Group SCALE4 Cross Sections).

```
=CSAS25
pkld41 THREE 13X8 CLUSTERS, 2.54  CM PITCH, 20.62  CM
SEPARATION
27GROUPNDF4 LATTICECELL
' U(4.306)02
U-234  1 0  5.1835-6 295 END
U-235  1 0  1.0102-3 295 END
U-236  1 0  5.1395-6 295 END
U-238  1 0  2.2157-2 295 END
O  1 0  4.6753-2 295 END
' water
H  2 0  6.6706-2 295 END
O  2 0  3.3353-2 295 END
' 6061 Al (clad)
AL  3 0  5.8433-2 295 END
CR  3 0  6.2310-5 295 END
CU  3 0  6.3731-5 295 END
MG  3 0  6.6651-4 295 END
MN  3 0  2.2115-5 295 END
TI  3 0  2.5375-5 295 END
'       (Zn replaced by Cu)
CU  3 0  3.0967-5 295 END
SI  3 0  3.4607-4 295 END
FE  3 0  1.0152-4 295 END
'  rubber end plug
C   4 0  4.3562-2 295 END
H   4 0  5.8178-2 295 END
CA  4 0  2.5660-3 295 END
S   4 0  4.7820-4 295 END
SI  4 0  9.6360-5 295 END
O   4 0  1.2461-2 295 END
' acrylic
H   5 0  5.6642-2 295 END
C   5 0  3.5648-2 295 END
O   5 0  1.4273-2 295 END
' lead
PB  6 0  3.2132-2 295 END
END COMP
SQUAREPITCH 2.540 1.265 1 2 1.415 3 1.283 0 END
pkld41 THREE 13X8 CLUSTERS, 2.540 CM PITCH, 20.62  CM
SEPARATION
READ PARA TME=200 GEN=160 NPG=1500 NSK=50
NUB=YES XS1=YES RUN=YES
END PARA
READ GEOM
UNIT 1
 COM=* FUEL PIN *
 CYLINDER  1 1  0.6325 92.075 0.0
 CYLINDER  0 1  0.6415 92.075 0.0
 CYLINDER  4 1  0.6415 94.2975 -2.2225
 CYLINDER  3 1  0.7075 94.2975 -2.2225
 CUBOID  2 1  4P1.27 94.2975 -2.2225
UNIT 2
 COM=* ARRAY OF FUEL PINS *
 ARRAY 1 0 0 -2.2225
UNIT 3
 COM=* WATER BETWEEN CLUSTERS *
 CUBOID  2 1  19.495   0 20.320 0 94.2975 -2.2225
GLOBAL
UNIT 4
 COM=* CLUSTERS WITH WATER BETWEEN *
 ARRAY 2 0 0 -2.2225
 CUBOID  5 1  138.050 0.0 20.320 0 94.2975 -4.7625
 CUBOID  2 1  151.025 -12.975 20.320 0 103.3375 -20.0625
 REPLICATE 6 1  2R0.0 2R10.2 2R0.0  1
 REPLICATE 2 1  2R30.5  2R20.3 6.16   0 1
END GEOM
READ ARRAY  ARA=1 NUX=13 NUY=8  FILL F1 END FILL
          ARA=2 NUX=5 NUY=1
          FILL  2 3 2 3 2
               END FILL
END ARRAY
READ PLOT
  XUL=-4 YUL=34 ZUL=20 XLR=97 YLR=-4
  ZLR=20  UAX=1  VDN=-1 NAX=120 NCH=' *~ctla~' END
END PLOT
END DATA
END
```

KENO-V.a Input Listing for Case 8 of Table 19 (27-Energy-Group SCALE4 Cross Sections).

```
=CSAS25
pku44 THREE 13x8  CLUSTERS, 2.540 CM PITCH, 13.49  CM
SEPARATION
27GROUPNDF4 LATTICECELL
' U(4.306)02
U-234  1 0  5.1835-6 295 END
U-235  1 0  1.0102-3 295 END
U-236  1 0  5.1395-6 295 END
U-238  1 0  2.2157-2 295 END
O  1 0  4.6753-2 295 END
' water
H  2 0  6.6706-2 295 END
O  2 0  3.3353-2 295 END
' 6061 Al (clad)
AL  3 0  5.8433-2 295 END
CR  3 0  6.2310-5 295 END
CU  3 0  6.3731-5 295 END
MG  3 0  6.6651-4 295 END
MN  3 0  2.2115-5 295 END
TI  3 0  2.5375-5 295 END
'       (Zn replaced by Cu)
CU  3 0  3.0967-5 295 END
SI  3 0  3.4607-4 295 END
FE  3 0  1.0152-4 295 END
'  rubber end plug
C   4 0  4.3562-2 295 END
H   4 0  5.8178-2 295 END
CA  4 0  2.5660-3 295 END
S   4 0  4.7820-4 295 END
SI  4 0  9.6360-5 295 END
O   4 0  1.2461-2 295 END
' acrylic
H   5 0  5.6642-2 295 END
C   5 0  3.5648-2 295 END
O   5 0  1.4273-2 295 END
' depleted uranium
U-235 6 0  9.5220-5 295 END
U-238 6 0  4.7151-2 295 END
END COMP
SQUAREPITCH 2.540 1.265 1 2 1.415 3 1.283 0 END
pkld44 THREE 13x8  CLUSTERS, 2.54 CM PITCH, 13.49  CM
SEPARATION
READ PARA TME=200 GEN=160 NPG=1500 NSK=50
NUB=YES XS1=YES RUN=YES
END PARA
READ GEOM
UNIT 1
 COM=* FUEL PIN *
 CYLINDER  1 1  0.6325 92.075 0.0
 CYLINDER  0 1  0.6415 92.075 0.0
 CYLINDER  4 1  0.6415 94.2975 -2.2225
 CYLINDER  3 1  0.7075 94.2975 -2.2225
 CUBOID  2 1  4P1.27 94.2975 -2.2225
UNIT 2
 COM=* ARRAY OF FUEL PINS *
 ARRAY 1 0 0 -2.2225
UNIT 3
 COM=* WATER BETWEEN CLUSTERS *
 CUBOID  2 1  12.365   0 20.320 0 94.2975 -2.2225
GLOBAL
UNIT 4
 COM=* CLUSTERS WITH WATER BETWEEN *
 ARRAY 2 0 0 -2.2225
 CUBOID  5 1  123.790 0.0 20.320 0 94.2975 -4.7625
 CUBOID  2 1  138.045 -14.255 20.320 0 101.8375 -20.0625
 REPLICATE 2 1  2R0.0   2R5.405 2R0.0    1
 REPLICATE 6 1  2R0.0 2R7.65 2R0.0  1
 REPLICATE 2 1  2R30.5  2R17.445 7.66   0 1
END GEOM
READ ARRAY  ARA=1 NUX=13 NUY=8  FILL F1 END FILL
          ARA=2 NUX=5 NUY=1
          FILL  2 3 2 3 2
               END FILL
END ARRAY
READ PLOT
  XUL=-4 YUL=34 ZUL=20 XLR=97 YLR=-4
  ZLR=20  UAX=1  VDN=-1 NAX=120 NCH=' *~ctla~' END
END PLOT
END DATA
END
```

KENO-V.a Input Listing for Case 17 of Table 20 (27-Energy-Group SCALE4 Cross Sections).

```
=CSAS25
sk49  THREE 12x16 CLUSTERS, 1.892 CM PITCH, 15.84  CM SEPARATION
27GROUPNDF4 LATTICECELL
' U(4.306)02
U-234  1 0  5.1835-6 295 END
U-235  1 0  1.0102-3 295 END
U-236  1 0  5.1395-6 295 END
U-238  1 0  2.2157-2 295 END
O  1 0  4.6753-2 295 END
' water
H  2 0  6.6706-2 295 END
O  2 0  3.3353-2 295 END
' 6061 Al (clad)
AL  3 0  5.8433-2 295 END
CR  3 0  6.2310-5 295 END
CU  3 0  6.3731-5 295 END
MG  3 0  6.6651-4 295 END
MN  3 0  2.2115-5 295 END
TI  3 0  2.5375-5 295 END
'       (Zn replaced by Cu)
CU  3 0  3.0967-5 295 END
SI  3 0  3.4607-4 295 END
FE  3 0  1.0152-4 295 END
'  rubber end plug
C   4 0  4.3562-2 295 END
H   4 0  5.8178-2 295 END
CA  4 0  2.5660-3 295 END
S   4 0  4.7820-4 295 END
SI  4 0  9.6360-5 295 END
O   4 0  1.2461-2 295 END
' acrylic
H   5 0  5.6642-2 295 END
C   5 0  3.5648-2 295 END
O   5 0  1.4273-2 295 END
'  STEEL WALLS
FE  6 0  8.1810-2 295 END
C   6 0  7.4686-4 295 END
MN  6 0  1.1000-3 295 END
P   6 0  6.0971-6 295 END
S   6 0  8.8332-6 295 END
SI  6 0  3.6983-4 295 END
NI  6 0  6.3552-4 295 END
MO  6 0  2.4114-4 295 END
CR  6 0  1.0896-4 295 END
CU  6 0  9.6587-5 295 END
END COMP
SQUAREPITCH 1.892 1.265 1 2 1.415 3 1.283 0 END
sk49  THREE 12x16CLUSTERS, 1.892 CM PITCH, 15.84  CM SEPARATION
READ PARA TME=200 GEN=160 NPG=1500 NSK=50
NUB=YES XS1=YES RUN=YES
END PARA
READ GEOM
UNIT 1
 COM=* FUEL PIN *
 CYLINDER  1 1  0.6325 92.075 0.0
 CYLINDER  0 1  0.6415 92.075 0.0
 CYLINDER  4 1  0.6415 94.2975 -2.2225
 CYLINDER  3 1  0.7075 94.2975 -2.2225
 CUBOID  2 1  4P.946 94.2975 -2.2225
UNIT 2
 COM=* ARRAY OF FUEL PINS *
 ARRAY 1 0 0 -2.2225
UNIT 3
 COM=* WATER BETWEEN CLUSTERS *
 CUBOID  2 1  15.363   0 30.272 0 94.2975 -2.2225
GLOBAL
UNIT 4
 COM=* CLUSTERS WITH WATER BETWEEN *
 ARRAY 2 0 0 -2.2225
 CUBOID  5 1  98.838  0.0 30.272 0 94.2975 -4.7625
 CUBOID  2 1  123.069 -24.231 30.272 0 101.8375 -20.0625
 REPLICATE 2 1  2R0.0   2R1.956 2R0.0    1
 REPLICATE 6 1  2R0.0 2R17.85  2R0.0  1
 REPLICATE 2 1  2R30.5  2R10.694 7.66   0 1
END GEOM
READ ARRAY  ARA=1 NUX=12 NUY=16  FILL F1 END FILL
          ARA=2 NUX=5 NUY=1
          FILL  2 3 2 3 2
              END FILL
END ARRAY
READ PLOT
  XUL=-4 YUL=34 ZUL=20 XLR=97 YLR=-4
  ZLR=20  UAX=1  VDN=-1 NAX=120 NCH=' *~ctla~' END
END PLOT
END DATA
END
```

A.2 MCNP Input Listings

MCNP4 was used.

Fuel rod clusters were created by filling cuboids with a universe containing an infinite lattice of fuel rods.

MCNP k_{eff} calculations used 110 generations of 1500 neutrons each after skipping 50 generations.

MCNP Input Listing for Case 1 of Table 19.

```
message:      outp=pmld41.o  runtpe=pmld41.r  srctp=pmld41.s

pmld41 THREE 13X8 CLUSTERS OF U(4.306)O2 RODS, 2.540 CM PITCH, 20.62  CM SEP
1     1 .06993052   -1 7 -8  u=1 imp:n=1 $ uo2 fuel
2     0   -2 1 7 -8  u=1 imp:n=1 $ gap
3     3 .0597516   -12 2  u=1 imp:n=1 $ clad
4     4 .1173416   -2 8 u=1 imp:n=1 $ rubber end plug (top)
5     4 .1173416   -2 -7 u=1 imp:n=1 $ rubber end plug (bottom)
6     2 .100059      12 u=1 imp:n=1 $ water
7     0  -4 3 -6 5  imp:n=1 lat=1 u=2 fill=1  $ lattice of fuel rods
8     0  -10 11 -20 19 -9 23 fill=2 imp:n=1  $ first rod cluster
9     0  -14 15 -20 19 -9 23 fill=2(52.515 0 0) imp:n=1  $ second rod cluster
10    0  -16 17 -20 19 -9 23 fill=2(105.03 0 0) imp:n=1  $ third rod cluster
11    2 .100059      10 -15 -20 19 -9 23  imp:n=1 $ water between clusters
12    2 .100059      14 -17 -20 19 -9 23  imp:n=1 $ water between clusters
13    5 .106563  19 -20 11 -16 -23 29  imp:n=1  $ acrylic support plate
14    6 .032132     33 -34 31 -37  35 -36  imp:n=1  $ lead reflector
15    6 .032174     33 -34 38 -32 35 -36  imp:n=1  $ lead reflector
16    2 .100059     (-11:16:20:-19:9:-29) -24 25 -26 27 -28 35
                                    #14 #15              imp:n=1 $ water
17    0  24:-25:26:-27:28:-35  imp:n=0

1     c/z  1.27 1.27 .6325  $ fuel cylinder
2     c/z  1.27 1.27 .6415  $ clad inner surface
3     px  0.0  $ fuel rod cell boundary
4     px  2.540  $ fuel rod cell boundary
5     py  0.0  $ fuel rod cell boundary
6     py  2.540  $ fuel rod cell boundary
7     pz  0.0  $ bottom of fuel
8     pz  92.075  $ top of fuel
9     pz  94.2975  $ top of clad
10    px  33.0199  $ farthest edge of first cluster  ***
11    px  .0001  $ closest edge of first cluster
12    c/z  1.27 1.
27 .7075  $ clad outer surface
14    px  85.5349  $ farthest edge of second cluster  ***
15    px  52.5151  $ closest edge of second cluster
16    px  138.0499 $ farthest edge of third cluster  ***
17    px  105.0301 $ closest edge of third cluster
19    py  0.00001  $ sides of clusters
20    py  20.31999 $ sides of clusters  ***
23    pz  -2.2225  $ bottom of fuel rod
24    px  181.525    $ side of water reflector   ***
25    px  -43.475 $ side of water reflector
26    py  50.820  $ side of water reflector   ***
27    py  -30.5  $ side of water reflector
28    pz  109.4975 $ top of water
29    pz  -4.7625  $ bottom of acrylic support plate
31    py  -10.20    $ lead
32    py   30.52    $ lead
33    px  -12.975  $ lead
34    px   151.025  $ lead
35    pz  -20.0625  $ lead
36    pz   103.3375 $ lead
37    py  -0.0      $ lead
38    py   20.32    $ lead
kcode  1500 1 50 160 50000
sdef  x=d1 y=d2 z=d3 cel=d4
si1   0 138
sp1   0 1
si2   0 31
sp2   0 1
si3   0 93
```

MCNP Input Listing for Case 1 of Table 19 (cont'd).

```
sp3   0 1
si4   l 8 9 10
sp4   v
print
c
c     MATERIALS FOR U(4.306)O2 RODS
c
c     m1 is UO2 fuel
m1    92234.50c 5.1835e-6 92235.50c 1.0102e-3
      92236.50c 5.1395e-6 92238.50c 2.2157e-2
      8016.50c  4.6753e-2
c     m2 is water
m2    8016.50c 3.3353e-2  1001.50c 6.6706e-2
mt2   lwtr.01t
c     m3 is 6061 Al (clad)
m3    13027.50c  5.8433e-2  24000.50c  6.2310e-5
      29000.50c  6.3731e-5  12000.50c  6.6651e-4
      25055.50c  2.2115e-5  22000.50c  2.5375e-5
c     Zn replaced by Cu, below
      29000.50c  3.0967e-5  14000.50c  3.4607e-4
      26000.50c  1.0152e-4                              c     m4 is rubber (end plugs)
m4    6000.50c   4.3562-2    1001.50c 5.8178e-2
      20000.50c  2.5660e-3  16032.50c 4.7820e-4
      14000.50c  9.6360e-5   8016.50c  1.2461e-2
mt4   poly.01t
c     m5 is acrylic (support plate)
m5    1001.50c 5.6642e-2  6000.50c 3.5648e-2
      8016.50c 1.4273e-2
mt5   poly.01t
c     m6 is lead
m6    82000.50c  3.2132e-2
```

MCNP Input Listing for Case 8 of Table 19.

```
message:      outp=pmu44.o  runtpe=pmu44.r  srctp=pmu44.s

pmu44 THREE 13X8 CLUSTERS OF U(4.306)O2 RODS, 2.540 CM PITCH, 13.49  CM SEP
1     1 .06993052   -1 7 -8  u=1 imp:n=1 $ uo2 fuel
2     0   -2 1 7 -8  u=1 imp:n=1 $ gap
3     3 .0597516   -12 2  u=1 imp:n=1 $ clad
4     4 .1173416   -2 8 u=1 imp:n=1 $ rubber end plug (top)
5     4 .1173416   -2 -7 u=1 imp:n=1 $ rubber end plug (bottom)
6     2 .100059      12 u=1 imp:n=1 $ water
7     0  -4 3 -6 5  imp:n=1 lat=1 u=2 fill=1  $ lattice of fuel rods
8     0  -10 11 -20 19 -9 23 fill=2 imp:n=1  $ first rod cluster
9     0  -14 15 -20 19 -9 23 fill=2(45.385 0 0) imp:n=1  $ second rod cluster
10    0  -16 17 -20 19 -9 23 fill=2(90.770 0 0) imp:n=1  $ third rod cluster
11    2 .100059      10 -15 -20 19 -9 23  imp:n=1 $ water between clusters
12    2 .100059      14 -17 -20 19 -9 23  imp:n=1 $ water between clusters
13    5 .106563  19 -20 11 -16 -23 29  imp:n=1  $ acrylic support plate
14    6 .04724622   33 -34 31 -37  35 -36  imp:n=1  $ uran reflector
15    6 .04724622   33 -34 38 -32 35 -36  imp:n=1  $ uran reflector
16    2 .100059     (-11:16:20:-19:9:-29) -24 25 -26 27 -28 35
                                    #14 #15              imp:n=1 $ water
17    0  24:-25:26:-27:28:-35  imp:n=0

1     c/z .946 .946 .6325  $ fuel cylinder
2     c/z .946 .946 .6415  $ clad inner surface
3     px  0.0  $ fuel rod cell boundary
4     px  2.540  $ fuel rod cell boundary
5     py  0.0  $ fuel rod cell boundary
6     py  2.540  $ fuel rod cell boundary
7     pz  0.0  $ bottom of fuel
8     pz  92.075  $ top of fuel
9     pz  94.2975  $ top of clad
10    px  33.0199  $ farthest edge of first cluster  ***
11    px  .0001  $ closest edge of first cluster
12    c/z .946 .946 .7075  $ clad outer surface
14    px  78.4049  $ farthest edge of second cluster  ***
15    px  45.3851  $ closest edge of second cluster
16    px  123.7899 $ farthest edge of third cluster  ***
17    px  90.7701  $ closest edge of third cluster
19    py  0.00001  $ sides of clusters
20    py  20.31999 $ sides of clusters  ***
23    pz  -2.2225  $ bottom of fuel rod
24    px  168.545  $ side of water reflector   ***
25    px  -44.755 $ side of water reflector
26    py  50.820  $ side of water reflector   ***
27    py  -30.5  $ side of water reflector
28    pz  109.4975 $ top of water
29    pz  -4.7625  $ bottom of acrylic support plate
31    py  -13.055   $ uran
32    py   33.375   $ uran
33    px  -14.255  $ uran
34    px   138.045 $ uran
35    pz  -20.0625  $ uran
36    pz   101.8375 $ uran
37    py   -5.405  $ uran
38    py   25.725   $ uran
kcode  1500 1 50 160 50000
sdef  x=d1 y=d2 z=d3 cel=d4
si1   0 96
sp1   0 1
si2   0 31
sp2   0 1
si3   0 93
sp3   0 1
```

MCNP Input Listing for Case 8 of Table 19 (cont'd).

```
si4   l 8 9 10
sp4   v
print
c
c     MATERIALS FOR U(4.306)O2 RODS
c
c     m1 is UO2 fuel
m1    92234.50c 5.1835e-6 92235.50c 1.0102e-3
      92236.50c 5.1395e-6 92238.50c 2.2157e-2
      8016.50c  4.6753e-2
c     m2 is water
m2    8016.50c 3.3353e-2  1001.50c 6.6706e-2
mt2   lwtr.01t
c     m3 is 6061 Al (clad)
m3    13027.50c  5.8433e-2  24000.50c  6.2310e-5
      29000.50c  6.3731e-5  12000.50c  6.6651e-4
      25055.50c  2.2115e-5  22000.50c  2.5375e-5
c     Zn replaced by Cu, below
      29000.50c  3.0967e-5  14000.50c  3.4607e-4
      26000.50c  1.0152e-4
c     m4 is rubber (end plugs)
m4    6000.50c   4.3562-2    1001.50c 5.8178e-2
      20000.50c  2.5660e-3  16032.50c 4.7820e-4
      14000.50c  9.6360e-5   8016.50c  1.2461e-2
mt4   poly.01t
c     m5 is acrylic (support plate)
m5    1001.50c 5.6642e-2  6000.50c 3.5648e-2
      8016.50c 1.4273e-2
mt5   poly.01t
c     m6 is depleted uranium
m6    92235.50c  9.5220-5  92238.50c 4.7151-2
```

MCNP Input Listing for Case 17 of Table 20.

```
message:      outp=sm49.o  runtpe=sm49.r  srctp=sm49.s

sm49 THREE 12X 16 CLUSTERS OF U(4.306)O2 RODS, 1.892 CM PITCH, 15.84  CM SEP
1     1 .06993052   -1 7 -8  u=1 imp:n=1 $ uo2 fuel
2     0   -2 1 7 -8  u=1 imp:n=1 $ gap
3     3 .0597516   -12 2  u=1 imp:n=1 $ clad
4     4 .1173416   -2 8 u=1 imp:n=1 $ rubber end plug (top)
5     4 .1173416   -2 -7 u=1 imp:n=1 $ rubber end plug (bottom)
6     2 .100059      12 u=1 imp:n=1 $ water
7     0  -4 3 -6 5  imp:n=1 lat=1 u=2 fill=1  $ lattice of fuel rods
8     0  -10 11 -20 19 -9 23 fill=2 imp:n=1  $ first rod cluster
9     0  -14 15 -20 19 -9 23 fill=2(38.067 0 0) imp:n=1  $ second rod cluster
10    0  -16 17 -20 19 -9 23 fill=2(76.134 0 0) imp:n=1  $ third rod cluster
11    2 .100059      10 -15 -20 19 -9 23  imp:n=1 $ water between clusters
12    2 .100059      14 -17 -20 19 -9 23  imp:n=1 $ water between clusters
13    5 .106563  19 -20 11 -16 -23 29  imp:n=1  $ acrylic support plate
14    6 .08512383   33 -34 31 -37  35 -36  imp:n=1  $ SS   reflector
15    6 .08512383   33 -34 38 -32 35 -36  imp:n=1  $ SS   reflector
16    2 .100059     (-11:16:20:-19:9:-29) -24 25 -26 27 -28 35
                                    #14 #15              imp:n=1 $ water
17    0  24:-25:26:-27:28:-35  imp:n=0

1     c/z .946 .946 .6325  $ fuel cylinder
2     c/z .946 .946 .6415  $ clad inner surface
3     px  0.0  $ fuel rod cell boundary
4     px  1.892  $ fuel rod cell boundary
5     py  0.0  $ fuel rod cell boundary
6     py  1.892  $ fuel rod cell boundary
7     pz  0.0  $ bottom of fuel
8     pz  92.075  $ top of fuel
9     pz  94.2975  $ top of clad
10    px  22.7039  $ farthest edge of first cluster  ***
11    px  .0001  $ closest edge of first cluster
12    c/z .946 .946 .7075  $ clad outer surface
14    px  60.7709  $ farthest edge of second cluster  ***
15    px  38.0671  $ closest edge of second cluster
16    px  98.8379  $ farthest edge of third cluster  ***
17    px  76.1341  $ closest edge of third cluster
19    py  0.00001  $ sides of clusters
20    py  30.27199 $ sides of clusters  ***
23    pz  -2.2225  $ bottom of fuel rod
24    px  153.569  $ side of water reflector   ***
25    px  -54.731 $ side of water reflector
26    py  60.772 $ side of water reflector   ***
27    py  -30.5  $ side of water reflector
28    pz  109.4975 $ top of water
29    pz  -4.7625  $ bottom of acrylic support plate
31    py  -19.806   $ SS
32    py   50.078   $ SS
33    px  -24.231  $ SS
34    px   123.069  $ SS
35    pz  -20.0625  $ SS
36    pz   101.8375 $ SS
37    py   -1.956  $ SS
38    py   32.228   $ SS
kcode  1500 1 50 160 50000
sdef  x=d1 y=d2 z=d3 cel=d4
si1   0 96
sp1   0 1
si2   0 31
sp2   0 1
si3   0 93
sp3   0 1
```

MCNP Input Listing for Case 17 of Table 20 (cont'd).

```
si4   l 8 9 10
sp4   v
print
c
c     MATERIALS FOR U(4.306)O2 RODS
c
c     m1 is UO2 fuel
m1    92234.50c 5.1835e-6 92235.50c 1.0102e-3
      92236.50c 5.1395e-6 92238.50c 2.2157e-2
      8016.50c  4.6753e-2
c     m2 is water
m2    8016.50c 3.3353e-2  1001.50c 6.6706e-2
mt2   lwtr.01t                                          c     m3 is 6061 Al (clad)
m3    13027.50c  5.8433e-2  24000.50c  6.2310e-5                29000.50c  6.3731e-5  12000.50c  6.6651e-4                25055.50c
2.2115e-5  22000.50c  2.5375e-5                c     Zn replaced by Cu, below                                    29000.50c  3.0967e-5  14000.50c
3.4607e-4
      26000.50c  1.0152e-4
c     m4 is rubber (end plugs)
m4    6000.50c   4.3562-2    1001.50c 5.8178e-2
      20000.50c  2.5660e-3  16032.50c 4.7820e-4
      14000.50c  9.6360e-5   8016.50c  1.2461e-2
mt4   poly.01t
c     m5 is acrylic (support plate)
m5    1001.50c 5.6642e-2  6000.50c 3.5648e-2
      8016.50c 1.4273e-2
mt5   poly.01t
c     m6 is steel
m6     26000.50c 8.1810e-2  6000.50c  7.4686e-4  25055.50c  1.1e-3
       15031.50c 6.0971e-6 16032.50c 8.8332e-6 14000.50c 3.6983e-4
       28000.50c 6.3552e-4  42000.50c 2.4114e-4 24000.50c 1.0896e-4
       29000.50c 9.6587e-5
```

A.3 ONEDANT/TWODANTInput Listings

Sample CSASIX, ONEDANT, AND TWODANT input listings for sensitivity studies are provided in Appendix D.

APPENDIX B: LOGBOOKS

Logbooks are stored at the Los Alamos National Laboratory Archives under the original experiment number. Logbooks for the experiments were listed on the July 16, 1993, inventory for the shipment from Hanford to Los Alamos as being in Boxes 6, 10, or 11. The 2.54-cm-pitch experiments from Reference 3 are probably included in the experiments numbered SSC (Simulated Shipping Cask) 4.3-000-029 to -042, dated 5/15/79 to 6/29/79 (Box 6). Experiments from Reference 5 are probably included in SSC 4.3-137 to -151, dated 3/11/80 to 4/23/80 (Box 10). Other experiments from References 3 and 5 are probably included in SSC-4.3-000-152 to -160, dated 9/2/80 to 11/20/80 (Box 11). Reference 6 experiments are likely included in SSC 4.3-000-161 to -172, dated 4/9/81 to 5/15/81 (Box 10).

APPENDIX C: EFFECT OF WATER IMPURITIES ON k_{eff}.

Results of analyses of water impurities from References 1-10 are given in Table C.1.

Note that two sets of results from Reference 8, the gadolinium-water experiments, are given. Two separate analyses, one of the gadolinium solution and the other of the gadolinium nitrate powder, were done. The first set of values is the largest amount of impurity found in any solution sample used in an approach-to-critical experiment (Reference 8, p. C.4). The second set of values is from the gadolinium nitrate powder analysis and is based on the highest gadolinium concentration used, which was 1.481 g Gd/liter (0.00148 g Gd/cm^3). Shaded concentrations are maximum values.

Concentrations of impurities in solution from their weight percent in gadolinium nitrate powder were calculated in the following manner: The molecular formula for the gadolinium nitrate powder is given as $Gd(NO_3)_3 \times 4.91\ H_2O$, giving a molecular weight of 431.72. Therefore, assuming a solution concentration of 1.481 g Gd/liter, the concentration of the impurity in solution from the given weight percent of the impurity in the gadolinium nitrate powder (Reference 8, p. C.3) is

$$0.001481\frac{g}{cm^3}\ \frac{(wt.\%\ impurity)}{(wt.\%\ Gd)} = \frac{.001481\frac{g}{cm^3}(wt.\%\ impurity)}{[100 - \sum(wt.\%\ impurities)]\frac{A_{W,Gd}}{M_{W,Gd\ powder}}}$$

$$= \frac{0.001481\frac{g}{cm^3}(wt.\%\ impurity)}{[100 - 0.4735]\frac{157.25}{431.72}} = 4.08534 \times 10^{-5}(wt.\%\ impurity)\frac{g}{cm^3}$$

Table C.1. Impurity Components of Water (g/m^3).[a] (Maximum values are shaded.)

Reference→ Component↓	1, p. 8[b]	2 (p. 6) and 3 (p. 7)[c]	4 (p. 8)[c]	5 (p. 9); 6 (p. 7); 7 (p. 6)[d]	8 (p. C.4)	8 (p. C.3)	9 (p. B.2)[e]	10 (p. B.2)
Cl	26.2±5.4	30.2±5.8	1.7±.6	≤ 5	-	-	11	18
NO_3^-	0.24±.12	0.42±.16	0.02±.01	0.02	-	-	<0.38[f]	2.83[f]
Cr	<0.028	<0.01	<0.01	<0.01	-	0.041	<0.01	<0.005
Zn	0.35±.05	0.26±.07	0.9±1.1	16	10.6	0.0613	<0.05	0.32
Mn	<0.55	<0.01	<0.01	<0.01	-	0.041	<0.01	<0.01
Pb	<0.015	<0.005	0.008±.001	<0.005	2.1	1.0220	<0.002	<0.005
F	0.21±.02	0.15±.04	0.15±.04	0.18	-	-	0.12	0.12
Fe	<0.06	<0.03	<0.03	24	-	0.21	0.12	0.20
Cu	<0.06	<0.01	<0.01	<0.01	18.2	0.123	<0.05	<0.05
Cd	0.004±.001	0.006±.001	0.020±.006	0.001	-	0.041	0.002	0.0006
Gd	-	-	10.4±3.6	-	-	-	-	<10
SO_3	6.7±.4	6.6±.04	13.4±5.0	14.5	-	-	21	16
$CaCO_3$	-	-	-	-	19.2[g]	1.02[g]	51.2	35
B	-	-	-	-	0.09	1.02	-	<25
Al	-	-	-	-	7.3	2.04	-	-
Eu	-	-	-	-	0.08	1.23	-	-
Mg	-	-	-	-	5.7	0.204	-	-
Nd	-	-	-	-	12.2	2.04	-	-
Si	-	-	-	-	3.1	2.04	-	-
Ni	-	-	-	-	6.8	0.204	-	-
Y	-	-	-	-	0.17	0.41	-	-

Reference→ Component↓	1, p. 8[b]	2 (p. 6) and 3 (p. 7)[c]	4 (p. 8)[c]	5 (p. 9); 6 (p. 7); 7 (p. 6)[d]	8 (p. C.4)	8 (p. C.3)	9 (p. B.2)[e]	10 (p. B.2)
Others	-	-	-	-	Nb 0.3	Ag .041 Au .041 Ba .041 Be 2.04 Ce .102 Co .041 Dy .204 Hf .041 K .204 Li .041 La .204 Mo .041 Na 1.02 Pt .204 Rh .102 Ru 1.02 Sm .204 Sn 1.02 Sr .041 Tb .204 Ti 2.04 U .204 V .041 W .102 Zr .041	-	-
Dissolved Solids (g/m^3)	-	137±5	113±28	61 ± 3	-	-	109	83

(a) If one cubic centimeter has a mass of 1 gram, then this is the same as PPM (parts per million) by weight.
(b) Average of samples taken at the beginning and near the end of the experiments.
(c) Error limits are standard deviations observed in three samples.
(d) In Reference 7, analysis is prior to boron additions (Reference 7, p. 2).
(e) Largest values of three samples.
(f) "Nitrate (as N) mg/liter."
(g) As Ca.

Effect Due to Water Density Reduction. The maximum amount of dissolved solids reported was 137 grams per cubic meter of solution. Assume that dissolved solids is 200 g/m^3, has the same density as water (~ 1 g/cm^3), and displaces the water. (These are all conservative assumptions: This concentration is greater than any measured total impurity concentration; also, many materials are denser than water and, when dissolved in water, do not displace as much water as their dry volume.) The percentage of water volume displaced by the solute is then $200/10^6 \times 100 = 0.02$ percent. To see the effect of reduced water density, the water volume fraction is reduced by this percentage. The resulting change in k_{eff} for this conservative model is less than 0.04 percent.[a]

[a] This is based on ONEDANT calculations of $U(2.35)O_2$ fuel rods in a cylindrical, water-reflected, near-optimal square-pitched array, using 27-group cross sections created by CSASIX.

Effect Due to Presence of Individual Impurities. Listed in Table C2 are the percent changes in k_{eff} for the addition of the maximum measured amounts of each impurity, as calculated by ONEDANT, for $U(2.35)O_2$ fuel rods at 2.032 cm pitch, using the 27-group cross sections processed by CSASIX.[a] No changes are greater than 0.005 percent except those from boron and gadolinium impurities, with Δk_{eff} values of 0.9 percent and 1.7 percent, respectively.

Additional calculations for Gd and B impurities in the water of arrays of 4.31 wt.% enriched fuel rod at two pitches, 2.54 cm and 1.892 cm, were performed. For $U(4.31)O_2$ rods at 2.54 cm pitch, B at 25 g/m^3 and Gd at 14 g/m^3 gave Δk_{eff} values of -0.81 percent and -1.48 percent, respectively. These same concentrations of B and Gd for $U(4.31)O_2$ rods at 1.892 cm pitch gave Δk_{eff} values of -0.41 percent and -0.69 percent, respectively. Therefore, critical configurations from the two references with these maximal possible impurity concentrations, References 4 and 10, should include these two impurities in the water.

[a] Because zinc and platinum were not in the Standard Composition Library for CSAS, copper was substituted for zinc and gold was substituted for platinum. (Copper and gold total cross sections appear to be similar, conservative substitutes for zinc and platinum.)

Table C.2. Calculated Effect of Impurities on Δk_{eff}.

Impurity	Concentration (g/cm^3)	Atom Density (atoms/barn-cm)	% Δk_{eff}
Ag	4.09×10^{-08}	2.281×10^{-10}	0
Al	7.30×10^{-06}	1.629×10^{-07}	0
Au	4.09×10^{-08}	1.249×10^{-10}	0
B	2.50×10^{-05}	1.393×10^{-06}	-0.885 -0.784[a]
	1.02×10^{-06}[b]	5.682×10^{-08}	-0.009
Ba	4.09×10^{-08}	1.791×10^{-10}	0
Be	2.04×10^{-06}	1.365×10^{-07}	0.002
$CaCO_3$	5.12×10^{-05}	3.081×10^{-07}	0.005
Cd	4.09×10^{-08}	2.189×10^{-10}	0
Ce	1.02×10^{-07}	4.390×10^{-10}	0.001
Cl	3.60×10^{-05}	6.115×10^{-07}	0.004
Co	4.09×10^{-08}	4.175×10^{-10}	0
Cr	4.09×10^{-08}	4.732×10^{-10}	0
Cu	1.82×10^{-05}	1.725×10^{-07}	0.002
Eu	1.22×10^{-06}	4.838×10^{-09}	-0.005
F	2.30×10^{-07}	7.291×10^{-09}	0
Fe	2.40×10^{-05}	2.588×10^{-07}	0.003
Gd	1.40×10^{-05}	5.361×10^{-08}	-1.653 -1.830[a]
	1.00×10^{-05}[c]	3.830×10^{-08}	-1.200
	5.00×10^{-06}[d]	1.915×10^{-08}	-0.592
Hf	4.09×10^{-08}	1.378×10^{-10}	0
K	2.04×10^{-07}	3.146×10^{-09}	0
Li	4.09×10^{-08}	3.544×10^{-09}	0
La	2.04×10^{-07}	8.856×10^{-10}	0

Impurity	Concentration (g/cm^3)	Atom Density (atoms/barn-cm)	% Δk_{eff}
Mg	$5.70x10^{-06}$	$1.412x10^{-07}$	0
Mn	$5.50x10^{-07}$	$6.029x10^{-09}$	0.002
Mo	$4.09x10^{-08}$	$2.564x10^{-10}$	0
N	$2.83x10^{-06}$	$1.217x10^{-07}$	0.002
Na	$1.02x10^{-06}$	$2.675x10^{-08}$	0.002
Nb	$3.00x10^{-07}$	$1.945x10^{-09}$	0
Nd	$1.22x10^{-05}$	$5.094x10^{-08}$	0.001
Ni	$6.80x10^{-06}$	$6.977x10^{-08}$	0.002
Pb	$2.10x10^{-06}$	$6.103x10^{-09}$	0
$Pt^{(e)}$	$2.04x10^{-07}$	$6.305x10^{-10}$	0
Rh	$1.02x10^{-07}$	$5.977x10^{-10}$	0.001
Ru	$1.02x10^{-06}$	$6.085x10^{-09}$	0.001
Si	$3.10x10^{-06}$	$6.647x10^{-08}$	0
Sm	$2.04x10^{-07}$	$8.179x10^{-10}$	0.001
Sn	$1.02x10^{-06}$	$5.182x10^{-09}$	0
SO_3	$1.84x10^{-05}$	$1.384x10^{-07}$	0.002
Sr	$4.09x10^{-08}$	$2.808x10^{-10}$	0.001
Tb	$2.03x10^{-07}$	$7.709x10^{-10}$	0.001
Ti	$2.04x10^{-06}$	$2.568x10^{-08}$	0
U	$2.04x10^{-07}$	$5.168x10^{-10}$	0
V	$4.09x10^{-08}$	$4.830x10^{-10}$	0

Impurity	Concentration (g/cm^3)	Atom Density (atoms/barn-cm)	% Δk_{eff}
W	1.02×10^{-07}	3.345×10^{-10}	0
Y	4.09×10^{-07}	2.767×10^{-09}	0
Zn[(f)]	1.60×10^{-05}	1.474×10^{-07}	0.003
Zr	4.09×10^{-08}	2.697×10^{-10}	0

(a) MCNP calculation.
(b) This is an actual measured value, from Reference 8.
(c) Measured maximum value from Reference 10.
(d) Half of measured maximum value from Reference 10.
(e) Because platinum was not in the cross section library, gold was substituted.
(f) Because zinc was not in the cross section library, copper was substituted.

APPENDIX D: SAMPLE CSASIX, ONEDANT, AND TWODANT INPUT LISTINGS FOR SENSITIVITY STUDIES

```
=CSASIX
csforl  4.31 wt%, 3 13x8
27GROUPNDF4 LATTICECELL
' U(4.31)02
U-234  1 0  5.1835-6 295 END
U-235  1 0  1.0102-3 295 END
U-236  1 0  5.1395-6 295 END
U-238  1 0  2.2157-2 295 END
O  1 0  4.6753-2 295 END
' water
H  2 0  6.6706-2 295 END
O  2 0  3.3353-2 295 END
' 6061 Al (clad)
AL  3 0  5.8433-2 295 END
CR  3 0  6.2310-5 295 END
CU  3 0  6.3731-5 295 END
MG  3 0  6.6651-4 295 END
MN  3 0  2.2115-5 295 END
TI  3 0  2.5375-5 295 END
'       (Zn replaced by Cu)
CU  3 0  3.0967-5 295 END
SI  3 0  3.4607-4 295 END
FE  3 0  1.0152-4 295 END
' lead
PB  4 0  3.2132-2 295 END
' water
H  5 0  6.6706-2 295 END
O  5 0  3.3353-2 295 END
END COMP
SQUAREPITCH 2.54 1.265 1 2 1.415 3 1.283 0 END
END
```

```
    1     0     0
fol1,slab of u(4.31)o2 fuel pins with lead reflecting walls
/  Block 1
igeom=slab ngroup=27 isn=16 niso=6 mt=6 nzone=6 im=4 it=144
T

/  Block 2
xmesh=0 15.136 16.136 26.336 41.336
xints= 50 4 30 60
zones=6 4 5 4 t

/ Block 3
 lib=xs27.p3
 chivec= .021 .188 .215 .125 .166 .18 .09 .014 .001 18z
 maxord=3 ihm=42 iht=3 ihs=16 ititl=1 ifido=2 i2lp1=1   t

/ Block 4
 matls=isos  assign=matls   t

/ Block 5
 ievt=1  isct=3  ibl=1 ibr=0 epsi=.000001 t

/ Block 6
 pted=0 zned=1 t

    1     0     0
for1,  4.31 wt% 3 13x8 clusters, 19.49 cm separation,
/      lead walls, 0 cm between fuel & wall
/  Block 1
igeom=6 ngroup=27 isn=8 niso=6 mt=6 nzone=6 im=6 it=200
jm=5
jt=170  maxscm=540000 maxlcm=4500000 t

/  Block 2
xmesh=0 16.51 36.005 69.025 82 92 112.5

xints= 30 40 60 30 20 20
ymesh=0.0 20.3 30.5 50.82 61.02 81.32
yints= 40 20 50 20 40
zones=6r5; 4r4 5 5;
     6 5 6 3r5; 4r4 5 5; 6r5  t

/ Block 3
 lib=xs27.p3
 chivec=.021 .188 .215 .125 .166 .180 .090 .014 .001 18z
 maxord=3 ihm=42 iht=3 ihs=16 ititl=1 ifido=2 i2lp1=1   t

/ Block 4
 matls=isos  assign=matls   t

/ Block 5
 ievt=1  isct=1 ith=0 ibl=1 ibr=0 ibt=0 ibb=0
 epsi=0.00001 oitm=120 bhgt=109.06  t
/ Block 6
 edoutf=3
 pted=1 zned=0  t
```